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PRES

Presidential Events

SUNDAY AFTERNOON

Leadership & Inclusive Excellence in STEM: Impact of Teacher-Scholars on Diversity

Sponsored by PROF, Cosponsored by PRES

MONDAY MORNING

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Sponsored by PROF, Cosponsored by AGFD, ANYL, BIOL, BIOT, CARB, CELL, CHED, CMA, COLL, COMP, ENVR, GEOC, I&EC, MEDI, MPPG, NUCL, ORGN, PHYS, PMSE, POLY, PRES, WCC and YCC

Excellence in Graduate Polymer Research

Biobased, Degradable & Chain-Exchange Polymers

Sponsored by POLY, Cosponsored by PRES, PROF[‡], SOCED[‡] and YCC[‡]

Excellence in Graduate Polymer Research

Biobased, Degradable & Chain-Exchange Polymers

Sponsored by POLY, Cosponsored by PRES, PROF[‡], SOCED[‡] and YCC[‡]

MONDAY AFTERNOON

Section A

Orange County Convention Center
Room W414C

The Chemistry of Disasters

Cosponsored by CCS and CHAS[‡]
J. M. Pickel, *Organizer, Presiding*

1:30 Introductory Remarks.

1:45 **PRES 1.** Caught in the Storm: Extreme Weather Hazards in the Chemical Enterprise. **K.M. Kulinowski**



TECHNICAL PROGRAM

2:30 PRES 2. Hurricane María: Forging the future of science in Puerto Rico. **I. Montes**

3:00 Intermission.

3:20 PRES 3. Looking Back to See Forward: Lessons from a Plant Explosion. **D. Mason**

3:50 PRES 4. Importance of Business Continuity and Emergency Planning for Research. **M.B. Koza**

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Sponsored by PROF, Cosponsored by AGFD, ANYL, BIOL, BIOT, CARB, CELL, CHED, CMA, COLL, COMP, ENVR, GEOC, I&EC, MEDI, MPPG, NUCL, ORGN, PHYS, PMSE, POLY, PRES, WCC and YCC

Excellence in Graduate Polymer Research

New Structures & Applications

Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC

TUESDAY MORNING

Section A

Orange County Convention Center
Room W414C

Bridging the (Safety) Gap between Academia & Industry

Cosponsored by CA, CCS, CHAS[†], CHED, PROF and YCC
J. M. Pickel, *Organizer, Presiding*
K. A. Miller, *Presiding*

8:30 Introductory Remarks.

8:45 PRES 5. Dow Lab Safety Academy: Promoting a positive safety culture in academia. **L. Seiler**

9:10 PRES 6. UMN Joint Safety Team, the Minnesota Model for lasting changes. **A. Sitek**

9:35 PRES 7. Identifying key factors of safety culture in academia from those identified in industry. **M.E. Gonzalez**, D.J. Casadonte

10:00 Intermission.

10:20 PRES 8. Peer to a mentor: Engaging graduate students in laboratory safety at northwestern. **X. Wang**

10:45 PRES 9. Cultivating a Safety Culture in Chemistry at Yale. **J. Freeze**

11:10 PRES 10. Impact of a pilot laboratory safety team workshop. **K.A. Miller**, K.I. Tyler



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

GSSPC: Artificial Molecular Machines & the Next Generation of Molecular Control

Sponsored by CHED, Cosponsored by COLL, I&EC, ORGN‡, PHYS, POLY and PRES

Excellence in Graduate Polymer Research

Approaches to Polymer Synthesis

Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC

TUESDAY AFTERNOON

Assessing Chemistry Outreach

Sponsored by CINF, Cosponsored by PRES and YCC

GSSPC: Artificial Molecular Machines & the Next Generation of Molecular Control

Sponsored by CHED, Cosponsored by COLL, I&EC, ORGN‡, PHYS, POLY and PRES

Excellence in Graduate Polymer Research

Conjugated & Electroactive Polymers

Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC

MPPG

Multidisciplinary Program Planning Group

M. Meador and L. Roberson, *Program Chairs*

SUNDAY MORNING

Interdisciplinary Chemistry for New Frontiers in Biology & Medicine

NanoBio

Sponsored by ANYL, Cosponsored by BIOL, COLL, MPPG, PHYS and PMSE‡



TECHNICAL PROGRAM

SUNDAY AFTERNOON

Section A

Orange County Convention Center
Valencia Ballroom A

Chemistry for New Frontiers Opening Session

M. A. Meador, M. Roberson, *Organizers, Presiding*

3:00 Introductory Remarks.

3:05 MPPG 1. Assembling materials charge-by-charge for targeted tissue delivery. **P.T. Hammond**

3:35 MPPG 2. Removing organic pollutants from water using polymers derived from corn. **W.R. Dichtel**

4:05 Intermission.

4:15 MPPG 3. Chemical systems out of equilibrium: From biology to electronics. **E.A. Weiss**

4:45 MPPG 4. Chemical catalysts for revolutionary agricultural research. **C. Jacobs-Young**

5:15 Q&A.

Interdisciplinary Chemistry for New Frontiers in Biology & Medicine

Microbia

Sponsored by ANYL, Cosponsored by BIOL, COLL, MPPG, PHYS and PMSE‡

Here We Are: Leading & Emerging Black Chemists in Analytical Chemistry

Sponsored by ANYL, Cosponsored by CMA‡, CTA‡ and MPPG‡

MONDAY MORNING

Section A

Orange County Convention Center
Room W314A

Third ACS NASA Symposium: Chemistry for Humanity's Next Giant Leap

C. J. Brumlik, G. L. Rodriguez, *Organizers*
K. Takhistova, *Organizer, Presiding*



TECHNICAL PROGRAM

8:30 Introductory Remarks.

8:40 MPPG 5. International Space Station's legacy and future. **R. Gatens**

9:05 MPPG 6. How can the chemical sciences support future human exploration of space? **M.A. Meador**

9:30 MPPG 7. Environmental Control and Life Support Systems (ECLSS). **M. Anderson**

9:55 Intermission.

10:05 MPPG 8. Low temperature burning of isolated fuel droplets in microgravity. **D. Dietrich**

10:30 MPPG 9. Microgravity materials science: The dynamics of coarsening processes. **P. Voorhees**

10:55 MPPG 10. Searching for life beyond Earth: Instruments and methods. **R.C. Quinn**

11:20 MPPG 11. O/OREOS nanosatellite space-environment effects on microbes and organic biomarkers. **A. Ricco**

Section B

Orange County Convention Center
Room W313

30th Anniversary of Chemistry of Materials - from 1989 to 2019

J. M. Buriak, C. Toro, *Organizers, Presiding*

8:30 MPPG 12. Chemistry of materials: The first 30 years. **J.M. Buriak**, C. Toro

8:45 MPPG 13. Programmable and smart sponges. **O.K. Farha**

9:15 MPPG 14. Studying complex supramolecular assembling behaviors of functional pi-conjugated molecules. **D. Zhao**, J. Xie, Y. Guo, H. Han

9:45 MPPG 15. Hydrogels for energy and environmental applications. **G. Yu**

10:15 Intermission.

10:30 MPPG 16. Amazing 3D and 2D halide perovskites: All the things they do. **M.G. Kanatzidis**

11:00 MPPG 17. Innovations in indium phosphide chemistry and characterization for emissive applications. **B.M. Cossairt**, J. Stein, N. Park, M. Friedfeld

11:30 MPPG 18. Organometallic optoelectronic materials. **K.S. Schanze**



TECHNICAL PROGRAM

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Sponsored by PROF, Cosponsored by AGFD, ANYL, BIOL, BIOT, CARB, CELL, CHED, CMA, COLL, COMP, ENVR, GEOC, I&EC, MEDI, MPPG, NUCL, ORGN, PHYS, PMSE, POLY, PRES, WCC and YCC

Interdisciplinary Chemistry for New Frontiers in Biology & Medicine

Biomarker Discovery

Sponsored by ANYL, Cosponsored by BIOL, COLL, MPPG, PHYS and PMSE‡

MONDAY AFTERNOON

Section A

Orange County Convention Center
Room W313

Pushing to the Extreme: Emerging Trends in Nanoscience, Materials Science & Photonics

P. Alivisatos, H. Atwater, J. M. Buriak, C. Toro, P. S. Weiss, *Organizers*
L. Fernandez, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 MPPG 19. Innovations in thin film assembly: “Pushing” metal ions and macromolecules to surfaces. **F. Caruso**

1:30 MPPG 20. Extreme regimes for nanoscience and photonics. **N.J. Halas**

1:55 MPPG 21. Recent strategies in the synthesis of 2D polymer and 2D COF. **K. Loh**

2:20 MPPG 22. Nanodiamond: Emerging material to solve biomedical challenges. **T. Weil**

2:45 MPPG 23. Breaking the walls between disciplines: towards new opportunities enabled by Nanoscience and Photonics. **R. Quidant**

3:10 MPPG 24. Design and self-assembly of photonic colloidal crystals. **S.C. Glotzer**

3:35 MPPG 25. Nanorobots for tumor microenvironment targeting and regulation. **G. Nie**

Section B

Orange County Convention Center
Room W314A

Third ACS NASA Symposium: Chemistry for Humanity’s Next Giant Leap



TECHNICAL PROGRAM

G. L. Rodriguez, K. Takhistova, *Organizers*
C. J. Brumlik, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 **MPPG 26.** In-situ resource utilization (ISRU): Overview. **J. Kleinhenz**

1:30 **MPPG 27.** Experimental insights into the geochemistry of Mercury. **K. Vander Kaaden**

1:55 Awards Presentation.

2:10 **MPPG 28.** Engineering self-assembly of protein polymers for functional materials. **S. Sim**

2:35 **MPPG 29.** Particular noncovalent bondings for self-healable materials. **T. Aida**

3:00 Awards Presentation.

3:15 **MPPG 30.** Dispersity under scrutiny: Exploring limits in block copolymer self-assembly. **B. van Genabeek**

3:40 **MPPG 31.** Supramolecular polymerizations: Chirality as a muse. **E.W. Meijer**

4:05 Concluding Remarks.

Section C

Orange County Convention Center
Valencia Ballroom A

The Kavli Foundation Emerging Leader in Chemistry Lecture

B. A. Charpentier, *Organizer, Presiding*

4:00 Introductory Remarks.

4:05 **MPPG 32.** Sensing human behavior with smart garments. **T.L. Andrew**

4:50 Q&A.

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Sponsored by PROF, Cosponsored by AGFD, ANYL, BIOL, BIOT, CARB, CELL, CHED, CMA, COLL, COMP, ENVR, GEOC, I&EC, MEDI, MPPG, NUCL, ORGN, PHYS, PMSE, POLY, PRES, WCC and YCC



TECHNICAL PROGRAM

MONDAY EVENING

Section A

Orange County Convention Center
Valencia Ballroom A

The Fred Kavli Innovations in Chemistry Lecture

B. A. Charpentier, *Organizer, Presiding*

5:00 Introductory Remarks.

5:05 MPPG 33. Chemistry of finding extraterrestrial life. **S.P. Kounaves**

5:50 Q&A.

5:55 Concluding Remarks.

TUESDAY MORNING

Section A

Orange County Convention Center
Room W414D

Applied Materials for New Frontiers: Ten Years of ACS Applied Materials & Interfaces

Cosponsored by COLL[‡], INOR[‡], PMSE[‡] and POLY[‡]
Financially supported by INOR, POLY, PMSE, COLL
M. Meador, S. S. Wong, K. Yu, *Organizers*
L. Fernandez, *Organizer, Presiding*

8:25 Introductory Remarks.

8:40 MPPG 34. Laser-induced graphene. **J.M. Tour**

9:05 MPPG 35. Silicon surfaces: From fundamentals to Applied Materials & Interfaces (AMI). **J.M. Buriak**, M. Hu, E. Lubber, B. Olsen, T. Hauger

9:30 MPPG 36. Critical role of solid-solid and solid-liquid interfaces and interphases on electrochemistry. **E.S. Takeuchi**, A.C. Marschilok, K.J. Takeuchi

9:55 Intermission.

10:10 MPPG 37. Suprastructures with Intrinsic Microporosity (SIM): Intriguing assemblies with infinite possibilities. **N.M. Khashab**

10:35 MPPG 38. Mechanically adaptive and adapting polymer systems. **C. Weder**



TECHNICAL PROGRAM

11:00 MPPG 39. Applied materials and interface studies of conjugated electroactive polymers. **J.R. Reynolds**

11:25 MPPG 40. Redox-active polymers for energy storage. **J.L. Lutkenhaus**, R. Verduzco

Section B

Orange County Convention Center
Room W314A

Third ACS NASA Symposium: Chemistry for Humanity's Next Giant Leap

C. J. Brumlik, K. Takhistova, *Organizers*
G. L. Rodriguez, *Organizer, Presiding*

8:30 MPPG 41. Industry panel: Future in space relies on advancing energy, materials and life science. **J. Green**

8:40 MPPG 42. New tools increase the pace and impact of chemical innovation at Dow. **A.N. Sreeram**

8:55 MPPG 43. Blurred lines: Applying technological leaps universally. **M. Krishnan**

9:10 MPPG 44. What can chemistry do to enable the next great leap in space science? **J. Arenberg**

9:25 MPPG 45. ExxonMobil: Finding opportunities in the space era. **T. Go**

9:40 MPPG 46. Johnson & Johnson: Innovative medicines & technologies. **P. Stoffels**

9:55 Panel Discussion.

10:15 Intermission.

10:25 MPPG 47. Industry panel: Reinventing research in space flight. **T. Ruttley**

10:35 MPPG 48. Opening the aperture: Research opportunities on Blue Origin commercial space platforms. **E. Wagner**

10:50 Panel Discussion.

11:40 Concluding Remarks.

TUESDAY AFTERNOON

Section A

Orange County Convention Center
Room W414D

Applied Materials for New Frontiers: Ten Years of ACS Applied Materials & Interfaces

Cosponsored by COLL[‡], INOR[‡], PMSE[‡] and POLY[‡]
Financially supported by INOR, POLY, PMSE, COLL



TECHNICAL PROGRAM

M. Meador, S. S. Wong, K. Yu, *Organizers*
L. Fernandez, *Organizer, Presiding*

1:30 MPPG 49. AIM-ing for design and assembly of heterogeneous catalyst with single-atom or near-single-atom precision. **J.T. Hupp**

1:55 MPPG 50. High current density niobium disulfide catalysts for hydrogen evolution. **M. Chhowalla**

2:20 MPPG 51. Acid compatible halide perovskite photocathodes: Solar assisted hydrogen production enabled by atomic layer deposition. I. Kim, M. Pellin, **A.B. Martinson**

2:45 MPPG 52. Sculpting photocatalysts on the nano scale. **L. Amirav**

3:10 Intermission.

3:25 MPPG 53. Langmuir protocol for advanced materials & interfaces: Molecular machine, nanocarbon, and cells. **K. Ariga**

3:50 MPPG 54. 3D printing and 4D stimuli-responsiveness in polymer materials. **R.C. Advincula**

4:15 MPPG 55. Plasmonic and magnetic nanoparticles for biomedical applications. **N. Thanh**

4:40 MPPG 56. Bicontinuous biphasic liquid emulsions for catalysis and separations. **D. Lee**

5:05 Concluding Remarks.

Section B

Orange County Convention Center
Valencia Ballroom A

Third ACS NASA Symposium: Chemistry for Humanity's Next Giant Leap

C. J. Brumlik, K. Takhistova, *Organizers*
G. L. Rodriguez, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 MPPG 57. Chemistry for the age of space exploration. **J. Green, T. Ruttley**

1:15 Fireside Chat.

1:30 MPPG 58. BASF: Research using the first super-computer in the chemical industry. **P. Eckes**

1:50 MPPG 59. American chemistry: Digitalization and re-skilled human capital to shape \$0.8 trillion. **D. Dickson**

2:10 Award Presentation.



TECHNICAL PROGRAM

2:15 **MPPG 60.** Microscopic explorations of inner space: The secret lives of cells. **E. Betzig**

2:45 Award Presentation.

2:50 **MPPG 61.** Advances in directed protein evolution. **F.H. Arnold**

3:20 Concluding Remarks.

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Sponsored by PROF, Cosponsored by ENVR, GEOC, I&EC, MEDI, MPPG, NUCL, ORGN, PHYS, PMSE, POLY, WCC and YCC

AGFD

Division of Agricultural & Food Chemistry

X. Fan, *Program Chair*

SUNDAY MORNING

Section A

Hyatt Regency Orlando
Florida Ballroom A

Second Global Symposium on Chemistry & Biological Effects of Maple Food Products

Chemistry & Neuroprotection

H. Ma, N. P. Seeram, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 **AGFD 1.** Current status and future prospects for maple research. **N.P. Seeram**

8:55 **AGFD 2.** Synthesis and characterization of quebecol and its analogues. **N. Voyer**, S. Cardinal, J. Azelmat, D. Grenier

9:25 **AGFD 3.** Characterization of biologically active proteins from red maple (*Acer rubrum*) leaves. S. Alshammari, Y. Khurshid, H. Ma, N.P. Seeram, **A. Ahmed**



TECHNICAL PROGRAM

9:55 AGFD 4. Isolation and characterization of major polysaccharides from maple sugar. M. Brochu, C.P. Lafrance, E. Landry, **M. Maheux**

10:25 Intermission.

10:40 AGFD 5. Phenolic-enriched red maple leaf extract (Maplifa™) prevents HFD-induced obesity, insulin resistance and inflammation via modulation of gut microbiota in mice. **J. Xu**, H. Ma, T. Liu, Z. Ding, W. Liu, Y. Mu, Z. Zhang, X. Huang, N.P. Seeram, L. Li

11:10 AGFD 6. Dietary intake of a phenolic-enriched extract of maple syrup reduces neuroinflammation in the 3xTg-AD mouse model of Alzheimer's disease. **K.N. Rose**, B.J. Barlock, N.A. DaSilva, S. Johnson, C. Liu, H. Ma, F. Akhlaghi, N.P. Seeram

11:40 AGFD 7. Potential neuroprotective effects of phenolic-enriched maple syrup (MSX) extract. **H.Y. Park**, S. Johnson, H. Ma, N.P. Seeram, D. Vatter

Section B

Hyatt Regency Orlando
Florida Ballroom B

Recent Advances in Food Fraud & Authenticity Analysis

H. Chun, *Organizer*
K. G. Lee, *Organizer, Presiding*
Y. Kim, *Presiding*

8:30 Introductory Remarks.

8:35 AGFD 8. Identification and analysis of food fraud and authenticity: Korean perspective. **H. Chun**

9:00 AGFD 9. Food authenticity, class analogy or class differentiation or both. **J. Zweigenbaum**

9:25 AGFD 10. Consensus ranking and fragmentation prediction for identification of unknowns in high resolution mass spectrometry. **A.J. Williams**, A. McEachran, T. Cathey, T. Transue, J. Sobus

9:50 Intermission.

10:05 AGFD 11. Targeted analytical methods for the authentication of perilla oil: Fatty acid, stable isotope, and FT-IR analysis approach. **B. Kim**, S. Ahn, H. Chun

10:30 AGFD 12. Qualitative and quantitative analyses of adulteration in Korean red ginseng (*Panax ginseng*) commercial products using HPLC and LC-MS. **J. Choi**, A. Islam, K. Kim

SUNDAY AFTERNOON

Section A



TECHNICAL PROGRAM

Hyatt Regency Orlando
Florida Ballroom A

Second Global Symposium on Chemistry & Biological Effects of Maple Food Products

From In Vitro & In Vivo Studies to Human Clinical Trials

H. Ma, N. P. Seeram, *Organizers, Presiding*

1:00 AGFD 13. Maple syrup-derived polyphenolics potentiate antibiotics *in vivo*. **N. Tufenkji**, V.B. Maisuria, D. Nguyen, E. Déziel, P. Casgrain, D. Houle

1:30 AGFD 14. Evaluation of a food grade phenolic-enriched maple syrup extract against diet-induced hepatic-steatosis and inflammation. **A. Slitt**, H. Ma, N.A. DaSilva, M. Pfohl, J. Agudelo, E. Marques, W. Wei, N.P. Seeram

2:00 Intermission.

2:10 AGFD 15. Maple syrup and other natural sweeteners alleviate insulin resistance and hepatic steatosis as compared to sucrose in diet-induced obese rats: Potential mechanisms of action. M. Valle, P. St-Pierre, G. Pilon, **A. Marette**

2:40 AGFD 16. Human intervention trial on maple syrup to evaluate its biological effects. **K. Abe**, A. Kamei, T. Toyoda

3:10 AGFD 17. Maple syrup as a substitute for commercial sports drinks: Can it be a viable solution for recreational and elite athletes? **J. Tremblay**, N. Leduc-Savard

3:40 Intermission.

3:50 AGFD 18. Strategies to communicate maple benefits for market development and promotion. **N. Langlois, J. Barbeau, Y. Ye, C. Ashley, N.P. Seeram**

4:50 Concluding Remarks.

Section B

Hyatt Regency Orlando
Florida Ballroom B

Recent Advances in Food Fraud & Authenticity Analysis

H. Chun, K. G. Lee, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 AGFD 19. Use of liquid chromatography quadrupole time-of-flight mass spectrometry and metabolomic profiling to discriminate coffee brewed by different methods. L. Xu, **Z. Xu**, X. Liao

2:00 AGFD 20. Analytical method to detect adulteration of ground roasted coffee. **K.G. Lee**



TECHNICAL PROGRAM

2:25 **AGFD 21.** Verification of the antioxidant polyphenolic detection method for ready to drink teas. **Y. Kim**

2:50 Intermission.

3:05 **AGFD 22.** Assessment of blueberry juice adulteration through LC-MS based metabolomic analysis. **J. Auh**

3:30 **AGFD 23.** Development of a 3D scanning method to differentiate artificial weight gained *Octopus minor*. C. Han, H. Choi, S. Jo, H. Na, M. Kim, M.K. Kim, **J. Lee**

3:55 **AGFD 24.** Challenges of adulteration and pesticide residues above MRL in Indian spices. S. Thakur, K. Gulati, **T. Jindal**

Section C

Hyatt Regency Orlando
Florida Ballroom C

Withycombe: Charalambous Graduate Student Symposium

K. Deibler, *Organizer, Presiding*

1:15 Introductory Remarks.

1:25 **AGFD 25.** Polysiloxanes modified thread-based microfluidic device for the development of an innovative immunoassay to detect *Salmonella* in food products. **K. Wang**, J.R. Choi, X. Lu

1:50 **AGFD 26.** Preparation, characterization and application of ovotransferrin nanofibrils. **Z. Wei**

2:15 **AGFD 27.** Parallel extraction of grape volatiles onto sorbent sheets prior to automated analysis by Direct Analysis in Real Time mass spectrometry. **M. Bee**, G.L. Sacks

2:40 Intermission.

2:55 **AGFD 28.** Engineering click-conjugated bacteriophages on magnetic nanoparticles for rapid detection of waterborne pathogens. **H. Zurier**, J.M. Goddard, S.R. Nugen

3:20 **AGFD 29.** Modification of food-safe glove surfaces with superhydrophobic nanotextures for enhanced food safety. J. Oh, **Y. Yegin**, W. Rapisand, M. Zhang, A. Castillo, L. Cisneros-Zevallos, M. Akbulut

3:45 **AGFD 30.** Understanding consumer acceptability in strawberry preserves using flavoromics. **G.A. Dubrow**, D.G. Peterson

4:10 Concluding Remarks.

SUNDAY EVENING

Section A



TECHNICAL PROGRAM

Orange County Convention Center
West Hall E2

General Posters

X. Fan, *Organizer*

5:30 - 7:30

AGFD 31. Utilization of a rapid-throughput monosaccharide analysis for the development of a food carbohydrate encyclopedia. **Y. Liu**, M. Amicucci, T. Vo, C.B. Lebrilla

AGFD 32. Physical state of almonds and method of oil extraction influence on peroxide values and conjugated dienes. **H. Chen**, T. Nguyen, A.E. Mitchell

AGFD 33. Isolation and formulation of radicinin as a microbial biopesticide against Pierce's Disease. **L. Lozano Salazar**, J.L. Cordoza, P. Rolshausen, M.C. Roper, K.N. Maloney

AGFD 34. Interaction between alpha-lactalbumin and human milk enzyme cathepsin D reveals specific peptide release at infant stomach pH. **J. Zheng**

AGFD 35. Optimizing extraction conditions and improving extraction yield of naringin and neohesperidin from Valencia and unripe mandarin oranges. **Y. Kim**, J.A. Manthey

AGFD 36. Enzyme inhibition, free radical scavenging and insecticidal activities of crude extracts and isolates from *Laportea aestuans* (Gaud). **G.K. Oloyede**

AGFD 37. Isolation of strawberry anthocyanins using high-speed counter-current chromatography and the copigmentation with catechin or epicatechin by high pressure processing. **Z. Xu**, H. Zou, X. Liao

AGFD 38. BooZi (molecular sieve) device's effect on aroma compounds in distilled spirits. **D. Budner**

AGFD 39. Comparison of extraction methods for antioxidant compounds from onion peel : Ultrasound-assisted and conventional extractions. **H. Heo**, U. Sim, J. Chung, J. Lee

AGFD 40. Biological activities of different solvent extracts from jujube (*Ziziphus jujuba* Mill.) fruits grown in Boeun area of Korea. **S. Hong**, D. Yeon, Y. Kim, J. Lee

AGFD 41. Investigation of tea chemistry. **R.J. Jalbert**, S. Hughes, S. Schmidt

AGFD 42. Diversity in optimum conditions of tea extraction upon expecting biological activities. Y. Jo, S. Hwang, **S. Lim**

AGFD 43. Proximate analysis and antioxidant properties of *Samanea saman* seeds. M. Malcolm, **A. Goldson-Barnaby**

AGFD 44. Flavonoids from Sea buckthorn (*Hippophae rhamnoides* L.) fruit with advanced glycation endproducts formation. Z. Li, Y. Nan, Z. Han, M. Lu, H. Ma, **L. Li**

AGFD 45. Factors affecting the phenolic composition and antioxidant properties of green and purple basil: soil bacteria, herbivory, and drought stress. **L. Ford**, A. Armeriv, T. Bilinski, E.D. Niemeyer



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- AGFD 46.** Changes in key odorants by the Lincoln County process (Tennessee whiskey). **T. Kerley**, J.P. Munafo
- AGFD 47.** Phytosterols and tocopherols content in unsaponifiable matter of okra seed cultivated in South Korea. **J. Yoon**, **Y. Kim**
- AGFD 48.** Synthesis and characterization of cinnamil and quinoxaline dyes for rapid detection of volatile amines. **X. Luo**, L. Lim
- AGFD 49.** Differences between artisanal and mass-produced cheese. **M.H. Tunick**, C.C. Cecilia Cirne, R. Trout
- AGFD 50.** Analysis of the amino acid content for beef, chicken and turkey bone broth. M. Shaw, **N.O. Flynn**
- AGFD 51.** Analysis of volatile compounds and antioxidant activities extracted from rice (*Oryza sativa* L.). **E. Han**, H. Lee, K.G. Lee
- AGFD 52.** Development and validation of a sensitive polyclonal antibody-based indirect competitive ELISA for determination of citrinin in grain-based foods. **G. Singh**, L. Velasquez, A. Huet, P. Delahaut, N. Gillard, T. Koerner
- AGFD 53.** Analysis of flavor compounds of caramel colorant with various manufacturing conditions. **H. Lee**, J. Kwon, K.G. Lee
- AGFD 54.** Detection of acrylamide in food using near infrared spectroscopy. C. Maranda, **M.M. Skinner**, O.M. McDougal
- AGFD 55.** Chemical analysis of an obscure *Rubus*: The thimbleberry (*R. parviflorus*). **T.A. Ruiz**, M.E. Gariepy, B.M. Canfield
- AGFD 56.** Biotin content of Korean beef in South Korea by immunoaffinity column/HPLC analysis. **J. Yoon**, N. Kim, A. Jeon, J. Kwon, S. Lee, Y. Choi, Y. Kim
- AGFD 57.** Method validation of immunoaffinity column-HPLC analysis for biotin in foods. **J. Kwon**, N. Kim, A. Jeon, J. Yoon, S. Lee, Y. Choi, Y. Kim
- AGFD 58.** Determining yeast cell-count & viability with varying smartphone cameras. **T. Ostrom**, D.J. Lecaptain
- AGFD 59.** Deterioration of tomato fruit quality during storage after dry gaseous ozone treatment to reduce populations of *Salmonella*. **X. Fan**, L. Wang, K. Sokorai, J. Sites
- AGFD 60.** Agro-based food packaging films: design and analyses. **H.N. Cheng**, A. Biswas, R.F. Furtado, C.R. Alves
- AGFD 61.** Improvement of storage stability of agricultural products through ethylene removal using non-thermal plasma and ZSM-5 supported palladium catalyst. S. Kim, **Y. Mok**
- AGFD 62.** Polyethylenimine precursor-loaded electrospun ethyl cellulose/poly(ethylene oxide) nonwovens for activated release of hexanal. **M. Dulvi**, L. Lim
- AGFD 63.** Flavor enhancement activity of the late-fall polypore: *Ischnoderma resinosum*. **P. Wickramasinghe**, C.R. Luckett, J.P. Munafo
- AGFD 64.** Determination of rate constants and activation energies associated with cannabidiol (CBD) formation and decomposition. **B. Bailey**, B.M. Canfield



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- AGFD 65.** Unsaponifiable matters from perilla seed meal protect against UVB-induced photoaging and promote collagen synthesis via stimulation of TGF- β /smad and inhibition of MAPK/AP-1 in human skin fibroblasts. **H. Lee**, Y. Kim, J. Lee
- AGFD 66.** Comparison of physicochemical and proximate properties of crude rice bran and processed rice (*oryza sativa*) oils. **S.A. Aderibigbe**
- AGFD 67.** Phytochemical, physicochemical composition, gas chromatography-mass spectrometry (GC-MS) analysis and anti-oxidant activity of the watermelon seed oil (*citrullus lanatus* L.). **S.A. Aderibigbe**
- AGFD 68.** Effect of kappa carrageenan on the oxidative stability of whey protein stabilized oil-in-water emulsions. **A. Ballard**, H. Congleton, H. Khouryieh
- AGFD 69.** Carotenoids fractionating from the tucumã (*Astrocaryum vulgare* Mart.) pulp oil by dry fractionation. **M. Mota**, M.J. Ferreira, C.M. Rezende, S.P. Freitas
- AGFD 70.** Characteristics of pesticide residues in spinach for establishing post-harvest residue level in Korea. **J. Lee**, S. Yang, T. Lee, H. Choi
- AGFD 71.** Establishment of analytical method for pesticide residues in meats. **S. Yang**, T. Lee, J. Lee, H. Choi
- AGFD 72.** Development of improved analytical method of residual pesticides in oriental herbal medicines. **T. Lee**, S. Yang, J. Lee, H. Choi
- AGFD 73.** Using fluorescence lifetime imaging microscopy for tracking translocation of small molecule pesticides in citrus seedlings. **G.S. Miller**, S. Santra, A.J. Gesquiere
- AGFD 74.** Risks of residual loads of restricted pesticides in soils of commercial farms in Akwa Ibom State, Nigeria. **A.I. Inyangudoh**, E. Inam, T. Arua, I. Udoekpo, C. Halsall, E. Ogwo
- AGFD 75.** Direct determination of paraquat, diquat, and related cationic polar pesticides in homogenized food samples using ion chromatography and high-resolution accurate mass spectrometry. **T.T. Christison**, J.E. Madden, J. Rohrer
- AGFD 76.** (Q)SAR, agrochemicals & regulation: The role of the computational and chemical biology group at Unam, Mexico. **A. Madariaga**, J. Barroso-Flores, F. Cortes-Guzman, K. Martinez Mayorga
- AGFD 77.** Intake, distribution, and retainment of the antibiotic oxytetracycline in citrus trees. **F. Hijaz**, F. Alrimawi, N. Killiny
- AGFD 78.** Uptake, translocation and stability of the antibiotic, streptomycin in citrus trees. **F. Alrimawi**, F. Hijaz, N. Killiny
- AGFD 79.** Biogenic silica extraction and comparison of agricultural residues for potential adsorbent material. **N. Lovanh**, J.H. Loughrin, G. Agga, B. Oh, G. Ruiz Aguilar
- AGFD 80.** Biotechnological aroma production using sesquiterpene *in situ* recovery. **M. Abrahão**, W.M. van Gulik, M.C. Cuellar, G.M. Pastore, L. van der Wielen
- AGFD 81.** Development of microencapsulation applied to flame resistance cotton fabric. **S. Chang**, B.D. Condon, J. Smith
- AGFD 82.** Protective effects of *Psidium guajava* L. leaves cultivated in South Korea on *tert*-butyl hydroperoxide-induced oxidative damage in HepG2 cells. **Y. Kim**, J. Yoon, N. Kim, J. Kwon, A. Jeon, J. Lee



TECHNICAL PROGRAM

- AGFD 83.** Bile salt binding ability of dietary fiber fractions from structurally modified common bean matrices: Impact on *in vitro* lipid digestion. **T. Lin**, S.F. Okeefe, C. Fernandez Fraguas
- AGFD 84.** Improvement via computational modeling of anti-microbial compounds for extending produce shelf-life. **S.M. Szewdo**, J.A. Darsey
- AGFD 85.** Effect of fermentation on the nutrient composition, invitro protein, digestibility and antioxidants properties of Opagha Seed(*Anthonota macrophylla*). **A.S. Oluwashina**
- AGFD 86.** Comparison of light emitting diodes colors on antioxidant property of red lettuce grown in closed soilless system. **S. Sawatdee**, C. Prommuak, T. Jarunlumert, P. Pavasant, A.E. Flood
- AGFD 87.** Heavy metal free quantum dots: A robust delivery vehicle for antibiotics for enhanced antibacterial activity. **T.J. Maxwell**, P. Rajasekaran, M. Young, M. Schaff, S. Santra
- AGFD 88.** Biopigments in sugarcane infected by borer-rot complex. **G.R. Manarim**, E.A. da Silva, C.P. da Silva, E.J. Pilau, C.L. de Aguiar
- AGFD 89.** Combination of plant pigments: Photophysical and redox consequences. **C.O. de Oliveira Machado**, A.E. Pagano, E.L. Bastos
- AGFD 90.** Effects of calcium chloride treatment on GABA accumulation and antioxidant activity during germination of brown rice. **H. Choe**, J. Song, Y. Kim, J. Lee
- AGFD 91.** Accumulation of cadmium in basil plants: urban vs. rural garden. **K. Couser**
- AGFD 92.** Effect of mechanical stress on anthocyanin production in living red raspberries. **C.C. Philipp**, A. Reardon, E. Stacy
- AGFD 93.** Identification of pulegone as the character impact odorant of hoary mountain mint, *Pycnanthemum incanum*. **M. Dein**, J.P. Munafo
- AGFD 94.** Bioassay-guided isolation of fungal natural products for fighting citrus greening disease. **V.D. Berry**, **J.L. Cordoza**, **J.J. Meloch**, A. Blacutt, M.C. Roper, P. Rolshausen, K.N. Maloney
- AGFD 95.** Ways to improve the humus status of different types of soils in Uzbekistan. T. Ortikov, **S. Pardaev**
- AGFD 96.** Scientific basis for improving the humus state of the soils of the Zeravshan valley of Uzbekistan. **T. Goziev**, T. Ortikov, S. Normamatov
- AGFD 97.** Regulation of humus balance by changing the balance of mobilization and immobilization processes. **T. Ortikov**, **S. Pardaev**, S. Normamatov
- AGFD 98.** On mechanism of isothiocyanates as H₂S donors. **Y. Lin**, X. Yang, D. Huang
- AGFD 99.** Local vs global models for the prediction of acute oral toxicity in rat. **B. Hernández**, G. Gómez-Jiménez, A. Madariaga, K. Martinez Mayorga
- AGFD 100.** Insight into the development of control strategy of aflatoxin through molecular mechanism of aflatoxin biosynthetic gene repression in *Aspergillus flavus* by molasses. **S.T. Hua**



TECHNICAL PROGRAM

AGFD 101. Inhibition of metal-mediated redox activity of Cu(II)-bacitracin with quercetin, salicylic acid and thiabendazole. **D. Cerrato**, C. Tang, S. Islam, L. Ming

AGFD 102. Enhanced sesqui- and triterpene accumulation by co-expression of HMG-CoA reductase and biotin carboxyl carrier protein (*BCCP1*) in tobacco (*Nicotiana benthamiana*). A. Lee, D. Ro, S. Kim, **J. Kim**

AGFD 103. Phenylpropanoid-CoA ligation by three isoforms of Pn4CL from *Piper nigrum* L. and corresponding substrates. Z. Jin, D. Ro, S. Kim, **J. Kim**

AGFD 104. Comprehensive theoretical investigation of alternariol and alternariol monomethyl ether. **Y. Tu**, Y. Tseng, M. Appell

AGFD 105. Residual characteristics of fungicide hexaconazole in minor crop mung bean during cultivation. S. Kim, Z. Jin, J. Lee, M. Rehan, X. Yuan, E. Park, R. Ko, B. Ju, **J. Kim**

AGFD 106. Dissipation pattern of fungicide chlorothalonil in *Sorghum bicolor* L. Moench after treatment of 75% wettable powder. J. Lee, M. Rehan, X. Yuan, Z. Jin, A. Lee, S. Kim, E. Park, R. Ko, B. Ju, **J. Kim**

AGFD 107. Withdrawn

MONDAY MORNING

Section A

Hyatt Regency Orlando
Florida Ballroom A

Flavor Chemistry of Chiral Compounds

S. Baoguo, T. Hongyu, M. C. Qian, *Organizers, Presiding*

8:15 Introductory Remarks.

8:20 AGFD 108. Flavor chemistry of heat-processed onions: Chiral aroma-active compounds can make the difference. **M. Granvogl**, M. Flaig

8:45 AGFD 109. Shedding new light on an old compound: Insights into the odor properties of *trans*-calamenene enantiomers and their occurrence in nature. **M. Steinhaus**, S.D. Neiens, S.M. Geißlitz

9:10 AGFD 110. Analytical and sensory characterization of chiral beta-mercaptoalkanones and beta-mercaptoalkanols. **A. Riegel**, C. Kiske, S. Nörenberg, K. Engel

9:35 AGFD 111. Sensory properties and asymmetric syntheses of chiral flavors by asymmetric oxydation. **H. Tian**, S. Baoguo, R. Ding, S. Liang, Y. Liu

10:00 Intermission.



TECHNICAL PROGRAM

10:15 AGFD 112. Chiral odorants from Cumberland rosemary (*Conradina verticillata*). M. Dein, **J.P. Munafo**

10:40 AGFD 113. Chiral aroma-active compounds in red raspberries. **M.C. Qian**

11:05 AGFD 114. Odor perception interactions between free monoterpene isomers and wine composition of Pinot gris wine. M. Song, C. Fuentes, J. Osborne, **E. Tomasino**

11:30 Concluding Remarks.

Section B

Hyatt Regency Orlando
Florida Ballroom B

Recent Advances in Food Fraud & Authenticity Analysis

K. G. Lee, *Organizer*
H. Chun, *Organizer, Presiding*
Y. Kim, *Presiding*

8:30 Introductory Remarks.

8:35 AGFD 115. Fingerprint approach in evaluation of adulteration and authenticity in dairy products. **S.D. Bhandari**, Z. Xie

9:00 AGFD 116. Simultaneous determination of bovine α -lactalbumin and bovine β -lactoglobulin in milk powders by ultra-high performance liquid chromatography tandem mass spectrometry. **Y. Zhang**, L. Mao, Y. Ren

9:25 AGFD 117. Development of portable sensor chip for toxic chemicals and microbial toxins in food and environment. **Y. Huh**, S. Oh, S. Kim, M. Lee, T. Park, H. Chun

9:50 Intermission.

10:05 AGFD 118. Development of real-time PCR method for six edible insects approved in Korea. **H. Kim**

10:30 AGFD 119. Withdrawn

Chemical Signaling in Plants

Sponsored by BIOL, Cosponsored by AGFD and AGRO

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium



TECHNICAL PROGRAM

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MONDAY AFTERNOON

Section A

Hyatt Regency Orlando
Florida Ballroom A

The Flavor of Subtropical & Tropical Fruits

G. K. Jayaprakasha, *Organizer*
Y. Wang, *Organizer, Presiding*
C. Hernandez-Brenes, *Presiding*

1:15 Introductory Remarks.

1:20 **AGFD 120.** Identification of the key odorants in jackfruit pulp by application of the sensomics approach. **M. Steinhaus**, J.E. Grimm

1:45 **AGFD 121.** Non-terpenes in citrus: Novel aldehydes and their sensory properties. **N.C. Da Costa**

2:10 **AGFD 122.** Characterization of volatile compounds from flowers and buds of Rio red grapefruits. **G.K. Jayaprakasha**, P. Chaudhary, B. Patil

2:35 **AGFD 123.** Rootstock effect on quality and consumer acceptance of Huanglongbing (HLB) affected orange juices. **L. Huang**, L. Reuss, Y. Wang

3:00 Intermission.

3:15 **AGFD 124.** Fatty acid composition and aroma volatile profiling of avocado germplasm from subtropical regions. **S. Ali**, **A. Plotto**, B. Scully, E. Stover, C. Pisani, M. Ritenour, J. Bai

3:40 **AGFD 125.** Aroma profiling of 'sweetheart' lychee using gas chromatography-olfactometry/mass spectrometry and aroma extract dilution analysis. **S. Feng**, M. Huang, J.H. Crane, Y. Wang

4:05 **AGFD 126.** Identification of aroma compounds in four Chinese mango juices, and effects of thermal and high-pressure processing on the mango juice aroma profiles. W. Zhang, **F. Lao**, J. Wu

Section B

Hyatt Regency Orlando
Florida Ballroom B

Antibiotic & Fungicide Resistance in Agriculture



TECHNICAL PROGRAM

Cosponsored by AGRO
X. Fan, X. He, *Organizers, Presiding*

1:15 AGFD 127. Antibiotic resistance research at the U.S. Department of Agriculture (USDA) Agricultural Research Service. **K. Cook**, R. Motroni, E. Thacker

1:45 AGFD 128. Opportunities to displace the need for antimicrobials in production. **K.E. Belk**

2:10 AGFD 129. Challenges to global surveillance and response to mobile colistin-resistance. **X. He**, S. Patfield, F.M. Rubio

2:30 AGFD 130. Tracking antimicrobial resistance in foodborne bacteria: Application of WGS in the US NARMS program. **S. Zhao**

2:55 Intermission.

3:10 AGFD 131. Management strategies for fungicide resistance in apple. **K. Cox**, S. Villani, K.M. Ayer

3:35 AGFD 132. Understanding antibiotic resistance in the context of urban agriculture. A. Mafiz, **Y. Zhang**

4:00 AGFD 133. Antimicrobial use and resistance in United States beef production. **J. Schmidt**, T. Wheeler, T. Arthur

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Sponsored by PROF, Cosponsored by AGFD, ANYL, BIOL, BIOT, CARB, CELL, CHED, CMA, COLL, COMP, ENVR, GEOC, I&EC, MEDI, MPPG, NUCL, ORGN, PHYS, PMSE, POLY, PRES, WCC and YCC

Chemistry in Space: Future Directions

Sponsored by YCC, Cosponsored by AGFD, ANYL, BIOT, BMGT, CHAS, ENVR, FLUO, GEOC, HIST, I&EC, MEDI, POLY and PROF

Undergraduate Research Posters

Agricultural & Food Chemistry

Sponsored by CHED, Cosponsored by AGFD and SOCED

MONDAY EVENING

Section A



TECHNICAL PROGRAM

Orange County Convention Center
West Hall C

Sci-Mix

X. Fan, *Organizer*

8:00 - 10:00

31-32, 34, 44, 48, 52, 55, 61-63, 83, 89, 92- 94, 98. See previous listings.

TUESDAY MORNING

Section A

Hyatt Regency Orlando
Florida Ballroom A

The Flavor of Subtropical & Tropical Fruits

Y. Wang, *Organizer*
G. K. Jayaprakasha, *Organizer, Presiding*
J. Suh, *Presiding*

8:15 Introductory Remarks.

8:20 AGFD 134. Characterization of grapefruit seed sprout off-flavor in grapefruit juice using GC-olfactometry and GC-MS. **R.L. Rouseff**, C. Emanuels

8:45 AGFD 135. Potential of aroma volatile compounds to improve the cantaloupe shelf-life and food safety. R. Metrani, G.K. Jayaprakasha, **B. Patil**

9:10 AGFD 136. Yield and fruit quality of commercial and alpine strawberry varieties grown in southern Florida. **A.H. Chambers**, Y. Fu, M. Brym, P. Moon, J. Bai, A. Plotto, E. Baldwin

9:35 AGFD 137. Flavor development in cocoa and chocolate: A review. **X. Tang**, Y. Wang

10:00 Intermission.

10:15 AGFD 138. Aroma volatile profiles in mango puree from different cultivars. **J. Sung**, A. Chambers, **Y. Wang**

10:40 AGFD 139. Identification of the major odor-active compounds in cajá. **S.D. Neiens**, S.M. Geißlitz, M. Steinhaus

11:05 AGFD 140. Chemical composition and biological activities of the root volatile oil of *Securidaca longipendiculata* fres. **A.A. Aliyu**, N.O. Olawore, L.O. Owolabi, A. Apoeso, S.Z. Ololade



TECHNICAL PROGRAM

Section B

Hyatt Regency Orlando
Florida Ballroom B

Food for Space Travel & Extreme Environments

N. C. Da Costa, *Organizer, Presiding*

8:15 Introductory Remarks.

8:25 AGFD 141. Exploration space food system: challenges and integrative solutions. **G. Douglas**

8:55 AGFD 142. (Very) long term vitamin stability in food prototypes developed for a mars mission. **A.H. Barrett**

9:25 AGFD 143. To Mars and back – with added flavour! **A.J. Taylor**, J. Beauchamp, L. Briand, V. Demaria Pesce, M. Heer, T. Hummel, S. McGrane, C. Margot, S. Pieters, P. Pittia, C. Spence

10:05 Intermission.

10:25 AGFD 144. In situ grown crops as a supplement to the astronaut diet. **M. Romeyn**

10:45 AGFD 145. Health and wellness on Russian spacecraft and stations: Setting space endurance records. **N.C. Da Costa**

11:25 AGFD 146. Novel high throughput nanoformulation platform technology to enhance water solubility and leaf/cuticle penetration of nutrients in extra-terrestrial hydroponic plantations. **E. Manek**, R.V. Jones, F. Darvas, J. Fail

Advanced Chemistry of "Non-Traditional" Polysaccharides

Sponsored by CELL, Cosponsored by AGFD, ANYL, BIOL and CARB

TUESDAY AFTERNOON

Section A

Hyatt Regency Orlando
Florida Ballroom A

The Flavor of Subtropical & Tropical Fruits

G. K. Jayaprakasha, *Organizer*

Y. Wang, *Organizer, Presiding*

S. Feng, *Presiding*



TECHNICAL PROGRAM

1:15 Introductory Remarks.

1:20 **AGFD 147.** *Garcinia xanthochymus* a potential functional tropical fruit beverage. P. Wickramasinghe, M. Dein, **A. Murray**, S. Manas, C.R. Lockett, V. Dia, J.P. Munafa

1:45 **AGFD 148.** Fruit quality in citrus: genetics and breeding for flavor and aroma. **X. Wei**, F.G. Gmitter, Y. Yu, Q. Yu, **C. Chen**, J. Bai, E. Baldwin, A. Plotto

2:10 **AGFD 149.** Avocado non-volatile flavor components (acetogenins) and their interaction with saltiness and bitterness perception. R. Villarreal-Lara, **C. Hernandez-Brenes**

2:35 Intermission.

2:50 **AGFD 150.** Classification of USDA orange-mandarin hybrids using volatile profiles. **J. Bai**, E. Baldwin, A. Plotto, R. Driggers, E. Stover

3:15 **AGFD 151.** Morphological distribution of individual polyphenols in 'Florida Radiance', Sweet Sensation® 'Florida127', and 'Florida Beauty' strawberries. K. Kelley, **A. Smith**, M. Nunes

3:40 **AGFD 152.** Simultaneous separation and identification of volatiles and coumarins from *Ageratum conyzoides* by UPLC-PDA. **S. Kumar**, T. Dhanani, S. Sharma, S. Shah, R. Singh, N. Gajbhiye, R. Kumar, S. Ghosh

Section B

Hyatt Regency Orlando
Florida Ballroom B

The Chemistry of Color in Foods

B. D. Guthrie, R. Tardugno, *Organizers, Presiding*

1:15 Introductory Remarks.

1:20 **AGFD 153.** Enzymatic acylation of anthocyanins isolated from alpine bearberry (*arctostaphylos alpina*) and lipophilic properties, thermostability and antioxidant capacity of derivatives. **W. YANG**, M. Kortensniemi, B. Yang, J. Zheng

1:50 **AGFD 154.** Formation and structure determination of polyphenol-derived red chromophores: Enhancing the color of processed cocoa powders. **D.C. Germann**, T.D. Stark, T. Hofmann

2:20 **AGFD 155.** Development of highly stable, water soluble food colorants from the peel of *Citrus limon*. **X. Chen**, **M.T. Hamann**

2:50 Intermission.

3:10 **AGFD 156.** Improving the performance of natural colorants to replace synthetics. **D. Dabas**

3:40 **AGFD 157.** Quantitative analysis of permitted and non-permitted color additives in different food matrices by a HPLC Method. **S.D. Bhandari**, B.P. Harp



TECHNICAL PROGRAM

4:10 AGFD 158. Contribution of anthocyanins to the anti-colitic activity of aronia berry. **B.W. Bolling**, J.C. Valdez, D. Martin, R. Pei

Advanced Chemistry of "Non-Traditional" Polysaccharides

Sponsored by CELL, Cosponsored by AGFD, ANYL, BIOL and CARB

WEDNESDAY MORNING

Section A

Hyatt Regency Orlando
Florida Ballroom A

Chemistry of Huanglongbing

J. A. Manthey, S. Raithore, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 AGFD 159. What have we learned about orange juice chemistry and sensory quality since huanglongbing was declared a disease in the State of Florida 13 years ago? **A. Plotto**, E. Baldwin, J. Bai, J.A. Manthey, S. Raithore, B. Dala Paula, M. Irej

8:30 AGFD 160. Impact of citrus greening on the flavor industry. **Z. Valappil**

9:00 AGFD 161. Mitigation of off-flavor in huanglongbing-affected orange juice using natural citrus non-volatile compounds. S. Raithore, J. Kiefl, B. Dala Paula, B. Gloria, J.A. Manthey, A. Plotto, J. Bai, W. Zhao, **E. Baldwin**

9:30 Intermission.

9:45 AGFD 162. Changes in volatile profile of peel oils in HLB affected oranges. **J. Bai**

10:10 AGFD 163. Metabolic dissecting of the tritrophic interactions between the huanglongbing pathogen, *Candidatus Liberibacter asiaticus*, its vector, *Diaphorina citri* and citrus host. **N. Killiny**

10:40 AGFD 164. Omics approach reveals altered host lipid metabolism against Huanglongbing disease. **J. Suh**, Y.S. Niu, Z. Wang, F.G. Gmitter, Y. Wang

11:05 AGFD 165. Could HLB-tolerant mandarins be used in Florida orange juice? **S. Feng**, L. Reuss, F.G. Gmitter, Y. Wang

Section B

Hyatt Regency Orlando
Florida Ballroom B



TECHNICAL PROGRAM

General Papers

Food & Health

X. Fan, *Organizer*

L. Howard, S. T. Hua, *Presiding*

8:00 Introductory Remarks.

8:05 AGFD 166. Isorhamnetin increases fat oxidation in *Caenorhabditis elegans* dependent on NHR-49. R. Farias-Pereira, J. Savarese, Y. Yue, S. Lee, **Y. Park**

8:25 AGFD 167. Bioactivity-guided isolation of anti-adipogenic compounds from Leaves of Shiya tea (*Adinandra nitida*). **C. Yuan**, Y. Wang

8:45 AGFD 168. Cross-link breaking activity and inhibitory effect of *Moringa oleifera* leaf crude extracts on fructose-derived advanced glycation endproducts. **O.I. Adeniran**, A. Mogale

9:05 AGFD 169. Isolation and identification of polymethoxylated flavones metabolites in rat urine and its evaluation on hepatic lipoprotein secretion. **D. Goncalves**, J.A. Manthey, P.I. Costa, T.B. Cesar

9:25 AGFD 170. Chlorophyll supplementation in a critical developmental window prevent diet-induced obesity and modulate gut microbiota in adult mice. Y. Li, Y. Cui, X. Hu, X. Liao, **y. zhang**

9:45 Intermission.

10:00 AGFD 171. Novel approaches to reduce bitterness in whole olives for environmentally sustainability. **A.E. Mitchell**, R. Johnson

10:20 AGFD 172. Non covalent binding of phenolic acids with oat β -glucans: impact on the physico-chemical properties of β -glucans. **N. Bordenave**

10:40 AGFD 173. Characterization of fatty acids of sesame, roselle and smooth loofah seeds flour. **H.O. Adubiaro**

11:00 AGFD 174. Influence of refining of vegetable oils on the stability, isolation and nutritional quality of tocopherols and tocotrienols. **R. Verhe**

11:20 AGFD 175. Polyphenol quantification in fruits: Determination of the contribution of individual polyphenols to quantitative results of four common analytical methods. **S. Ma**, C. Kim, A. Neilson, S.F. Okeefe, G.M. Peck, A.C. Stewart

Nanocellulose: From Fundamentals to Function

Sponsored by CELL, Cosponsored by AGFD, ANYL and BIOL

WEDNESDAY AFTERNOON



TECHNICAL PROGRAM

Section A

Hyatt Regency Orlando
Florida Ballroom A

Chemistry of Huanglongbing

J. A. Manthey, S. Raithore, *Organizers, Presiding*

1:15 AGFD 176. Seasonal changes in trifoliolate orange (*Poncirus trifoliata*) leaf polyphenols. **J.A. Manthey**, D.G. Hall

1:40 AGFD 177. Exogenous application of methyl jasmonate and salicylic acid on citrus foliage: Effects on foliar volatiles and aggregation behavior of Asian citrus psyllid (*Diaphorina citri*). **J. Patt**, P. Robbins, G. McCollum, R.T. Alessandro

2:10 AGFD 178. Chemistry of oak (*Quercus* spp.) water extract and its effect on HLB infected citrus trees. **C. Dorado**, J.A. Manthey, M. Pitino, L. Cano, R. Shatters, L. Rossi

2:35 Intermission.

2:50 AGFD 179. Advances in treatments to manage Huanglongbing: Targeting Liberibacter bacteria and psyllid endosymbionts. **W.B. Hunter**, A. Sandoval Mojica, G. Miles, G. McCollum, T. Paris, V. Aishwarya, M. Boyle, S. Altman, K. Pelz-Stelinski, C.S. Holland

3:20 AGFD 180. Bactericides as tools in the fight against Citrus HLB Disease: Getting these molecules where they need to be, when they need to be there. **R. Shatters**

3:50 AGFD 181. Recovering value-added co-products from culled HLB symptomatic and preharvest dropped citrus fruit. **R.G. Cameron**, H. Chau, A.T. Hotchkiss, C. Dorado, J.A. Manthey, J. Bai

4:20 Concluding Remarks.

Section B

Hyatt Regency Orlando
Florida Ballroom B

General Papers

Analytical Methods

X. Fan, *Organizer, Presiding*
S. T. Hua, *Presiding*

1:00 Introductory Remarks.

1:05 AGFD 182. Belgian chocolate as a model system for food analysis by atom probe tomography. **C. Barroo**, A.J. Akey, D.C. Bell



TECHNICAL PROGRAM

1:25 AGFD 183. Using triacylglycerols for detecting olive oil adulteration using UHPLC-CAD and PCA. **H. Green**, X. Li, M. De Pra, K. Lovejoy, F. Steiner, I. Acworth, S. Wang

1:45 AGFD 184. Differentiating the cultivar of processed olives using DNA, fatty acid profile and NMR fingerprinting methods. **L. Crawford**, E. Hatzakis, T. Reiter, S. Wang

2:05 AGFD 185. Seeing the whole picture: A multi-platform screening approach for contaminants in food. **A. Andrianova**, B.D. Quimby, M. Churley, J. Westland, C. Milner

2:25 AGFD 186. Calibration-free double-pulse laser-induced breakdown spectroscopy (CF DP-LIBS) for nutritional characterization of soybean leaves. A. Ranulfi, G. Senesi, P. Villas-Boas, M. Meyer, **D.M. Milori**

2:45 Intermission.

3:00 AGFD 187. Comparative analysis of dried fruit by molecular and atomic spectroscopy. **J. Mierzwa**

3:20 AGFD 188. Determination of brominated vegetable oils in beverages using pyrolytic combustion coupled to ion chromatography. **T.T. Christison**, S.P. Patil, J. Rohrer

3:40 AGFD 189. Selective optical detection of free sulfites in aqueous and non-aqueous environments. **L.D. Schmitt**

4:00 AGFD 190. Polar pesticide analysis by ion chromatography coupled with triple quadrupole mass spectrometer. **B. Huang**, J. Rohrer

4:20 AGFD 191. Characterization of sugars and sugar alcohols using hydrophobic interaction liquid chromatography coupled with charge aerosol detection. **S. Chakraborty**, M. Phan, E. Abreu, A. Gould, K. Blascyk

Nanocellulose: From Fundamentals to Function

Sponsored by CELL, Cosponsored by AGFD, ANYL and BIOL

THURSDAY MORNING

Section A

Hyatt Regency Orlando
Florida Ballroom A

General Papers

Plants & their Environment

X. Fan, *Organizer, Presiding*
S. T. Hua, *Presiding*

8:30 Introductory Remarks.



TECHNICAL PROGRAM

8:35 AGFD 192. GYY-4137 and dithiophosphates to increase the growth and harvest yields of four key plants. J. Carter, E.M. Brown, J.P. Grace, E.E. Irish, **N.B. Bowden**

8:55 AGFD 193. Untargeted metabolomics for the differentiation of healthy sweet potatoes from fungi infected sweet potatoes. **C. Gamlath Mohottige**

9:15 AGFD 194. Noninvasive diagnosis of tomato late blight via smartphone fingerprinting of leaf volatiles. **Z. Li**, R. Paul, T. Ba Tis, A. Saville, J. Hansel, **J. Ristaino**, Q. Wei

9:35 Intermission.

9:50 AGFD 195. Development and characterization of gold nanoparticles for plant genetic engineering. **S. Butrus**, G. Demirer, N. Goh, H. Zhang, F. Cunningham, M. Landry

10:10 AGFD 196. Identification, synthesis and initial field evaluation of the sex pheromone produced by *Thelosia camina* (LEPIDOPTERA:EUPTEROTIDAE). **D.M. Vidal**, E.B. Saad, M.D. Coracini, M.P. Bosch, C. Quero, Á. Guerrero, P. Zarbin

10:30 AGFD 197. Nanotechnology application to remediation of soils and plant nutrition through amphiphile enantiomeric colloids. **L.A. Lightbourn Rojas**

Section B

Hyatt Regency Orlando
Florida Ballroom B

General Papers

Biotechnology, Utilization of Agricultural by products, etc.

X. Fan, *Organizer*
L. A. Colaruotolo, S. T. Hua, *Presiding*

8:00 Introductory Remarks.

8:05 AGFD 198. Breakthrough of the final conundrum in China's milk powder adulteration incident: Formation mechanism and solutions of infant kidney stones. **W. Dong**, Y. Zhang, P. Hu, Q. Wu

8:25 AGFD 199. Extraction and characterization of nanocellulose from cotton gin motes and cotton gin waste. **J.H. Jordan**, M.W. Easson, B.D. Condon

8:45 AGFD 200. Cottonseed can be a useful source of plant polyphenols. **H. Cao**, K. Sethumadhavan

9:05 AGFD 201. Role of caffeine and alcohol in the formation of glucose from starch- α -Amylase reaction: Application of a two-step model. **A. Khan**

9:25 Intermission.



TECHNICAL PROGRAM

9:40 AGFD 202. Coproporphyrins, novel interphylum growth factors released by *Sphingopyxis* sp., enable laboratory cultivation of previously uncultured *Leucobacter* sp.. R. Takai, N.I. Bhuiyan, **K. Shigetomi**, S. Mitsuhashi, Y. Kamagata, M. Ubukata

10:00 AGFD 203. Brighter side of biodegradable food packaging: Luminescent probes to monitor structural properties. **L.A. Colaruotolo**, C. Gonzalez Martinez, R.L. Bueno Lopez, H. Ball, R. Enfield, M. Corradini

10:20 AGFD 204. Tailoring material chemistry to reduce fouling and microbial cross-contamination in food production. B. Werner, J.Y. Wu, **J.M. Goddard**

10:40 AGFD 205. Development of nanotechnology enabled locally systemic pesticide (LSP) particles. **A. Ozcan**, M. Young, M. Doomra, S. Santra

11:00 AGFD 206. Studies on the effect of processing method on loss of nutrients in some grains and legumes. **M.C. Azih**

Nanocellulose: From Fundamentals to Function

Sponsored by CELL, Cosponsored by AGFD, ANYL and BIOL

THURSDAY AFTERNOON

Nanocellulose: From Fundamentals to Function

Sponsored by CELL, Cosponsored by AGFD, ANYL and BIOL

ANYL

Division of Analytical Chemistry

K. Agnew-Heard and M. Bush, *Program Chairs*

SUNDAY MORNING

Section A

Hyatt Regency Orlando
Orlando Ballroom M

Advances in Ion Mobility Spectrometry

New Developments



TECHNICAL PROGRAM

C. Bleiholder, F. Fernandez-Lima, *Organizers*
F. C. Liu, *Presiding*

8:00 Introductory Remarks.

8:05 ANYL 1. Applications of native nESI-TIMS-MS for structural biology. **F. Fernandez-Lima**

8:35 ANYL 2. Enhancing disaccharide ion mobility separations through shift reagents and frequency modulation. **K.R. McKenna**, L. Li, K.A. Morrison, B. Clowers, F.M. Fernandez

9:00 ANYL 3. Fourier transform ion mobility-orbitrap for native mass spectrometry. **J. McCabe**, M.L. Poltash, M. Shirzadeh, D.H. Russell

9:25 ANYL 4. Improvements in metabolomics and proteomics separations and quantitation using Structures for Lossless Ion Manipulations (SLIM) IM-MS. **C.D. Chouinard**, G. Nagy, I.K. Attah, Y.M. Ibrahim, R.D. Smith

9:55 Intermission.

10:15 ANYL 5. Determination of ion mobilities in complex gas mixtures: Evaluation of Blanc's law for polyatomic ions. C. Naylor, T. Reinecke, **B. Clowers**

10:45 ANYL 6. Differential mobility spectrometry-mass spectrometry for isotope ratio analysis. **I. Ayodeji**, T.G. Evans-Nguyen, S. Badal, G. MacLean, J. Shelley

11:10 ANYL 7. Gated trapped ion mobility spectrometry. **M.E. Ridgeway**

Section B

Hyatt Regency Orlando
Orlando Ballroom N

Interdisciplinary Chemistry for New Frontiers in Biology & Medicine

NanoBio

Cosponsored by BIOL, COLL, MPPG, PHYS and PMSE[‡]
X. Xu, *Organizer, Presiding*

8:00 ANYL 8. Rational vaccinology: In pursuit of the perfect vaccine. **C.A. Mirkin**

8:30 ANYL 9. Surface chemistry of gold nanorods: From purification to siRNA delivery. **A. Wei**, J. Wang

9:00 ANYL 10. Design of aptamer micelles targeting fractalkine-expressing cancer cells in vitro and in vivo. **E. Kokkoli**

9:30 ANYL 11. Real-time probing of cytotoxic and therapeutic effects of single nanoparticles on single tumor cells. **X. Xu**, P. Songkiatisak, P. Cherukuri, R.M. Richardson, K.K. Raut, A. Zourou

10:00 Intermission.



TECHNICAL PROGRAM

10:10 ANYL 12. Graded surfaces and materials for biological and biomedical applications. **Y. Xia**

10:40 ANYL 13. Nano plus bacteria: How do they connect? **C.J. Murphy**

11:10 ANYL 14. Interrogating immune functions with designer Janus interfaces. **Y. Yu**

11:40 ANYL 15. Three-dimensional nanostructured architectures enable efficient neural differentiation of mesenchymal stem cells via mechanotransduction. **Z. Wang**, M. Poudineh, S.O. Kelley

Section C

Hyatt Regency Orlando
Orlando Ballroom L

Extraterrestrial Organic Analysis: Past, Present & Future

Past & Present

Cosponsored by YCC[‡]
A. M. Stockton, *Organizer, Presiding*
C. J. Bennett, *Presiding*

8:00 Introductory Remarks.

8:10 ANYL 16. Legacy of Cassini-Huygens' ion neutral mass spectrometry at Saturn. **J.H. Waite**, R. Perryman, C. Glein, K. Miller

8:50 ANYL 17. Discovery of organics on Mars with the SAM experiment on the Curiosity rover. **P.R. Mahaffy**

9:30 ANYL 18. Pulsed triboelectric nanospray ionization for analysis of complex organics. **M. Bouza Arces**, A. Li, Z.L. Wang, F.M. Fernandez

9:55 Intermission.

10:10 ANYL 19. Extraterrestrial contributions to the prebiotic inventory of the early earth from meteorites. **C.J. Bennett**, A. LeBleu-DeBartola, B. Ferrari, C. Pirim, J. Noble, Y. Carpenter, C. Focsa, L. Tetard, A. Schulte, D. Britt

10:35 ANYL 20. Fabricating a portable microfluidic cell counter for Icefin, an autonomous underwater vehicle for exploring under Antarctic ice. **N. Speller**, M. Cato, J.L. McNeice, T. Cantrell, M.R. Meister, B. Schmidt, A.M. Stockton

11:00 ANYL 21. Laser desorption mass spectrometry: MOMA-MS and beyond. **S.A. Getty**

Engineered Lignocellulosic Materials & Multiphase Systems: Anselme Payen Award Symposium in Honor of Orlando Rojas

Sustainable Nanofibers



TECHNICAL PROGRAM

Sponsored by CELL, Cosponsored by ANYL and COLL

New Horizons: Early-Career Researchers in Renewable Materials: Symposium in honor of the Kingfa & PhD Student Prize Winners

Sponsored by CELL, Cosponsored by ANYL and PROF

Bio-Based Materials for Energy Conversion & Storage Applications

Electrolyte & Separators for Battery Applications

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Bio-Based Materials for Energy Conversion & Storage Applications

Electrodes for Battery Applications

Sponsored by CELL, Cosponsored by ANYL and BIOL

Advances in Renewable Materials

Sponsored by CELL, Cosponsored by ANYL and CARB

Interplay of Cellulose & Other Biopolymers in Biological & Designed Materials Systems

Interactions of Plant Polymers in Model Systems

Sponsored by CELL, Cosponsored by ANYL, BIOL and CARB

SUNDAY AFTERNOON

Section A

Hyatt Regency Orlando
Orlando Ballroom M

Advances in Ion Mobility Spectrometry



TECHNICAL PROGRAM

Structure

C. Bleiholder, F. Fernandez-Lima, *Organizers*
I. K. Webb, *Presiding*

1:00 Introductory Remarks.

1:05 ANYL 22. Assembly of amyloid systems: The TDP-43 and SOD 1 proteins associated with Amyotrophic Lateral Sclerosis (ALS); key fragments and mutants. **M.T. Bowers**, V. Laos, K.L. Lazar Cantrell, T. Do

1:35 ANYL 23. Top-top-down sequencing of native protein complex in tandem trapped ion mobility spectrometry – mass spectrometry (TIMS-TIMS/MS). **F.C. Liu**, C. Bleiholder

2:00 ANYL 24. Insights on the structural integrity of knot proteins using trapped ion mobility spectrometry – mass spectrometry. **K. Jeanne Dit Fouque**, F. Leng, F. Fernandez-Lima

2:30 Intermission.

2:50 ANYL 25. Collision induced unfolding: New tools for structural biology and drug discovery. **B.T. Ruotolo**, D. Polasky, S. Dixit, S. Fantin, D. Vallejo, K. Parson, C. Zhao

3:20 ANYL 26. Selective binding of a toxin and phosphatidylinositides to a mammalian potassium channel. **A. Laganowsky**

3:50 ANYL 27. Use of ion mobility mass spectrometry for the investigation of the effects of geometries, shapes, apparent densities, and dipole moments on the CCS of small metal complexes. **C. Kune**, J.R. Haler, S. Rappe, A. Demonceau, L. Delaude, J. Far, E. De Pauw

4:15 ANYL 28. Advancing neuropeptide research via novel application of Ion Mobility Mass Spectrometry (IM-MS). **L. Li**, G. Li

Section B

Hyatt Regency Orlando
Orlando Ballroom N

Interdisciplinary Chemistry for New Frontiers in Biology & Medicine

Microbia

Cosponsored by BIOL, COLL, MPPG, PHYS and PMSE‡
X. Xu, *Organizer, Presiding*

1:00 ANYL 29. Multiscale spatiotemporal signaling in microbial communities. T. Cao, J. Jia, H. Do, N. Morales-Soto, J. Ellis, J. Sweedler, J. Shrout, **P.W. Bohn**

1:30 ANYL 30. Effects of antimicrobials on bacteria membrane permeability probed by second harmonic light scattering. **H. Dai**



TECHNICAL PROGRAM

2:00 ANYL 31. SERS monitoring of quorum sensing in bacteria colonies. **L. Liz Marzan**

2:30 ANYL 32. Heme acquisition pathways for rapid pathogen detection and antimicrobial photodynamic therapy. **A. Wei,** A.V. Morales, T.R. Maltais, L. Lin, W. Younis, M.N. Seleem

3:00 Intermission.

3:10 ANYL 33. Understanding and manipulating bacterial toxin efflux at single-molecule single-cell level. **P. Chen**

3:40 ANYL 34. Hybrid structured illumination expansion microscopy reveals microbial cytoskeleton organization. **J.C. Vaughan**

4:10 ANYL 35. Probing the interaction of small molecules with living cell membranes using second harmonic generation. **T.R. Calhoun,** L.N. Miller

4:40 ANYL 36. Antimicrobial natural products from ancient actinomycete bacteria. **A. Hoffman,** E.J. Valente

5:10 ANYL 37. Fluorescent bead-based method to study the phospholipase A2 -lipid membrane interaction. **S. Hossain,** K. Pai, M.E. Piyasena

Section C

Hyatt Regency Orlando
Orlando Ballroom L

Here We Are: Leading & Emerging Black Chemists in Analytical Chemistry

Cosponsored by CMA[‡], CTA[‡] and MPPG[‡]
C. Bridge, R. A. Robinson, *Organizers, Presiding*

1:00 Introductory Remarks.

1:05 ANYL 38. Drugs and explosives identify differentiation in ion mobility spectrometry. **A. Kanu**

1:30 ANYL 39. Directional surface-plasmon-coupled Raman spectroscopy: A new laboratory instrument for combined adsorption and sensitive Raman detection of thin films on smooth planar surfaces. **C.K. Nyamekye,** S.C. Weibel, E.A. Smith

1:55 ANYL 40. Fabrication of a surface plasmon resonance platform for the development of an electrokinetic surface plasmon resonance (EK-SPR) biosensor. **O. Sathoud,** K.S. Booksh

2:20 ANYL 41. Targeted DART ionization for rapid analytical screening. **C. Bridge,** J. Sprague, D.S. Hernandez Funes, K. Foon

2:45 Intermission.

3:00 ANYL 42. Nanostructured biosensors for diagnosis and prediction of pain biomarkers. **O.A. Sadik,** I. Yazgan, L. Yin, P. Gerhardstein



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

3:25 ANYL 43. Hydroxyl radical footprinting coupled with mass spectrometry: Application for in-cell protein. **L. Jones**

3:50 ANYL 44. Comprehensive 'Omics strategies to study disparities in Alzheimer's Disease. **R.A. Robinson**

4:15 ANYL 45. Leveraging emerging mass spectrometry (MS)-based technologies for multi-scale mapping of the lung. **C. Ansong**, G. Clair, J. Kyle, Y. Zhu, E. Nakayasu

4:40 Concluding Remarks.

Section D

Hyatt Regency Orlando
Plaza International Ballroom K

New Frontiers in Teaching Analytical & Bioanalytical Chemistry

N. J. Ronkainen, *Organizer, Presiding*
S. Kradtap, *Presiding*

1:00 ANYL 46. Intercultural virtual exchange for multidimensional learning outcomes in chemistry teaching. **S. Kradtap**, K. Watla-iad

1:20 ANYL 47. Sustainability and social responsibility themed quantitative analysis course. **N.J. Ronkainen**

1:40 ANYL 48. Integrated lecture and laboratory structured project-based analytical chemistry curriculum. **D. Budner**, B.K. Simpson

2:00 Intermission.

2:10 ANYL 49. Introducing a MATLAB®-based chemometrics curriculum for use in undergraduate analytical chemistry. **A. Figueroa Navedo**, P.A. Mabrouk

2:30 ANYL 50. 3D printable open-source optical cage assembly for undergraduate instrument design. **B.J. Winters**

2:50 ANYL 51. Calibration in context: Using beer analysis to introduce standardization methods. **R.A. Hunter**

3:10 ANYL 52. Learning new bioanalytical laboratory skills with new tools. **R. Georgiadis**, N. Eckart

3:30 Intermission.

3:40 ANYL 53. Ultra-HPLC in the advanced analytical chemistry laboratory course. **M.C. Koether**, S.I. Richardson

4:00 ANYL 54. pH-regulated optical performances in organic/inorganic hybrid: A dual-mode sensor array for pattern recognition-based biosensing. **Q. Yan**

4:20 ANYL 55. Label-free fluorescent pattern discrimination of metal ions in biofluids using bioinspired copolymers-based nose/tongue-mimic chemsensor. **Z. Lin**



TECHNICAL PROGRAM

4:40 ANYL 56. Bioinspired Copolymers-Cu²⁺ hybrid sensor array for fluorescent pattern discrimination of thiols and chiral recognition of cysteine enantiomers in biofluids. **Z. Lin**

Engineered Lignocellulosic Materials & Multiphase Systems: Anselme Payen Award Symposium in Honor of Orlando Rojas

Cellulose Nanocrystals Enabling Sustainable Materials

Sponsored by CELL, Cosponsored by ANYL and COLL

New Horizons: Early-Career Researchers in Renewable Materials: Symposium in honor of the Kingfa & PhD Student Prize Winners

Sponsored by CELL, Cosponsored by ANYL and PROF

Bio-Based Materials for Energy Conversion & Storage Applications

Lignin-Based Materials for Supercapacitor & other Applications

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Bio-Based Materials for Energy Conversion & Storage Applications

Electroconductive Hydrogels

Sponsored by CELL, Cosponsored by ANYL and BIOL

Advances in Renewable Materials

Sponsored by CELL, Cosponsored by ANYL and CARB

Interplay of Cellulose & Other Biopolymers in Biological & Designed Materials Systems

Structure & Mechanics of Plant Cell Walls

Sponsored by CELL, Cosponsored by ANYL, BIOL and CARB



TECHNICAL PROGRAM

SUNDAY EVENING

Section A

Orange County Convention Center
West Hall C

Analytical Division Poster Session

Cosponsored by CTA⁺
K. Agnew-Heard, *Organizer*

7:00 - 9:00

ANYL 57. Detection of amino acid biosignatures using capillary electrophoresis. **J.S. Creamer**, M.F. Mora, P.A. Willis

ANYL 58. Withdrawn

ANYL 59. Novel approach to automotive paint analysis using direct analysis in real time mass spectrometry. **K. Jones**, M. Maric, C. Bridge

ANYL 60. Space-time analysis of optical responses of liquid crystal sensors. **A. Smith**, J. Sheavly, N.L. Abbott, R. Van Lehn, V. Zavala

ANYL 61. Analysis of organic and inorganic anions and cations by capillary electrophoresis with contactless conductivity detection for planetary science applications. **E. Oberlin**, M.S. Ferreira Santos, A.C. Noell, M.F. Mora

ANYL 62. Formation of heterocyclic compounds by electrochemically induced intramolecular cyclization. **A. Vasquez**

ANYL 63. Screen-printed electroluminescent display modified with graphene oxide for sensing applications. **A. Yakoh**, R.Á. Diduk, O. Chailapakul, A. Merkoci

ANYL 64. Proximate analysis of phytochemical screening and antimicrobial activities of solvent extract of tiger nut (*Cyprus esculentus*). **M.A. Yoonus**

ANYL 65. Smartphone-based mobile detection platform for rapid molecular diagnostics and spatiotemporal disease mapping. **S. Jinzhao**

ANYL 66. Characterization of sexual assault lubricants: Lubricant database use in an operational setting. **B. Baumgarten**, M. Maric, C. Vadell-Orsini, C. Bridge

ANYL 67. Rapid antibiotic susceptibility testing of patient urine samples using large volume free-aolution light scattering microscopy. **M. Mo**

ANYL 68. Distribution pattern and health risk assessment of polycyclic aromatic hydrocarbons in the water and sediment of Algoa Bay, South Africa. **A.O. Adeniji**, O.O. Okoh, A. Okoh

ANYL 69. Distribution of the stereoisomers of VX in guinea pig tissues following intravenous exposure. **J.M. McGuire**, L. Wright, R. Kristovich, M. Busch



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- ANYL 70.** Label-free impedimetric immunosensor based on N, S-GQDs decorated Au-PANI for selective detection of carcinoembryonic antigen. **A.B. Ganganboina**, R. Doong
- ANYL 71.** Studies on the minearology of some solid minerals found in selected locations in Nigeria. **I. Asia**
- ANYL 72.** Correlational studies of some effluent quality parameters in a petroleum industry in Nigeria. **I. Asia**
- ANYL 73.** Detection of heavy metals utilizing modified CNT electrodes with nanoparticles. **S.K. Lunsford, T. Mangold**, M. Kanthak, K. Muran, L. Zhai
- ANYL 74.** Development of aerosolized monodisperse radioactive particles to track particle deposition. **V. Alstadt**, J. Kesavan, J. Bottiger
- ANYL 75.** Semi-quantitative determination of two fentanyl analogs using fentanyl as a surrogate reference material. **S.E. Voelker**, L.M. Lorenz
- ANYL 76.** Detection of extracellular proteolytic cathepsin L activity using full length histone H3 conjugated electrochemical biosensor. **K. Lee**
- ANYL 77.** Asymmetric flow field flow fractionation to assess the impact of manufacturing process variables on the globule size distribution of cyclosporine ophthalmic emulsions. **H. Qu**, D. Patel, D. Kozak, R. Walenga, S. Choi, P.J. Faustino, M. Ashraf, C.N. Cruz, X. Xu
- ANYL 78.** Development of automatic alternate-current electrochemical etching system for the platinum/irridium probe of scanning tunneling microscopy. **T. Takami**, S. Oki, R. Kitamura
- ANYL 79.** Transition metal oxide nanoparticles as surfaces for the SALDI-MS analysis of real world samples and complex mixtures. **S. Ward**, M.P. Lapak, J.I. Schwieg, B.A. Zanca, L. Barnes, A. McCoy, J.R. Yount, A. Olaitan, K.S. Molek
- ANYL 80.** Analysis of illicit substances found at fatal overdose scenes and their relationship to victim toxicology reports. **T. Cleary**, A. Ballew, B. Ray, M. Lieberman
- ANYL 81.** Simultaneous determination of pharmaceuticals by solid-phase extraction and liquid chromatography–tandem mass spectrometry: A case study from Sharjah sewage treatment plant. **M. Semreen**, A. Shanableh, L. Semerjian, H. Alniss, M. Mousa, X. Bai, K. Acharya
- ANYL 82.** Co-immunocapture and electrochemical quantitation of total and phosphorylated amyloid- β_{40} monomers. **S. Wang**, Z. Yin, B. Shen, **J. Xiang**
- ANYL 83.** Analysis of thyroid hormones in commercial dog food by high performance liquid chromatography with inductively coupled plasma mass spectrometry detection. **R. Wilson**, E.G. Yanes Santos, J. Brueggemeyer
- ANYL 84.** Self-powered enzymatic biosensor for detection of glutathione. J.L. Rutherford, **B.G. Roy**, A. Weaver, K.J. Beaver, M. Rasmussen
- ANYL 85.** Evaluation of the effect of common rice cooking-practices (stove top pasta method) on its metal content. **W.M. Alrawi**, Y. Eltayb, N. Al-jabir, A. Al-shraim
- ANYL 86.** Rapid characterization of insulin modifications and sequence variations by proteinase K digestion and UHPLC-ESI-MS. **W. Tang**, R. Yang, H. Sheng, F. Meng



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

ANYL 87. Case study of green earth pigments as authentic reference materials. **H. Kastenholz**, G.D. Smith, A.M. Wilson, V.J. Chen

ANYL 88. Ion mobility-mass spectrometry and ozone-Induced dissociation (OzID) methods for improved lipidomics analysis. **K. Baker**, **R. Fraser Carris**, **S. Maddox**, C.D. Chouinard

ANYL 89. Electrochemical detection of common neurotransmitters by green synthesized nanoparticles coated onto a modified conductive polymer electrode. **S.K. Lunsford**, **M. Kanthak**, **T. Mangold**, K. Muran, L. Zhai

ANYL 90. Spectrophotometric determination of trace amount of nitrite in water with 4-aminophenylacetic acid and oxine. **D.B. Khadka**

ANYL 91. Measuring the environmental degradation of traditional drug and new psychoactive substance (NPSs) residues. **E. Robinson**, E. Sisco, D. Samarov

ANYL 92. Torus circles on relationships between vicinal constant couplings $^3J_{HH}$ and torsional angles θ_{HnHn+1} . **C. Mitan**, E. Bartha, C. Draghici, M. Caproiu, P. Filip, R.M. Moriarty

ANYL 93. Golden ratio and tetrahedral angles: Relationships between the ^{13}C -RMN chemical shift and tetrahedral angles. **C. Mitan**, E. Bartha, P. Filip, C. Draghici, M. Caproiu, R. Moriarty

ANYL 94. Investigating the anti-fouling properties of carbon nanotube yarn electrodes with FSCV. **R.A. Krevh**, M. Weese, A.E. Ross

ANYL 95. Studies in non-invasive blood glucose determination by micro-Raman, FTIR-ATR spectroscopy and multivariate statistics. **M. Cook**, G.H. Naisbitt

ANYL 96. Determination of catechins in green tea extracts using high performance liquid chromatography coupled with photodiode array and electrospray ionization mass spectrometry. **S. Vest**, Z. Zajickova

ANYL 97. Spectrophotometric and spectrofluorimetric determination of L-Ornithine in pure form and dietary supplements: A chemometric approach. **H.A. Aly**, **A.S. El-Shafie**, M. Elazazy

ANYL 98. Investigation of the sequential flow analysis and the use of chemical reductants for the determination of nitrate in sea water and salt water aquaria. **P.J. Iles**, R. Kochambilli, K. Starr, P. Tiffany, N.R. Bastian, R.V. Valcarce, L.D. Giddings

ANYL 99. Super-resolution imaging of nanoscale chemical heterogeneity on zymosan particles. **W. Li**, H. Wang, S. Lee, X. Xu, Y. Yu

ANYL 100. Identification of pharmaceuticals in Utah's Jordan River. **C.W. Peak**, **B. Luecker**, **B. Schnopp**, **I. Nidawi**, **L. Long**, **P. Tiffany**, **N. Elmore**, L.D. Giddings, R.V. Valcarce, P.J. Iles

ANYL 101. Determination and comparison of antioxidant levels in *Moringa oleifera* leaves and fermented seeds. **A.G. Gonzalez**, H.M. Morales, A. Mar

ANYL 102. Effects of citric acid on the mechanical and corrosion properties of Ni-Y₂O₃ coatings for enhanced corrosion protection. N.K. Ngo, A. Couch, **H. Conrad**, T.D. Golden



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- ANYL 103.** Analysis of fluoride by FIA in dental products. **P.J. Iles**, S. Moore, K. Green, R.V. Valcarce, L.D. Giddings, C. Anderson, S. Dulaney, J. Hughes, C. Sorenson, G. McCormack, R. Kochambilli
- ANYL 104.** Multi-chamber plasma oxidation apparatus for radiocarbon dating of ancient rock art paintings. **A. Arykbayeva**, K.L. Steelman
- ANYL 105.** Analysis of fluoride in dietary samples flow injection analysis employing a fluoride ion-selective electrode. **P.J. Iles**, S. Moore, S. Dulaney, J. Marble, K. Green, J. Hughes, G. McCormack, R.V. Valcarce, L.D. Giddings, R. Kochambilli
- ANYL 106.** Gas chromatography-tandem mass spectrometry method for the selective determination of 2-nitropropane in mainstream cigarette smoke. **G. Chapman**, J. Giraldo Junco, R. Bravo, C.H. Watson, L. Valentin-Blasini
- ANYL 107.** Sticker electrode: A novel disposable device for electrochemical biosensing. L.O. Orzari, R. Freitas, I. Andreotti, **B. Janegitz**
- ANYL 108.** Smartphone-based electrochemical immunosensor for hepatitis B virus detection. **P. Teengam**, O. Chailapakul, N. Ngamrojanavanich
- ANYL 109.** Assessment of ionic content and nutrients in the plant extracts of *Tetraena qatarense* (*Zygophyllum qatarense*) by ICP-OES and ion chromatography. **H. AlThani**, H. Nimir, H. Hassan, H. Al Easa
- ANYL 110.** Sandwich structure of plasmonic paper for surface enhanced Raman spectroscopy. **J. Harms**, D. Burr, W. Fatigante, C.C. Mulligan, J.D. Driskell, J. Kim
- ANYL 111.** DNA nanostructure-based label-free detection of cancer miRNA-21 biomarker. **S. Han**, S. Yang, W. Liu, R. Wang
- ANYL 112.** Analyzing plasmonic and photonic coupling in butterfly wings using surface-enhanced Raman spectroscopy. **L. Palmer**, J.L. Brooks, R.R. Frontiera
- ANYL 113.** Influence of transition metal oxide nanoparticle size on surface-assisted laser desorption/ionization mass spectrometry of small biomolecules. **J.I. Schwieg**, **M.P. Lapak**, S. Ward, S. Varnum, K.S. Molek
- ANYL 114.** Rapid formation of plasmonic paper for SERS applications. **W. Jang**, J.A. Lartey, H. Byun, J. Kim
- ANYL 115.** Development of colorimetric sensor array for discrimination of heavy metal ions. **Y. Huang**, **P. Cheng**, **C. Tan**, **Y. Tan**
- ANYL 116.** Multipronged strategy to identify HIV protein phosphorylation sites using MALDI mass spectrometry. **K.J. Mark**, P. Rathod, H. Ho, E.J. Chang
- ANYL 117.** Indirect determination of biologically significant aminothiols by high performance liquid chromatography coupled with fluorescence detection using a 3-hydroxyflavone derivative. **L. Mikaliunaite**, D.B. Green
- ANYL 118.** Comparison of the temporal dynamics of caspase activity during multiple pathways of apoptosis. **R.D. Reif**, C. Zwemer, S. Morris
- ANYL 119.** Detection limit of a portable Raman spectrophotometer for SERS detection of gunshot residue. **E. Hondrogiannis**, **E. Thayer**, M. Devadas, W. Turner, D. Baird



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

ANYL 120. Use of peak ion ratios measured by gas chromatography-mass spectrometry for the quantitative determination of gasoline target compounds recovered from weathered gasoline spiked onto burnt nylon carpet for forensic purposes. **E. Hondrogiannis, R. Alibozek, C. Newton**

ANYL 121. Preparation of nanoflower-like MoS₂-Ag-CNF by electrospinning and hydrothermal method and its application in VB2 electrochemical sensor. **Y. Ding**

ANYL 122. Capillary electrophoretic analysis of dyes in textile fibers. C.L. Copper, **E. Deglau, G. Gosney, M. Moini**

ANYL 123. Analytical determination of sulfate ions and its attack impact on concrete structures. **A.N. Kawde, A. Abd El Fattah, S. AlDulaijan**

ANYL 124. How the primary structure of related heptapeptides affects their charge states, tertiary structure, and collision-induced dissociation as investigated by ion mobility-mass spectrometry and density functional theory. Y. Lin, J.M. Zahnow, **E. Torres, E. Yousef, L.A. Angel**

ANYL 125. Novel colorimetric and fluorescent assay for aromatic aldehydes detection. **A.N. Marciano Delgado, E. Fasoli**

ANYL 126. Expression, purification, and isolation of mouse Notch1 EGF27. **J. Grennell, M. Macnaughtan**

ANYL 127. Fabrication of LSPR sensor chip based on glass substrate for highly sensitive detection of C-reactive protein. **S. Oh, Y. Huh**

ANYL 128. Composition-dependent photocatalytic activity of Pd/*m*-BiVO₄/BiOBr nanosheets: Degradation of polychlorinated biphenyls. **S. Bachas-Daunert, S. Angaramo, M.R. Knecht, E.M. Zahran, E. Williamson**

ANYL 129. Examination of ionic liquid water dilution effects using differential scanning calorimetry. **N. Walker, J. Wrona, B.J. Bellott, S.K. Shaw**

ANYL 130. Phosphate determination in a stream near a water treatment facility. **R. Haughey, B.J. Bellott**

ANYL 131. Spherical gold nanoparticle-based LSPR sensing chips for rapid and sensitive detection of hepatitis B virus surface antigens (HBsAg). **S. Oh, Y. Huh**

ANYL 132. Highly sensitive aptamer-based nanobiosensors for the detection of human odontogenic ameloblast-associated (ODAM) as a biomarker for periodontal diseases. **B. Lee, S. Kim, Y. Ko, J. Park, S. Ji, M. Gu**

ANYL 133. Method development for the determination of Hg solvation during the cyanidation of Hg⁰-contaminated tailings. **S. Aljic, C.S. Seney, A.M. Kiefer**

ANYL 134. Stability study of an extemporaneous suspension of olmesartan medoxomil. **P. Bhattarai, T. McPherson, M.J. Nieto, W.M. Kolling**

ANYL 135. Microspectroscopy of nanomaterials, biological species, and live cells. **J. Oleske, J. Cooper**

ANYL 136. Combating cyanide fishing: Methods for cyanide detection in common clownfish (*Amphiprion ocellaris*). **S. Hunt, A. Bonanno, J. Grossman, N.E. Breen, A. Rhyne**

ANYL 137. Regional new particle formation measurements with an arduino multisensor device. **K. Rodriguez, L. Montgomery, D. Yordanova, R. Smith, A. Cole, N.M. Kidwell**



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- ANYL 138.** Application of Super Resolution Radial Fluctuation (SRRF) imaging to measurement of single molecule kinetics. **J. Cooper**
- ANYL 139.** Analysis of the metal content of white wines by region using ICP-OES. **C. Hall**
- ANYL 140.** Adaptable xerogel-layered amperometric biosensor platforms on wire electrodes for clinically relevant measurements. **L. Hughes**, N. Labban, M.B. Wayu, J.A. Pollock, M.C. Leopold
- ANYL 141.** Investigating decoherence pathways in $\text{Ho}(\text{W}_5\text{O}_{18})_2$ via magneto-infrared spectroscopy. **A. Blockmon**, K. Hughey, K. O'Neal, Y. Duan, A. Ullah, L. Moreno, M. Ozerov, S. Hill, A. Gaita-Arino, E. Coronado, J. Musfeldt
- ANYL 142.** Development of *in vitro* permeation method for nasally insufflated abuse deterrent formulation. **N.S. Kamal**, A. Zidan, X. Feng, X. Xu, C.N. Cruz, M. Ashraf
- ANYL 143.** Identification of small immunosuppressive molecules produced by chytridiomycosis-causing fungal pathogens. **B.M. Gillard**, J. Tasca, J. Feliciano, T.P. Umile, L. Rollins-Smith, K.P. Minbiole
- ANYL 144.** Analytical results for an insoluble polyacrylic acid ion exchange powder for removal of lead from aqueous systems. **C.C. Philipp**, B. Buchanan, A. Reardon
- ANYL 145.** Optimization of an LC-MS method for the detection of pyrrolizidine alkaloids and their *N*-oxides in herbarium-preserved apocynaceae leaves. **J. Tasca**, H.A. Sanchez, C.R. Smith, T. Livshultz, K.P. Minbiole
- ANYL 146.** Colorimetric, paper-based detection of phosphate in marine environments. **J. Racicot**, T. Mako, M. Levine
- ANYL 147.** Screening and rapid enantiomeric separation of different classes of chiral drugs by convergence chromatography. **A. Masood**, J. Eby, P.J. Faustino
- ANYL 148.** Determination of amino acid content in defatted soybean meal by U-HPLC. **V.R. Spourdalakis**, **B.J. Bellott**, M.A. Berhow
- ANYL 149.** Comparison of UV-photochemical vapor generation and chemical hydride generation for Cd(II) determination. **S. Gilman**, E. Novakova, V. Cervený, J. Hranicek
- ANYL 150.** Detection of cocaine and cocaine simulants on clothing with ion mobility spectrometry (IMS). **N. Remke**, N. Fujimoto, K. Carson, O. Suski, E. Weaver, J.D. Brown, G. Frysinger
- ANYL 151.** Using surface-enhanced Raman scattering of gold nanostars for encoding molecular information. **S. Curry**, Y. Huo, C. Jiang
- ANYL 152.** Simultaneous determination of aflatoxin B1 and its major metabolite aflatoxin M1 in body fluids using dispersive pipette extraction (DPX) followed by high-performance liquid chromatography (HPLC) analysis. **H. Guan**, Q. Cai
- ANYL 153.** Molecular analysis of the induced DNA damage in *Bacillus subtilis* by nanoscale complex metal oxide. **T. Pho**, K.N. Hoang, T.A. Qiu, V. Guidolin, M. Hang, R.J. Hamers, S. Balbo, C.L. Haynes, V. Feng
- ANYL 154.** Surface chemistry and spectroscopic study of the NAC part α -synuclein. **O.S. Olaluwoye**, c. Wang



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- ANYL 155.** Evaluation of the stability of warfarin sodium crystallinity using X-ray diffractometer. **A. Alayoubi**, S. Mattson, C.N. Cruz, M. Ashraf, P.J. Faustino, D. Shakleya
- ANYL 156.** Colorimetric and fluorescent sensing of NADPH in cancer cells. **S. Bae**, S. Shin, S. Kim
- ANYL 157.** Application of novel excited-state CH_2Cl_2 -induced chemi-ionization coupled with time-of-flight mass spectrometry for the real-time detection of volatile organics. **J. Huang**, J. Shu, B. Yang, Z. Zhang, K. Jiang, Z. Li
- ANYL 158.** Decomposition of a nerve agent simulant using UiO-66/PU composite films. **S. Shin**, S. Bae, K. Kim
- ANYL 159.** Determination of fluoride in sodium fluoride tooth gel by ion chromatography. **M. Aggrawal**, J. Rohrer
- ANYL 160.** Detection loop-mediated isothermal amplification was used in the adulteration of duck source. C. Yan, X. Zhao, **C. Ma**
- ANYL 161.** Examining the chiral selectivity of dipeptide surfactant undecyl alanine valine in the presence of diamine counterions. **R. Zoe**, F.H. Billiot, K.F. Morris, E. Billiot
- ANYL 162.** Quantification of beta-galactosidase activity in ovarian cancer cell monolayers. **S. Hayes**, R.L. McCarley
- ANYL 163.** Chemical analysis of tampons. **K. Carlin**, S.T. Shipman
- ANYL 164.** Colorimetric detection of *Bacillus cereus* based on whatman filter paper and LAMP reaction. **S. Liu**, S. Kuang
- ANYL 165.** Evaluation of fibrous silica particles for liquid chromatography. **N.A. Lopez**, L.A. Colon
- ANYL 166.** Mass spectrometric characterization and monitoring the charge variants of rApolipoprotein A-I Milano dimer by anion exchange chromatography. **C. Ramineni**, J. Xu
- ANYL 167.** Determination of nicotine content in e-cigarettes and e-liquid refills utilizing HPLC methods. N. Golob, P. Bhattarai, J. Kerr, T. McPherson, **M.J. Nieto**
- ANYL 168.** Development of a weak anion exchange stationary phase using 2-(Dimethylamino)ethyl methacrylate-co-N-(Hydroxymethyl) acrylamide copolymer for separation of ovalbumin and antibody charge variants. **C. Schwartz**
- ANYL 169.** Decoration of gold nanoparticles onto $\text{Ti}_3\text{C}_2\text{T}_x$ for highly efficient surface-enhanced Raman scattering. **M. Garcia Cervantes**, T. Limbu, F. Yan
- ANYL 170.** Determination of sodium monofluorophosphate in toothpaste using ion chromatography. **H. Yang**, J. Rohrer
- ANYL 171.** Anionic conjugated polyelectrolyte mediated apoptosis imaging in cancer cells. **P. Wu**
- ANYL 172.** Prediction of the vicinal constant couplings $^3J_{\text{HH}}$ and torsional angles ($\theta_{\text{HnHn+1}}$) from the ^{13}C -NMR chemical shifts. **C. Mitan**, P. Filip, C. Deleanu, R. Moriarty, C. Draghici, M. Teodor, E. Bartha
- ANYL 173.** Instrumental assay as a prelude to automated field anion testing. **L.A. Marlowe**, S.K. O'Shea, S.C. MacConnell, C.M. Masse
- ANYL 174.** Withdrawn



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

ANYL 175. Screening of aptamers binding to a cell membrane receptor transiently expressed on the surface of the human cells. **E. Kim**, S. Lee, M. Gu

ANYL 176. Electrochemical-biosensor for the detection of coliform presence in drinking water. **T. Bigham**, J. Davis

ANYL 177. Composite microneedle arrays modified with palladium nanoclusters for electrocatalytic detection of hydrogen peroxide. **C. Hegarty**, S. McKillop, T. Dooher, D. Dixon, J. Davis

ANYL 178. Gold microtubes to electrolessly synthesize manganese dioxide particles. **E. Johnson**, J. Experton, C.R. Martin

ANYL 179. Study of evaporative emissions of ethanol-blended gasoline using headspace-SPME coupled with GC-MS. **A. Ahmed**, D.E. Raynie

ANYL 180. Pressurized liquid extraction: A robust extraction method for cannabinoid analysis and in-extraction chemical modification of acidic cannabinoids. **D. Seifried**, C.A. Kinney

ANYL 181. Synthesis, spectroscopic characterization, biological activity, and dye on cotton and wool fabrics of mixed ligand metal complexes derived from l-phenyl alanine, and 4-chlorobenzophenone Schiff base and anthranilic acid. **T.H. Jasim Al-noor**

ANYL 182. Determination of trace elements in red and white wine samples by graphite furnace atomic absorption spectroscopy. **S.M. Abegaz**

ANYL 183. Colorimetric calcium probe with comparison to an ion-selective optode. **H. ManLing**, X. Xie, C. Zhu

ANYL 184. Comparison of amplification efficiency of different templates using denaturation bubble-mediated strand exchange amplification. **X. Zhao**, **C. Ma**, **C. Yan**

ANYL 185. Superparamagnetic iron oxide nanoparticles allied to gold nanoparticles in the detection of Zika virus by surface-enhanced Raman spectroscopy. **J.J. Santos**, R.L. Silveira, S.H. Toma, K. Araki, A.G. Brolo, P. Corio

ANYL 186. Detection of exosomes using chemiluminescence assay based on competitive hybridization with aptamer. **L. He**, X. Yu, N. He, Z. Li

ANYL 187. ^{13}C NMR analysis of $^{13}\text{C}_2$ molecules to model in-situ sediment halogenated organic carbons transformations. **C. Masse**, L.A. Marlowe, S.C. MacConnell, S.K. O'Shea

ANYL 188. Assay development for N_2 -Ethylguanine using liquid chromatography- triple quadrupole (LC-TQ) mass spectrometry instrumentation. **A.M. Newman**, J. Wilhide, W.R. Lacourse

ANYL 189. Atomic force microscopy (AFM) and scanning electron microscopy (SEM) studies of ganglioside-phospholipid mixed vesicles. **A. Sunda-Meya**, N. Phambu, B.M. Almarwani, E. Gatune, A. Fashola

ANYL 190. Development of thiol specific fluorogenic agent for lysosome thiol imaging in live cells. **Y. Alqahtani**

ANYL 191. Gas chromatography-mass spectrometry and inductively coupled plasma - mass spectrometry analysis of dokha, Middle-Eastern tobacco product, to measure nicotine. **E. Hondrogiannis**, **R. Alibozeq**, A. Belunis



TECHNICAL PROGRAM

- ANYL 192.** Bandgap tunability with transition metal cation exchange for zinc oxide nanostructures morphology, optical and crystallinity studies. **K. Davis**, H.P. Rathnayake
- ANYL 193.** Instrument-free sample preparation system for clinical use. **Y. Shin**
- ANYL 194.** Development of a novel near-infrared fluorescent hydrogen sulfide probe for live cells and tissues imaging. **X. Huang, J. Zhang, Y. Tan, N. Xu**
- ANYL 195.** Fabrication of redox pH probes for use in microbial reactors. **C. Casimero**, A. McConville, J. Fearon, C. Lawrence, C. Taylor, R. Smith, J. Davis
- ANYL 196.** Withdrawn
- ANYL 197.** Analytical method development and analysis of tricyclazole residue *Proso Millet* using LC-MS/MS. **R. Ko**, Z. Jin, J. Lee, A. Lee, E. Park, X. Yuan, M. Rehan, S. Kim, B. Ju, J. Kim
- ANYL 198.** Analytical method development and analysis of bitertanol residue in *Sorghum* using GC-MS/MS. **X. Yuan**, Z. Jin, J. Lee, A. Lee, E. Park, R. Ko, M. Rehan, S. Kim, B. Ju, J. Kim
- ANYL 199.** Characterizing natural molecule intramolecular bonding using NMR equilibrium isotope effect. **E. Lund**, D.J. O'Leary
- ANYL 200.** Infrared and Raman studies of ganglioside-peptide interactions. **N. Phambu**, B.M. Almarwani, A. Sunda-Meya
- ANYL 201.** Comparative extraction techniques of volatile and semi-volatile halogenated organic arrays from marine sediments by solid phase, Soxhlet and microwave protocols determined by GC/MS.. **S. MacConnell**, C. Masse, L.A. Marlowe, S.K. O'Shea
- ANYL 202.** Self-assembled monolayer of 3-Mercaptopropionic acid on a gold electrode for prostate cancer detection applications. **M.M. Santana Rivera**, S. Alonso Sevilla, C. Colon, M.B. Santiago-Berrios
- ANYL 203.** Chiral analysis of amino acid distributions in Europa and Enceladus analogues using analyte pre-concentration. **K.M. Seaton**, A. Stockton
- ANYL 204.** Interactions of carbamate insecticides with hydrophilic and hydrophobic surfaces using surface-selective spectroscopy. **J.L. Cartagena**, L. Bromley III, A. Fernando, P. Videla, V.S. Batista, L.A. Velarde
- ANYL 205.** Au nanotubule plated polycarbonate membranes for the study of cation transference. **S. Walters**, J. Experton, C.R. Martin
- ANYL 206.** Interaction of brilliant cresyl blue with gold nanoparticles modified with B-cyclodextrin as a sensor for warfarin. **N. Gonzalez Velez**
- ANYL 207.** Characterization of organosilane nanostructures with atomic force microscopy. **A.M. Arcement**, N. Kuruppu Arachchige, Z.L. Highland
- ANYL 208.** Differentiation between ZIKA lineages using electrochemical biosensors based on nucleic acid detection. **A.M. Balcarcel**, M.V. Foguel, C.E. Ledezma, P. Calvo-Marzal, K.Y. Chumbimuni Torres



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- ANYL 209.** Development of a microfluidic device for quantitation of nitrate/nitrite in water and soil. **R. Martinez, T. Gyaltsen, K. Frederick**
- ANYL 210.** Determination of total and free mycophenolic acid in human plasma by high-performance liquid chromatography with fluorescence detection. **P. Tang**
- ANYL 211.** HPLC analysis for antioxidant properties of beer and the impact on shelf life. **A. Zielinski, D.J. Lecaptain**
- ANYL 212.** Flavonoids in *Pinus taeda* (loblolly pine), *Quercus Virginiana* (Southern live oak), *Carya illinoensis* (pecan), *Acer Negundo* (box alder), *Quercus palustris* (pin oak), and *Populus alba* (white poplar). **C. McCullum**
- ANYL 213.** Evaluating the influence of NAD(P)H: Quinone oxidoreductase-1 and metastatic phenotype on ovarian cancer metastasis. **M. Jackson**
- ANYL 214.** Saponins in the bark of *Pinus taeda* (loblolly pine), *Quercus virginia* (southern live oak), *Carya illinoisensis* (pecan), *Acer negundo* (box alder), *Quercus palustris* (pin oak), and *Populus alba* (white poplar). **C. McCullum**
- ANYL 215.** Tannins from the bark of *Pinus taeda* (loblolly pine), *Quercus virginiana* (southern live oak), *Carya illinoensis* (pecan), *Acer negundo* (box alder), *Quercus palustris* (pin oak), and *Populus alba* (white poplar). **C. McCullum**
- ANYL 216.** Phytochemistry of bark collected from *Pinus taeda* (loblolly pine), *Quercus virginiana* (Southern live oak), *Carya illinoensis* (pecan), *Acer negundo* (box alder), *Quercus palustris* (pin oak), and *Populus alba* (white poplar). **C. McCullum**
- ANYL 217.** Chemometric analyses for electrochemical signal amplification for the detection of cancer biomarker. **S. Turner, M. Boza, M.V. Foguel, P. Calvo-Marzal, K.Y. Chumbimuni Torres**
- ANYL 218.** Expression, purification, and separation of Notch1 EGF25. **K.D. Jenkins, M. Macnaughtan**
- ANYL 219.** Optimizing sol-gel derived Si-based nanoparticles for use in luminescence-based chemical sensing. **E.M. Berni, P.S. Palencia, J.F. Destino**
- ANYL 220.** Detection of amines in air with ion chromatography and thermal desorption gas chromatography. **P.J. Silva**
- ANYL 221.** Identification of metal cations in solution using acid-base titration. **R.K. Lynch, A. Altman**
- ANYL 222.** Advanced urine testing using conductometric techniques to assess renal function. **M.S. McAfee**
- ANYL 223.** Influence of hydrogen assisted method for copper electrodeposition. **S. Rosa**
- ANYL 224.** Charge remote analysis of lignin model compounds in gas phase by mass spectroscopy. **S. Mistry, C.J. Conder, P.G. Wenthold**
- ANYL 225.** Aromatic analysis of lavender essential oil using nanofiber sensors. **M. Vaughn, N. Stevens**
- ANYL 226.** Cyclic voltammetric determination of acetaminophen, a quantitative analysis course laboratory. **N.T. Hart, W.C. Lane, L. De La Garza**
- ANYL 227.** Neutral red as a pH luminescent sensor for carbon dioxide studies. **M.N. Ericson, S. Marpu, M.A. Omary**



TECHNICAL PROGRAM

ANYL 228. Work towards an electrogenerated chemiluminescence -DNA biosensor labeled with a ruthenium complex. **G. Stark, H. Bui**, K.N. Hipp, R.Y. Lai, E.M. Gross

ANYL 229. Novel molecular complexes for the selective detection of Perfluorooctanoic acid. **T.S. Saeed**, S.O. Obare

ANYL 230. Development and evaluation of mobile phone camera as an electrogenerated chemiluminescence detection method for biogenic amines using a ruthenium complex. **N. Heckenlaible**, A. Kava, C. Henry, E.M. Gross

ANYL 231. Results from testing an icy moon penetrator organic analyzer. M. Cato, N. Speller, Z. Duca, P. Putman, S. Foreman, J. Kim, B. Schmidt, **A.M. Stockton**

General Posters

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General Posters

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MONDAY MORNING

Section A

Hyatt Regency Orlando
Orlando Ballroom M

Advances in Ion Mobility Spectrometry

Complex Mixtures & Post-Translational Modifications

C. Bleiholder, F. Fernandez-Lima, *Organizers*
K. Jeanne Dit Fouque, *Presiding*

8:00 Introductory Remarks.

8:05 ANYL 232. On-line nanoLC-ion mobility-electron capture dissociation-QTOF MS/MS Analysis of biopolymers and mixtures. J.A. Hill, R. Glaskin, C. Heckendorf, K.B. Chandler, D.R. Leon, M.E. McComb, **C.E. Costello**

8:35 ANYL 233. Liquid chromatography-ion mobility-mass spectrometry for the improved analysis of isomeric anabolic androgenic steroids. **A. Levy**, N.R. Oranzi, R.A. Yost

9:00 ANYL 234. Combination of capillary electrophoresis and ion mobility coupled to mass spectrometry to theoretical calculations for cysteine connectivity identification in peptides bearing two intra-molecular disulfide bonds. C. Delvaux, P. Massonnet, C. Kune, G. Upert, G. Mourier, J.R. Haler, N. Gilles, L. Quinton, E. Béchet, **J. Far**, E. De Pauw



TECHNICAL PROGRAM

9:30 Intermission.

9:50 ANYL 235. Tandem-trapped ion mobility spectrometry / mass spectrometry for structural biology applications. **C. Bleiholder**

10:20 ANYL 236. Integration of gas-phase covalent ion/ion reactions with ion mobility spectrometry. V. Carvalho, L. Keeling, I.K. **Webb**

10:50 ANYL 237. Native ion mobility mass spectrometry: Adding new dimensions. **M.F. Bush**

Section B

Hyatt Regency Orlando
Orlando Ballroom N

Interdisciplinary Chemistry for New Frontiers in Biology & Medicine

Biomarker Discovery

Cosponsored by BIOL, COLL, MPPG, PHYS and PMSE‡
X. Xu, *Organizer, Presiding*

8:00 ANYL 238. Beyond biomarkers: Array-based profiling for diagnostics and geno- and phenotypic screening for precision medicine. **V.M. Rotello**

8:30 ANYL 239. Wearable bands as passive sweat sensors. **S. Yang**

9:00 ANYL 240. Rare cell analysis using magnetic ranking cytometry: A new approach to liquid biopsy. **S.O. Kelley**, M. Labib, R. Mohamadi, M. Poudineh

9:30 ANYL 241. Surface-enhanced Raman scattering on paper test strips for quantitative detection of biomarkers in clinical blood samples. X. Gao, K. Curtin, **N. Wu**

10:00 Intermission.

10:10 ANYL 242. Sweetening the process of biomarker discovery in Alzheimer's disease: Development of improved chemical strategies for probing glycosylation patterns in AD. **L. Li**, Z. Chen, X. Zhong

10:40 ANYL 243. Pulsed isotopic labeling of hypoxic and normoxic cellular populations. **A.B. Hummon**

11:10 ANYL 244. Searching for non-invasive volatile biomarkers for colorectal cancer in stool headspace and exhaled breath: Standardised sampling and analysis. **J. Beauchamp**, A. Smolinska, R. van Vorstenbosch, T. Ligor, L. Schlund, B. Buszewski, F. van Schooten

11:30 ANYL 245. Metabolomics of *Oxalobacter formigenes* to characterize intestinal oxalate secretion. **C.A. Chamberlain**, M. Hatch, T.J. Garrett

Section C



TECHNICAL PROGRAM

Hyatt Regency Orlando
Orlando Ballroom L

Extraterrestrial Organic Analysis: Past, Present & Future

Planned & Proposed

Cosponsored by YCC†
A. M. Stockton, *Organizer, Presiding*
C. J. Bennett, *Presiding*

8:00 ANYL 246. Scanning Habitable Environments with Raman and Luminescence for Organics and Chemicals (SHERLOC) on Mars 2020. **L. Beegle**, R. Bhartia, W. Abbey, J. Razzell Hollis, S.A. Asher, M. Fries, A. Burton

8:40 ANYL 247. Enceladus: Life signatures and habitability. **A. Davila**, J. Eigenbrode, T. Hurdford, C. McKay

9:20 ANYL 248. Solid contact ion selective electrodes for planetary science applications. **E. Oberlin**, A.C. Noell, M.F. Mora

9:45 Intermission.

10:00 ANYL 249. Microfabricated Organic Analyzer for Biosignatures (MOAB). **R.A. Mathies**, M. Golozar, A. Butterworth, J. McCauley, A.M. Stockton, J. Kim, J. New, M. Burchell, M. Price

10:45 ANYL 250. Microchip electrophoresis hardware for spaceflight missions of exploration. **M.F. Mora**, F. Kehl, E. Tavares da Costa, N. Bramall, P.A. Willis

11:10 ANYL 251. In-situ desalination using ion exchange chromatography for detection of biosignatures in planetary environments. **J. Skerritt**, K. Craft, T. VanVolkenburg, K. Ohiri

11:35 ANYL 252. Fragmentation mapping for molecular complexity metrics with flight capable ion traps. **H.V. Graham**, P.R. Mahaffy, S. Johnson, G. Cooper, C. Kempes, E. Libby

Section D

Hyatt Regency Orlando
Plaza International Ballroom K

Advances in the Characterization of Electronic Nicotine Delivery Systems (ENDS)

K. Agnew-Heard, *Organizer*
J. Lisko, *Organizer, Presiding*

8:00 Introductory Remarks.

8:10 ANYL 253. Characterization of Electronic Nicotine Delivery Systems (ENDS): Implications for public health and regulatory science. **R. Oconnor**



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

8:40 ANYL 254. Universal e-cigarette test: standardized research materials, testing devices and testing methods. **B. Koszowski**

9:10 Intermission.

9:25 ANYL 255. Identification and quantification of flavoring chemicals in ENDS refill solutions. **M.L. Goniewicz**, T. Vanderbush, N. Leigh

9:55 ANYL 256. Free radical and carbonyl formation in electronic cigarette aerosols. **J.P. Richie**, Z.T. Bitzer, R. Goel, S. Reilly, N. Trushin, J. Foulds, J. Muscat, R. Elias

10:25 Intermission.

10:40 ANYL 257. Reporting formaldehyde in electronic cigarette aerosol and the relevance of formaldehyde hemiacetals and acetals. **M.S. Melvin**, K. Avery, R. Ballentine, W.P. Gardner, X. Jin, W. McKinney, Y.B. Pithawalla, D.C. Smith, K.A. Wagner

11:10 ANYL 258. Impact of device variability on the determination of aldehyde compounds in e-cigarette emissions. **I.G. Gillman**, A.S. Pennington, K.E. Humphries

Engineered Lignocellulosic Materials & Multiphase Systems: Anselme Payen Award Symposium in Honor of Orlando Rojas

Creating Sustainable Polymers & Composites

Sponsored by CELL, Cosponsored by ANYL and COLL

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Sponsored by PROF, Cosponsored by AGFD, ANYL, BIOL, BIOT, CARB, CELL, CHED, CMA, COLL, COMP, ENVR, GEOC, I&EC, MEDI, MPPG, NUCL, ORGN, PHYS, PMSE, POLY, PRES, WCC and YCC

New Horizons: Early-Career Researchers in Renewable Materials: Symposium in honor of the Kingfa & PhD Student Prize Winners

Sponsored by CELL, Cosponsored by ANYL and PROF

Understanding Cellulose Crystallinity & Non-Crystalline Aggregated States of Cellulose

Sponsored by CELL, Cosponsored by ANYL



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

Advances in Renewable Materials

Sponsored by CELL, Cosponsored by ANYL and CARB

Interplay of Cellulose & Other Biopolymers in Biological & Designed Materials Systems

Xylan & Lignin Interactions with Cellulose

Sponsored by CELL, Cosponsored by ANYL, BIOL and CARB

MONDAY AFTERNOON

Section A

Hyatt Regency Orlando
Orlando Ballroom M

Frank H. Field & Joe L. Franklin Award for Outstanding Achievement in Mass Spectrometry

Cosponsored by PROF[‡]
E. R. Williams, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 ANYL 259. **Award Address** (Frank H. Field and Joe L. Franklin Award for Outstanding Achievement in Mass Spectrometry sponsored by the Waters Corporation). Ultraviolet photodissociation mass spectrometry for characterization of proteins and protein complexes. **J. Brodbelt**

1:40 ANYL 260. High throughput chemical reactions in droplets and thin films. **R.G. Cooks**, Z. Wei, Y. Li, D. Logsdon, R. Hilger

2:15 ANYL 261. Understanding the molecular defect in Cystic Fibrosis. S. Pankow, C. Bamberger, D. Calzolari, S. Martinez de Bartolome Izquierdo, M. Lavallee-Adams, **J.R. Yates**

2:50 Intermission.

3:10 ANYL 262. Role of surface-induced dissociation in a native MS workflow. **V.H. Wysocki**

3:45 ANYL 263. Mass, mobility and MS^N measurements of individual ions with charge detection mass spectrometry. **E.R. Williams**, C. Harper, A. Elliot

Section B

Hyatt Regency Orlando
Orlando Ballroom N



TECHNICAL PROGRAM

Interdisciplinary Chemistry for New Frontiers in Biology & Medicine

DNA/RNA & Disease Diagnosis

Cosponsored by BIOL, COLL, PHYS and PMSE
X. Xu, *Organizer, Presiding*

1:00 ANYL 264. Imaging of disease targets in cells via stimulus-responsive molecular probes. **R.L. McCarley**

1:30 ANYL 265. Specific DNA aptamers selected for molecular classification of breast cancer subtypes. **N. He**, M. Liu, Y. Deng, Z. Wang

2:00 ANYL 266. Development of a miniaturized system for DNA-based sepsis diagnosis. **A. Woolley**, R.L. Hanson, D. Harris, R. Knob, O.B. Tateoka, R.L. Wood, R.A. Robison, W.G. Pitt

2:30 ANYL 267. Visually probing restriction engineered biological nanopores in a high-throughput nanopore array. **S. Huang**

3:00 ANYL 268. Programmable DNA-semiconductor nanostructures for molecular delivery. **L. Zhang**, S.O. Kelley

3:20 Intermission.

3:30 ANYL 269. Passive implantable fluidic sensor for non-invasive monitoring of tibial plate strain via plain radiography. **A. Rajamanthrilage**, M. Arifuzzaman, P. Millhouse, J. DesJardins, C. Behrend, J.N. Anker

3:50 ANYL 270. Development of lipobead-based phospholipase D biosensor for diagnostic applications. **R. Gurung**, T. Ogas, P. Patidar, M.E. Piyasena

4:10 ANYL 271. Characterizing differentiation potential of adipose-derived stem cells using gold nanorods by dark-field hyperspectral scattering microscopy. **S. Sahu**, N. Mehta, S. Shaik, R. Devireddy, M.R. Gartia

4:30 ANYL 272. Acoustophoretic separation of cell samples exploiting the differences in biomechanical properties. **G.P. Gautam**, T. Ogas, **P. Patidar**, M.E. Piyasena

4:50 ANYL 273. Mechanical manipulation of Caco-2 Cell behavior on centrifugal microfluidic platforms. **D.L. Cavazos-Elizondo**, **A.V. Martínez-Dibildox**, S.O. Martinez-Chapa, M. Aeinehvand, J. Villela, H. Aguirre Soto, S. Serna

5:10 ANYL 274. New strategies for early diagnosis and prognosis of acute myocardial infarction. **S. Khor**, W. Lim, T. Thevarajah, B. Goh

Section C

Hyatt Regency Orlando
Orlando Ballroom L

Student Organized Symposium: New Analytical Approaches for Environmental Chemistry

A. V. Morales, *Organizer*



TECHNICAL PROGRAM

M. Misovich, C. West, *Organizers, Presiding*
A. C. Morales, *Presiding*

1:00 ANYL 275. Probing molecular composition of Iron-organic complexes and their photochemical products in laboratory mimics of atmospheric aerosol and cloud water. **C. West**, M. Misovich, P. Lin, A. Hettiyadura, A. Laskin

1:20 ANYL 276. Yields and fate of OH radical-initiated oxidation of β -ocimene in the presence of NO_x at different relative humidities. **A.C. Morales**, T. Jayarathne, J. Slade, A. Laskin, P.B. Shepson

1:40 ANYL 277. Highly sensitive, colorimetric, paper-based devices for the dual detection of nitrate and nitrite. **T. Mako**, J. Racicot, A. Levenson, M. Levine

2:00 ANYL 278. Quartz crystal microbalance based virtual sensor array for detection and discrimination of VOCs using phosphonium ionic liquid composites. **S. Vaughan**, R. Pérez, P. Chhotaray, I.M. Warner

2:20 Intermission.

2:35 ANYL 279. Ambient aerosol optical properties throughout the UV-Vis spectral region derived via photoacoustic spectroscopy and broadband cavity-enhanced spectroscopy. **M. Pogash**, G.D. Smith

2:55 ANYL 280. Exploring the chemistry of hydrocarbon: Organic acid and carbonyl formation from γ -ketohydroperoxide decomposition in n-butane oxidation. **D. Popolan-Vaida**

3:15 ANYL 281. Measuring the influence of surfactants on the growth of individual aqueous coarse mode aerosol particles. **A. Frossard**, R. Bramblett, W.C. Hudson, T. Burdette, V. Gerard, B. Noziere, R.C. Cohen

3:35 ANYL 282. Widening the window for environmental analysis: On-line HPLC monitored by 21 tesla Fourier transform ion cyclotron resonance mass spectrometry. **A.G. Marshall**, M.L. Chacon, Y. Corilo, C.L. Hendrickson, L.C. Krajewski, S.F. Niles, J.C. Putman, S.M. Rowland, D.F. Smith, R. Ware, C.R. Weisbrod, R.P. Rodgers

3:55 Concluding Remarks.

Section D

Hyatt Regency Orlando
Plaza International Ballroom K

Advances in the Characterization of Electronic Nicotine Delivery Systems (ENDS)

J. Lisko, *Organizer*
K. Agnew-Heard, *Organizer, Presiding*

1:00 Introductory Remarks.

1:10 ANYL 283. Parameters affecting nicotine and toxicant fluxes in electronic cigarettes. **N.A. Saliba**, A. El Hellani, R. El Hage, R. Salman, S. Talih, N. Karaoghlanian, J. Zeaiter, A. Shihadeh

1:40 ANYL 284. Characterization of nicotine, carbonyl, and carbon monoxide emissions from four types of electronic cigarette devices. **A. Khlystov**, Y. Son, V. Samburova, C. Bhattarai



TECHNICAL PROGRAM

2:10 Intermission.

2:25 ANYL 285. Non-targeted analysis using gas chromatography mass spectrometry to evaluate chemical composition of e-vapor products. **N.H. Shah**, M.R. Noe, J.H. Miller, K.A. Agnew-Heard, M. Crosswhite, Y.B. Pithawalla, W.P. Gardner

2:55 ANYL 286. Real-time characterization and quantification of electronic cigarette aerosol and VOC using proton transfer mass spectrometry. **N. Heine**

3:25 Intermission.

3:40 ANYL 287. Oral cell-based biomarkers for assessing e-cigarette-derived exposures and effects. **I. Stepanov**

4:10 ANYL 288. Development of spectrometric methods for e-liquids authentication. **M. Funck**

Engineered Lignocellulosic Materials & Multiphase Systems: Anselme Payen Award Symposium in Honor of Orlando Rojas

Creating 21st Century Sustainable Materials from Lignin

Sponsored by CELL, Cosponsored by ANYL and COLL

Kathryn C. Hach Award for Entrepreneurial Success

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LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Sponsored by PROF, Cosponsored by AGFD, ANYL, BIOL, BIOT, CARB, CELL, CHED, CMA, COLL, COMP, ENVR, GEOC, I&EC, MEDI, MPPG, NUCL, ORGN, PHYS, PMSE, POLY, PRES, WCC and YCC

Chemistry in Space: Future Directions

Sponsored by YCC, Cosponsored by AGFD, ANYL, BIOT, BMGT, CHAS, ENVR, FLUO, GEOC, HIST, I&EC, MEDI, POLY and PROF

New Horizons: Early-Career Researchers in Renewable Materials: Symposium in honor of the Kingfa & PhD Student Prize Winners

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TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

Emerging Frontiers in Fluorescence Microscopy: From Single Molecules to Super Resolution

Sponsored by PHYS, Cosponsored by ANYL

Ionic-Liquids Processing of Polysaccharides

Sponsored by CELL, Cosponsored by ANYL and CARB

Fluorescence Techniques Applied to Lignocellulose Characterization

Sponsored by CELL, Cosponsored by ANYL and BIOL

Hemp Processing: From Weed to Values

Sponsored by CELL, Cosponsored by AGRO and ANYL

Undergraduate Research Posters

Analytical Chemistry

Sponsored by CHED, Cosponsored by ANYL and SOCED

MONDAY EVENING

Section A

Orange County Convention Center
West Hall C

Sci-Mix

K. Agnew-Heard, M. F. Bush, *Organizers*

8:00 - 10:00

1, 6, 9, 15, 16, 17, 19, 26, 36, 40, 49, 57, 58, 60, 61, 65, 67, 246, 248, 251, 254, 255, 264, 265, 267, 268, 269, 271, 272, 274, 275, 276, 277, 288. See previous listings.



TECHNICAL PROGRAM

ANYL 289. Distinctive fluorescence of water-soluble flavonol induced by the surface bonding on ZrO₂nanoparticle and its application to a test strip for fluoride ion detection. **Y. Takahashi**, W. Ando, K. Takano

ANYL 290. Phenolics, Antioxidant Capacity and Bioaccessibility of Kombucha Tea. **N. Değirmencioğlu**, E. Yıldız, Y. Sahan, M. Güldas, O. Gurbuz

ANYL 291. Geometry and energy: Relationships between the ¹³C-NMR chemical shift and tetrahedral angles. **C. Mitan**, R.M. Moriarty, P. Filip, E. Bartha, C. Draghici, M.T. Caproiu

295, 298, 301, 302, 303, 304, 306, 307, 308, 309, 310, 312, 313, 318, 319, 322, 326, 328, 330, 332, 337, 338, 344, 347, 350, 351, 353, 354, 357, 358, 359, 360, 361, 362, 365, 366, 367, 369, 370, 374, 375, 376, 377, 378, 380, 381, 384, 385, 386, 387, 388, 392, 393, 397, 398, 399. See subsequent listings.

TUESDAY MORNING

Section A

Hyatt Regency Orlando
Orlando Ballroom M

ACS Award in Chromatography

Cosponsored by PROF[‡]
S. G. Weber, *Organizer, Presiding*

8:00 Introductory Remarks.

8:10 ANYL 292. Award Address (ACS Award in Chromatography sponsored by MilliporeSigma). UHPLC: Where to go Next with Particles, Columns and Instruments? **G. Desmet**, S. Deridder, K. Broeckhoven

8:50 ANYL 293. Design and development of an online-liquid chromatography mass spectrometry workflow to enable manufacturing of synthetic peptides. **S. Groskreutz**, G. Lambertus, J. Dieringer, M. Johnson, T. Maloney

9:30 ANYL 294. Miniaturizing liquid chromatography columns and instrumentation. **J.P. Grinias**

10:10 Intermission.

10:25 ANYL 295. Vacuum-Jacketed Columns: An opportunity for better LC/MS integration. **F. Gritti**

11:05 ANYL 296. Use of active temperature control in capillary liquid chromatography. **S.G. Weber**, A.R. Horner, S. Groskreutz, M. Rerick

Section B

Hyatt Regency Orlando
Orlando Ballroom N



TECHNICAL PROGRAM

Interdisciplinary Chemistry for New Frontiers in Biology & Medicine

Structure, Imaging & Sensing

Cosponsored by BIOL, COLL, PHYS and PMSE‡
X. Xu, *Organizer, Presiding*

8:00 ANYL 297. Development of a mass spectrometry-guided structural biology workflow. **V.H. Wysocki**

8:30 ANYL 298. Global measurements of protein folding stability for the characterization of aging and disease. **M.C. Fitzgerald**

9:00 ANYL 299. Functional roles of topoisomerases in transcription: Relevance for basis and treatment of human diseases. **Y. Tse-Dinh**

9:30 ANYL 300. PicoNewton oscillatory and compressive mechanical force manipulation of single-molecule protein structure and functions. **H. Lu**

10:00 Intermission.

10:10 ANYL 301. Near-infrared nerve-specific fluorophores for fluorescence image-guided surgery. **L. Wang**, C.W. Barth, V. Shah, A.W. Alani, A. Antaris, J. Sorger, S.L. Gibbs

10:30 ANYL 302. Optical sensors for detecting signaling phospholipids. **A. Chandra**, S. Mondal, R. Venkatramani, A. Datta

10:50 ANYL 303. Converting green fluorescent protein based biosensors to red in a general way. **S. Zhang**, H. Ai

11:10 ANYL 304. Molecular modelling approach to access organophosphate toxicity with human acetylcholinesterase. **T. Jindal**

Section C

Hyatt Regency Orlando
Orlando Ballroom L

Advances in Electrochemistry

L. A. Baker, J. Experton, *Organizers, Presiding*

8:00 ANYL 305. Novel electrochemical sensor based on CuO/H-C₃N₄/rGO nanocomposite for efficient electrochemical sensing nitrite. **Y. Li**

8:30 ANYL 306. Initial steps towards the development of a miniaturized amperometric sensor capable of selective H₂S detection. **J.A. Bennett**, H. Pharathikoune, M. Rodriguez

9:00 ANYL 307. Prussian blue zinc oxide carbon nanotube composite for rapid hydrogen peroxide assaying. **R.R. Pandey**, Y. Guo, Y. Gao, C. Chusuei



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

9:30 ANYL 308. Fabrication of molecular imprinted polymer modified glassy carbon electrode for electrochemical detection of 4-nitrophenol. **S. Ata**, M. Feroz

10:00 Intermission.

10:10 ANYL 309. Electropolymerization of molecularly imprinted polypyrrole for sensing explosive compounds. **N. Holubowitch**, S.P. Beaudoin, G. Medina, J. Wray

10:40 ANYL 310. Aptamer electrochemical biosensor for cadmium ions detection. **Y. Liu**, Y. Deng, N. He

11:10 ANYL 311. Rapid and selective detection of Zika virus circulating in the Americas using electrochemical RNA-sensor along with NASBA. **M.V. Foguel**, C.A. Lynch, A. Reed, A.M. Balcarcel, P. Calvo-Marzal, Y. Gerasimova, K.Y. Chumbimuni Torres

11:40 ANYL 312. Preparation of novel redox dye modified aptamers and their application to construct wash-free electrochemical biosensing technologies. **J. Lee**, N. Loew, K. Sode

Section D

Hyatt Regency Orlando
Plaza International Ballroom K

Frontiers in Forensic Mass Spectrometry

K. Evans-Nguyen, *Organizer, Presiding*

8:00 ANYL 313. On the tandem mass spectrometry of cathinones and mass spectrometric identification of drugs. **G.P. Jackson**, J.T. Davidson, Z.J. Sasiene, Y. Abiedalla, C.R. Clark

8:30 ANYL 314. Towards on-site drug evidence confirmation using ambient sampling, portable mass spectrometry. **C.C. Mulligan**, W. Fatigante, A.R. Stelmack, D. Burr, J. Harms, J. Kim, J.D. Driskell, J.R. Wieland

9:00 ANYL 315. Automated dye extraction microfluidics device coupled to a quadrupole time-of-flight mass spectrometer enables the direct analysis of dyes from trace single fibers and single fiber threads. **N.R. Vinueza**

9:30 ANYL 316. Targeted rapid sample preparation of fentanyl for mass spectrometric analyses. E. Seyyal, N. Grimes, **T.G. Evans-Nguyen**

10:00 Intermission.

10:10 ANYL 317. Temperature Controlled Ambient Ionization of Lubricants for Increased Match Determination. **C. Bridge**, M. Maric

10:40 ANYL 318. Detection of ricin and abrin toxin by laboratory-based and portable direct analysis in real-time mass spectrometry (DART-MS). **J. Sekowski**

11:10 ANYL 319. DART-HRMS/Kendrick mass defect analysis applied to the sourcing of plastic bonded explosives. G. Gaiffe, R.B. Cole, **M.C. Bridoux**



TECHNICAL PROGRAM

11:40 ANYL 320. Applications of the US EPA's CompTox chemicals dashboard to support structure identification and chemical forensics using mass spectrometry. **A.J. Williams**, A. McEachran, J. Sobus, E. Schymanski

Engineered Lignocellulosic Materials & Multiphase Systems: Anselme Payen Award Symposium in Honor of Orlando Rojas

Sustainable Materials in High Performance Applications

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Exploring the Frontiers of Chemistry through NASA Research

Getting There: Advanced Materials for Space Travel

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ACS Sustainable Chemistry & Engineering: Symposium in honor of Dr. Silvia Vignolini

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Emerging Frontiers in Fluorescence Microscopy: From Single Molecules to Super Resolution

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Understanding Cellulose Crystallinity & Non-Crystalline Aggregated States of Cellulose

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Failed Brilliance in Nanocellulose Science & Technology



TECHNICAL PROGRAM

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Advanced Chemistry of "Non-Traditional" Polysaccharides

Sponsored by CELL, Cosponsored by AGFD, ANYL, BIOL and CARB

Transforming the Undergraduate Chemistry Laboratory to Teach Transferable Skills & Develop Young Scientists

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TUESDAY AFTERNOON

Section A

Hyatt Regency Orlando
Orlando Ballroom M

ACS Award in Analytical Chemistry

Cosponsored by PROF
A. Woolley, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 ANYL 321. Award Address (ACS Award in Analytical Chemistry sponsored by the Battelle Memorial Institute). Half a century of column technology. **M.L. Lee**

1:45 ANYL 322. Analytical glycoscience: Still a promising field with unmet needs. **M.V. Novotny**

2:25 Intermission.

2:40 ANYL 323. Separations at extreme conditions: Fast and high pressure. **R. Kennedy**

3:20 ANYL 324. In-depth proteome profiling of single cells including circulating tumor cells by nanodroplet sample processing and ultrasensitive LC-MS. **R.T. Kelly**, Y. Zhu, G. Clair, J. Podolak, R. Zhao, R. Moore, G. Thomas, C. Ansong, Y. Cong

4:00 ANYL 325. Miniaturized separation systems for chemical analysis: With multiple assists from my award winning colleague, Milton Lee. **A. Woolley**, M.J. Beauchamp, E.K. Parker, A.V. Nielsen, J.B. Nielsen, V. Sahore, H.M. Almughamsi, H. Gong, G.P. Nordin

Section B

Hyatt Regency Orlando
Orlando Ballroom N



TECHNICAL PROGRAM

Advances in Ligand-Binding Assays Involving Integral Membrane Proteins

C. Chen, A. Vaish, *Organizers, Presiding*

1:00 Introductory Remarks.

1:05 ANYL 326. MLKL: A study of conformational changes. B. Ma, D. Marcotte, P. Murugan, K. Michelsen, T. Wang, A. Bertolotti-Ciarlet, J.H. Jones, B. Moree, M. Butko, J. Salafsky, X. Sun, T. McKee, **L. Xue**, L.F. Silvan

1:35 ANYL 327. Hydroxyl radical footprinting-mass spectrometry (HRF-MS): Probing solvent accessibility changes for the elucidation of membrane-ligand interactions. **A.T. Wecksler**

2:05 ANYL 328. Lysosomal integral membrane protein-2 as a phospholipid receptor revealed by structural, biophysical and cellular studies. **S. Liu**

2:35 Intermission.

2:50 ANYL 329. Binding affinity determination of therapeutic antibodies to membrane protein targets. A. Vaish, **C. Chen**, P.J. Grandsard

3:20 ANYL 330. Withdrawn

3:50 ANYL 331. Native ion mobility mass spectrometry of membrane protein complexes. Y. Liu, W. Liu, M.L. Poltash, D.H. Russell, **A. Laganowsky**

4:20 Panel Discussion.

Section C

Hyatt Regency Orlando
Orlando Ballroom L

Advances in Electrochemistry

L. A. Baker, J. Experton, *Organizers, Presiding*

1:00 ANYL 332. Single molecule detection of markers with a label-free bio-electronic sensor. **L. Torsi**

1:30 ANYL 333. Real-time electrochemical detection of *Pseudomonas aeruginosa* phenazine metabolites using transparent carbon ultramicroelectrode arrays. **O. Simoska**, J.J. Shear, K.J. Stevenson

2:00 ANYL 334. Single molecule profiling of molecular recognition at a model electrochemical biosensor. **T. Ye**, Q. Gu, W. Nanney, H. Cao

2:30 ANYL 335. Development of an “lab-on-a-chip” device using electrochemistry. **V. Arau**, Y. Cheng, S. Basuray, S. Chatterjee



TECHNICAL PROGRAM

3:00 Intermission.

3:15 ANYL 336. Neurotransmitter detection at near the theoretical performance limit of electroenzymatic sensors. **I. Huang**, M. Clay, H.G. Monbouquette

3:45 ANYL 337. Construction of fungus FADGDH harboring electron transfer domain and its application for direct electron transfer type enzyme sensor. **J. Okuda-Shimazaki**, T. Yanase, W. Tsugawa, K. Sode

4:15 ANYL 338. Controlling the mediator diffusion in disposable enzyme sensor strips by utilizing interdigitated array microelectrodes. **N. Loew**, M. Hatada, J. Okuda-Shimazaki, W. Tsugawa, Y.I. Takahashi, K. Sode

4:45 ANYL 339. Development of a novel open circuit potential type sensor employing 2.5th generation enzyme. **I. Lee**, N. Loew, W. Tsugawa, K. Ikebukuro, K. Sode

Section D

Hyatt Regency Orlando
Plaza International Ballroom K

Advances in Mass Spectrometry

M. F. Bush, *Organizer*
C. Chouinard, *Presiding*

1:00 ANYL 340. Expanding molecular coverage of cholesterol derivatives and eicosenoids using structure-selective reactions and ion mobility-mass spectrometry. S. Maddox, R. Fraser Carris, K. Baker, **C.D. Chouinard**

1:30 ANYL 341. Expanding chemical coverage of a single cell by combining MS techniques. **M. Philip**, H. Tian, E. Neumann, J. Ellis, S. Rubakhin, J. Sweedler

1:55 ANYL 342. Using native top-down nESI FTICR-MS to characterize the interaction of tau protein with assembly modulator CLR01. **M. Nshanian**

2:20 Intermission.

2:35 ANYL 343. Identification and accurate quantification of structurally related peptide impurities in synthetic B-type natriuretic peptide by mass spectrometry. **P. Xiao**

3:00 ANYL 344. Tetrodotoxin production and stress response in newts as analyzed by LC-MS. **J. Tasca**, B. LaBumbard, A. Poltronetti, D.C. Woodhams, K.P. Minbirole

3:25 ANYL 345. Quantitation of tryptophan degradation products using wide isolation MS/MS via UHPLC-HRMS/MS. **V.Y. Rubio**, G.P. Wang, R.A. Yost, T.J. Garrett

3:50 ANYL 346. Separation and characterization of marine dissolved organic matter (DOM) by combination of Fe(OH)₃ co-precipitation and solid phase extraction followed by ESI FT-ICR MS. **L. Li, Z. Fang, C. He, Q. Shi**



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

Engineered Lignocellulosic Materials & Multiphase Systems: Anselme Payen Award Symposium in Honor of Orlando Rojas

Lignocellulosic Materials & Multiphase Systems

Sponsored by CELL, Cosponsored by ANYL and COLL

Exploring the Frontiers of Chemistry through NASA Research

Living There: Science for the Future of Manned Space Exploration

Sponsored by COMSCI, Cosponsored by ANYL, BIOL[‡], BIOT, CELL, COLL, ENFL[‡], I&EC[‡], INOR[‡], NUCL[‡], PHYS[‡], PMSE[‡] and POLY[‡]

Exploring the Frontiers of Chemistry through NASA Research

Living There: Science for the Future of Manned Space Exploration

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Ionic-Liquids Processing of Polysaccharides

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Understanding Cellulose Crystallinity & Non-Crystalline Aggregated States of Cellulose

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TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

Advanced Chemistry of "Non-Traditional" Polysaccharides

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Transforming the Undergraduate Chemistry Laboratory to Teach Transferable Skills & Develop Young Scientists

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WEDNESDAY MORNING

Section A

Hyatt Regency Orlando
Orlando Ballroom M

Advances in Spectroscopy

Novel Applications of Raman Spectroscopy

Cosponsored by CTA
A. D. Campiglia, *Organizer, Presiding*

8:00 Introductory Remarks.

8:10 ANYL 347. Characterizing virus-induced gene silencing at the cellular level with *in situ* multimodal imaging. **S. Burkhow**, N. Stephens, Y. Mei, M. Duenas, D. Freppon, G. Ding, S. Smith, Y. Lee, B.J. Nikolau, S.A. Whitham, E.A. Smith

8:30 ANYL 348. Mechanism of remarkable surface enhanced raman scattering based on graphene-TiO₂ nanocomposites and application to real-time monitoring of cancer cell related telomerase and PD-L1 expression at single-cell level. **E. Feng**, T. Zheng, Y. Tian

8:50 ANYL 349. Directional Raman scattering: A tool for measuring adsorption and chemical content at smooth interfaces. **E.A. Smith**, C.K. Nyamekye, S.C. Weibel

9:10 ANYL 350. Simultaneous Raman and photothermal infrared spectroscopy at submicron spatial resolution. **C.A. Marcott**, C. Prater, E. Dillon, M. Kansiz

9:30 Intermission.

9:50 ANYL 351. Variable temperature Raman micro-spectroscopy as a nanoanalytical tool for studying 2D materials. **C.G. Wall**

10:10 ANYL 352. Withdrawn



TECHNICAL PROGRAM

10:30 ANYL 353. Accessible mycotoxin identification by label-free SERS nanoaptasensors in solution. **B.C. Galarreta**, Y. Hernández, L. Lagos, L. Veliz

10:50 Concluding Remarks.

Section B

Hyatt Regency Orlando
Orlando Ballroom N

Advances in Ligand-Binding Assays Involving Integral Membrane Proteins

C. Chen, *Organizer*
A. Vaish, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 ANYL 354. Second-harmonic generation and its application to integral membrane proteins. **B. Moree**, D. Shaya, T. Young

8:35 ANYL 355. Fluorescent agonists and antagonists for probing purinergic adenosine and P2Y receptors. **K.A. Jacobson**, F. Ciruela

9:05 ANYL 356. Salipro system for stabilization of membrane proteins. A. Heuer, **R. Loving**

9:35 Intermission.

9:50 ANYL 357. Label-free quantification of small molecule interactions with membrane proteins in single cells by mechanical amplification. **F. Zhang**, W. Jing, A. Hunt, Y. Yang, S. Wang, N. Tao

10:20 ANYL 358. Graphene-based field effect biosensing: An orthogonal approach for measuring integral membrane proteins. **B. Goldsmith**

10:50 ANYL 359. Measuring ligand binding kinetics to membrane proteins using Virion-oscillators. **G. Ma**, G. Syu, X. Shan, B. Henson, S. Wang, P. Desai, H. Zhu, N. Tao

11:20 Panel Discussion.

Section C

Hyatt Regency Orlando
Orlando Ballroom L

Advances in Electrochemistry

L. A. Baker, J. Experton, *Organizers, Presiding*



TECHNICAL PROGRAM

8:00 ANYL 360. Understanding the metal nanoparticles size effect for electrochemically induced ostwald ripening: A case study with Au nanoparticles. **D.K. Pattadar**, F.P. Zamborini

8:30 ANYL 361. Withdrawn

9:00 ANYL 362. Analyzing metal nanoparticle transformations by anodic stripping voltammetry. **F.P. Zamborini**, D.K. Pattadar, J. Sharma

9:30 ANYL 363. Earthworm-like N, S-Doped carbon tubeencapsulated Co_9S_8 nanocomposites derived from nanoscaled metal–organic frameworks for highly efficient bifunctional oxygen catalysis. **T. Liu**, L. Zhang, Y. Tian

10:00 Intermission.

10:15 ANYL 364. Probing electrocatalytic reactions at individual metallic nanostructures via optically enhanced electrochemical methods. **C.M. Hill**, P. Saha, J.D. Walmsley, J.W. Hill

10:45 ANYL 365. Inverse metal-assisted chemical etching for suspended III-V nanofoils. **T.S. Wilhelm**, C.W. Soule, M.A. Baboli, P.K. Mohseni

11:15 ANYL 366. Synthesis, characterization, and the effects of cerium oxide grafted ferrocene-nickel nanocomposite coatings. **H. Conrad**, N.K. Ngo, T.D. Golden

11:45 ANYL 367. Corrosion inhibition of mild steel in acidic medium by simple triazole- and imidazole-based aromatic compounds. **E. Caldona**, M. Zhang, T. Hollis, C.E. Webster, D. Wipf, D.W. Smith

Section D

Hyatt Regency Orlando
Plaza International Ballroom K

Advances in Mass Spectrometry

M. F. Bush, *Organizer*
C. Chouinard, *Presiding*

8:00 ANYL 368. Mechanism of thermal decomposition of tetramethylsilane: A flash pyrolysis vacuum ultraviolet photoionization time-of-flight mass spectrometry and density functional theory study. X. Liu, **J. Zhang**, A. Vazquez, D. Wang, S. Li

8:25 ANYL 369. Next-generation spacecraft propellant performance and the ultimate fate of their exhaust plumes: Insights from mass spectrometry and collision-induced dissociation. **A.L. Patrick**

8:50 ANYL 370. Excited-state CH_2Cl_2 -induced chemi-ionization: A novel high-efficient ionization method applied for mass spectrometry. **B. Yang**, J. Shu, J. Huang, Z. Zhang, K. Jiang, Z. Li

9:15 ANYL 371. Thermal desorption-pyrolysis gas chromatography mass spectrometry: An approach to speciation and closing carbon mass balance. **A. Kubatova**, B. Nesporek, A.L. LaVallie, T. Berg, E. Kozliak

9:40 Intermission.



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

9:55 ANYL 372. Elucidation of source components of dissolved organic compounds in precipitation samples by gas chromatography-mass spectrometry and factor analysis. **S.F. Li**, X. Lee, O. Woo, D. Carlos, S. Watts

10:20 ANYL 373. Mass spectroscopic analysis of phenol derivatives by Gibbs reaction. **S. Mistry**, P.G. Wenthold

10:45 ANYL 374. Determination of the total purity of a high-purity copper material to be used as a primary standard for element determination. **T. Zhou**, J. Zhang, Y. Tang, Y. Cui

11:10 ANYL 375. Integrated method developments for *in vitro* evaluation of sunscreen products. **Y. Yang**, J. Zhang, J. Wang, H. Hsu, J. Wang, P.J. Faustino, C.N. Cruz, M. Ashraf

Nanocellulose: From Fundamentals to Function

Sponsored by CELL, Cosponsored by AGFD, ANYL and BIOL

Bioactive Delivery: Frontiers in Biomaterials

Sponsored by CELL, Cosponsored by ANYL, BIOL and CARB

Emerging Frontiers in Fluorescence Microscopy: From Single Molecules to Super Resolution

Sponsored by PHYS, Cosponsored by ANYL

Bio-Based Gels & Porous Materials

3D printing & Rheology of Cellulose & Nanocellulose

Sponsored by CELL, Cosponsored by ANYL, BIOL and COLL

Valorization of Renewable Resources & Residuals into New Materials & Multiphase Systems

Sponsored by CELL, Cosponsored by AGRO and ANYL

Wood-Based Polymers: From Functional Structures to Applications

Lignin



TECHNICAL PROGRAM

Sponsored by CELL, Cosponsored by ANYL

WEDNESDAY AFTERNOON

Section A

Hyatt Regency Orlando
Orlando Ballroom M

Advances in Spectroscopy

Novel Applications of Fluorescence, Absorption & SEM-EDS Spectroscopy

Cosponsored by CTA
A. D. Campiglia, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 ANYL 376. Probing and manipulating enzyme activity and conformational dynamics by single-molecule AFM-FRET and magnetic tweezers-FRET ultramicroscopy. **H. Lu**, M. Wu, S.R. Chowdhury, Y. He

1:25 ANYL 377. Multi-analysis: From sensing to perception. **F. Li**

1:45 ANYL 378. New insights to optical properties of fluorescent quantum dots by polarized resonance synchronous spectroscopy and polarized Stokes'-shifted fluorescence spectroscopy. **J. Xu**, Y. Yuan, O. Chen, D. Zhang

2:05 ANYL 379. High impact chemistry: Design and testing an icy moon penetrator organic analyzer. **A.M. Stockton**, M. Cato, Z. Duca, T. Cantrell, S. Foreman, J. Kim, P. Putman, B. Schmidt

2:25 Intermission.

2:40 ANYL 380. In silico interpretation of endogenous fluorescence spectra from a live organism. **E. Heider**, S. Alheety, D. Valenti, N. Mujumdar, A.D. Campiglia, J. Harper

3:00 ANYL 381. Using cyclodextrins for toxicant detection in commercial products: from menstrual cups to macaroni and cheese. **M. Levine**, D.J. DiScenza, J. Lynch, L. Intravia

3:20 ANYL 382. Identification of glitter and shimmer cosmetic particles using SEM-EDS. **K. Najjar**, C. Bridge

3:40 Concluding Remarks.

Section C

Hyatt Regency Orlando
Orlando Ballroom L

Advances in Electrochemistry



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

L. A. Baker, J. Experton, *Organizers, Presiding*

1:00 ANYL 383. Large-area SECM imaging based on scanning band electrodes. A. Dorfi, H. Kuo, G. O'Neil, J. Wright, **D. Esposito**

1:30 ANYL 384. Elucidating the properties of the solid-liquid interface in aqueous and organic solvents using polystyrene spheres and the resistive-pulse technique. **W.S. Russell**, J.W. Polster, A.J. Souna, J.T. Fourkas, Z. Siwy

2:00 ANYL 385. Reduction of anthelmintic drug (Methyl carbamate- albendazole) on electrodes electrode surfaces and analysis of chromatographic reduction products. **A.M. Mugweru**, Z. Mazzochette

2:30 ANYL 386. Integrating particle gating and electrochemical rectification within attoliter volume nanopore electrode arrays. **K. Fu**, D. Han, S. Kwon, P.W. Bohn

3:00 Intermission.

3:15 ANYL 387. Synthesis, electrochemical and structural characterization of manganese oxide particles on gold microtubes for battery applications. **J. Experton**, X. Wu, G. Wang, A. Teyssendier de La Serve

3:45 ANYL 388. In-situ analysis and simulation of heat generation during charging and discharging of Ni-rich layered oxide cathode. **G. Kim**

4:15 ANYL 389. Variation in electrical conductivity of novel Li-ion battery electrode based on copper thickness and composition. **E. Bonyi**, Z. Camielle, Z. Kukoyi, F. Coleman, k. aslan, F. Forohtar

4:45 ANYL 390. Withdrawn

Nanocellulose: From Fundamentals to Function

Sponsored by CELL, Cosponsored by AGFD, ANYL and BIOL

Bioactive Delivery: Frontiers in Biomaterials

Sponsored by CELL, Cosponsored by ANYL, BIOL and CARB

Bio-Based Gels & Porous Materials

Gels in Medical Applications

Sponsored by CELL, Cosponsored by ANYL, BIOL and COLL



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

Valorization of Renewable Resources & Residuals into New Materials & Multiphase Systems

Sponsored by CELL, Cosponsored by AGRO and ANYL

Wood-Based Polymers: From Functional Structures to Applications

Hierarchies & Assembly, Films & Fibers

Sponsored by CELL, Cosponsored by ANYL

THURSDAY MORNING

Section A

Hyatt Regency Orlando
Florida Ballroom C

Advances in Spectroscopy

Advances in EPR, NMR & Infrared Spectroscopy

Cosponsored by CTA
A. D. Campiglia, *Organizer, Presiding*

8:00 Introductory Remarks.

8:10 ANYL 391. Direct and accurate quantitative analysis of paramagnetic species in crude oil by EPR spectroscopy. **M.A. Morsy**, A.N. Kawde, E. Al-Shafei

8:30 ANYL 392. Relationships between vicinal constant couplings $^3J_{HH}$, 1H and ^{13}C -NMR chemical shifts and torsional angles. **C. Mitan**, E. Bartha, P. Filip, C. Draghici, M. Caproiu, R. Moriarty

8:50 ANYL 393. Error analysis of solution state three-dimensional structures determined using residual dipolar coupling NMR. **D. Gardner**, W. Carroll

9:10 ANYL 394. Portable high speed mid-IR spectrometer. **T. Jeon**, A. Nateghi, A. Scherer

9:30 Intermission.

9:45 ANYL 395. Fourier transform infrared microspectroscopy imaging to study *C. elegans* nematode. A. Bouyanfif, S.P. Liyanage, E. Hequet, N. Moustaid-Moussa, **N. Abidi**

10:05 ANYL 396. GC-MS and FTIR characterization of the different fractions of *Jatropha tangorensis* leaf extract. **C. Unegbu**

10:25 ANYL 397. Fermi resonance of p-azido-benzonitrile. **D.G. Hogle**, M.J. Tucker



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

10:45 ANYL 398. Fourier transform infrared spectroscopy applied to the analysis of data-encoded mixtures. **H.D. Stout,** T. Brinzer, B.C. Kyle, D.J. Scott, K.C. Gronborg, H. Geng, S. Cho, W.W. Clark, S. Garrett-Roe, T.Y. Meyer

11:05 ANYL 399. Modulation of vibrational energy transfer between azido- and cyano- reporters through an aromatic scaffolds. **F. Chalyavi,** A. Schmitz, E.E. Fenlon, S.H. Brewer, M.J. Tucker

11:25 Concluding Remarks.

Nanocellulose: From Fundamentals to Function

Sponsored by CELL, Cosponsored by AGFD, ANYL and BIOL

Additive Manufacturing of Bio-based & Renewable Materials

Sponsored by CELL, Cosponsored by AGRO, ANYL and BIOL

Bio-Based Gels & Porous Materials

Nanostructuring of Gels & Aerogels & their Use as Sensors

Sponsored by CELL, Cosponsored by ANYL, BIOL and COLL

Valorization of Renewable Resources & Residuals into New Materials & Multiphase Systems

Sponsored by CELL, Cosponsored by AGRO and ANYL

Wood-Based Polymers: From Functional Structures to Applications

From Biomass to Materials: Global Challenges

Sponsored by CELL, Cosponsored by ANYL

Emerging Frontiers in Fluorescence Microscopy: From Single Molecules to Super Resolution

Sponsored by PHYS, Cosponsored by ANYL



TECHNICAL PROGRAM

THURSDAY AFTERNOON

Nanocellulose: From Fundamentals to Function

Sponsored by CELL, Cosponsored by AGFD, ANYL and BIOL

Additive Manufacturing of Bio-based & Renewable Materials

Sponsored by CELL, Cosponsored by AGRO, ANYL and BIOL

Bio-Based Gels & Porous Materials

Gels, Aerogels & Carbogels

Sponsored by CELL, Cosponsored by ANYL, BIOL and COLL

Valorization of Renewable Resources & Residuals into New Materials & Multiphase Systems

Sponsored by CELL, Cosponsored by AGRO and ANYL

Wood-Based Polymers: From Functional Structures to Applications

Films & Fibers

Sponsored by CELL, Cosponsored by ANYL

Emerging Frontiers in Fluorescence Microscopy: From Single Molecules to Super Resolution

Sponsored by PHYS, Cosponsored by ANYL

BIOT

Division of Biochemical Technology

J. Neville and B. Pflieger, *Program Chairs*



TECHNICAL PROGRAM

SUNDAY MORNING

Section A

Rosen Centre Hotel
Grand A

Emerging Frontiers in BIOT

Bioprocessing in 2024: Disruptive Technological Innovation in Industry & Academia

M. A. Blenner, C. A. Eckert, D. J. Roush, *Organizers*
J. Erickson, C. Haynes, *Presiding*

8:30 BIOT 1. Harvesting today's technology to guide tomorrow's innovations. **J. Hubbuch**

9:10 BIOT 2. Applications of a CHO metabolic model for cell culture process development. **J.V. Price**, J. Bucher, K.A. Barnthouse, P. Hu, J. Cunningham, E.J. Schaefer, R. Shivappa

9:30 BIOT 3. Honey, I shrunk the biologics manufacturing facility! **A. Andar**, V. Chopda, B. Punshon-Smith, D. Burgenson, M. Al-Adhami, S. Deldari, S. Borhani, E. Gutierrez, R. Adiga, X. Ge, L.M. Tolosa, D.D. Frey, G. Rao

9:50 Intermission.

10:10 BIOT 4. Continuous multi-column displacement chromatography for separation of charge variants of monoclonal antibodies. **O. Khanal**, V. Kumar, F. Schlegel, P. Rolandi, O. Kaltenbrunner, A.M. Lenhoff

10:30 BIOT 5. Towards antibody capture via continuous integrated target precipitation-filtration. Q. Gu, Z. Li, J.L. Coffman, **T.M. Przybycien**, A.L. Zydney

10:50 BIOT 6. Production of tandem-core virus-like particles using *Escherichia coli*-based cell-free protein synthesis. **N. Colant**, J. Teneb Lobos, O. Ogonah, A. Ramirez, S. Frank, W. Rosenberg, D.G. Bracewell

11:10 BIOT 7. Decisional tools for predictive data-mining and cost-effective design for biopharma facilities of the future. **S. Farid**

Section B

Rosen Centre Hotel
Grand B

Downstream Processing

Novel Therapeutic Modalities



TECHNICAL PROGRAM

S. Chollangi, M. Gruvegard, C. Heldt, *Organizers*
M. Bakhshayeshi, C. Peixoto, B. J. Roman, *Presiding*

8:30 BIOT 8. Performance of chromatography beads, monoliths and membrane adsorbers in the purification of enveloped virus-like particles. **P. Pereira Aguilar**, K. Reiter, P. Steppert, A. Jungbauer

8:50 BIOT 9. Downstream process development for a clinical stage retrovirus-like particle. **M. Fitchmun**, M.A. Snyder

9:10 BIOT 10. Combination of membrane-based and chromatographic methods to achieve pure and concentrated oncolytic measles viruses. D. Loewe, H. Dieken, T. Grein, **D. Salzig**, P.M. Czermak

9:30 BIOT 11. Non-enveloped virus partitioning in osmolyte enhanced aqueous two-phase systems. **P. Joshi**, M. Schroeder, B.M. Jones, S. Kriz, C. Heldt

9:50 Intermission.

10:10 BIOT 12. Optimizing the clarification process for viral vectors feed streams for use in gene therapy. **B. Raghavan**, M. Collins, T. Sanderson, S. Bergheim-Pietza

10:30 BIOT 13. Evaluation of continuous chromatographic purification of therapeutic extracellular vesicles. **M. Moleirinho**, R.J. Silva, M.J. Carrondo, P. Alves, C. Peixoto

10:50 BIOT 14. Development of a second generation process for the production of clinical-grade exosomes. **A. Noyes**, K. Ellis, M. Doherty, K. DeSanty, R. Bourdeau, S. Estes, K. Konstantinov

11:10 BIOT 15. Developing affinity peptide-based cell separation using phage display. **R. Ghosh**, A. Mullerpatan, T. Baltazar, P. Karande, S.M. Cramer

Section B

Rosen Centre Hotel
Grand B

Spotlights on Research Areas

Welcome to 2018 BIOT

J. Neville, B. Pflieger, *Organizers*
T. M. Przybycien, *Presiding*

11:30 BIOT 16. Perlman Award: Past, present and future of biomanufacturing. **A. Hanly**

Section C

Rosen Centre Hotel
Salon 4

Upstream Processes



TECHNICAL PROGRAM

Microbial Metabolic Engineering

P. Peralta Yahya, A. Russo, C. T. Trinh, *Organizers*
Z. Rui, Z. Shao, K. Solomon, *Presiding*

8:30 BIOT 17. Designing modular synthetic metabolons via dCas9-guided assembly. **E. Berckman**

8:50 BIOT 18. Functional production of solvent transporters sourced from non-conventional fungi in model yeast. **S. Seppala**, J.I. Yoo, D. Yur, M.A. O'Malley

9:10 BIOT 19. Engineering the early secretory pathway for increased protein secretion in *Saccharomyces cerevisiae*. P.B. Besada-Lombana, **N.A. Da Silva**

9:30 BIOT 20. Kinetically guided, ratiometric tuning of fatty acid biosynthesis. A. Ruppe, **J.M. Fox**

9:50 Intermission.

10:10 BIOT 21. Production of bioherbicides by *in vivo* and *in vitro* synthetic biology approaches. **Y. Ding**

10:30 BIOT 22. Rapid optogenetic circuits to enable dynamic control in metabolic engineering using light. E.M. Zhao, R.J. Lovelett, J. Toettcher, Y. Kevrekidis, **J.L. Avalos**

10:50 BIOT 23. B&B DIC Wang Award: Systems and synthetic biology: constructing programmable cells. **T. Moon**

Section D

Rosen Centre Hotel
Salon 2

End-to-End Biomanufacturing

Scale-Up, Scale-Out & Tech Transfer Case Studies

J. Bender, J. C. Love, V. Roy, *Organizers*
P. R. Smith, M. Stone, *Presiding*

8:30 BIOT 24. Lower temperature and sufficient oxygenation at clarification step ease antibody disulfide reduction and aggregate formation: A pilot-scale case study for manufacturing process transfer. **J. Tian**, S. Yakubu, C. Rives, F. Deer, J. Lee, S. Gu, B. Baynes, Y. Xiong, Y. Wang, A. Shukla

8:50 BIOT 25. Scale-up and scale-down of a mammalian cell culture based fed-batch process: Case study. **M. Paranandi**

9:10 BIOT 26. CO₂ control strategy at 3L bench scale for cell culture process development and scale-up. **B. Russell**, K. Hahn, S. Ahuja

9:30 BIOT 27. Challenges in facility fit: Establishing a robust process for filtration of process intermediates. **M. Goetz**, T. Parker



TECHNICAL PROGRAM

9:50 Intermission.

10:10 BIOT 28. Technical Evaluation to understand overall yield variability in a mAb manufacturing process and potential opportunities for yield improvement. **M. Stone**, S. Siva, J. Easson, J. Alvarado, S.A. Tobler

10:30 BIOT 29. Lyophilization process development and transfer enabled by equipment characterization and process modeling. **F. Schlegel**, C. Ruitberg, G. Scalzo

10:50 BIOT 30. Speed to GMP: Moving from rapid process development to high throughput tech transfer. **N. Bubna**, J. Kim, D. Chang, S. Mostafa

11:10 BIOT 31. Bringing a commercial process back home: Tech transferring from an external CMO for internal manufacture. **R. Procopio-Melino**

Section E

Rosen Centre Hotel
Salon 6

Biomedical Technologies

Precision Medicine: Biomarkers, Imaging & Diagnostics

R. D. Sheth, G. Thurber, M. Westoby, *Organizers*
K. Orcutt, S. L. Servoss, *Presiding*

8:30 BIOT 32. Ultra-sensitive platinum nanoparticle based digital assay for point-of-care diagnostics. **H. Chen**, Z. Li, L. Zhang, P. Sawaya, J. Shi, P. Wang

8:50 BIOT 33. Lateral flow assay ruler for instrument-free quantitative and rapid point-of-care testing. **Z. Li**, H. Chen, P. Wang

9:10 BIOT 34. Real time monitoring of NASBA reaction using split hybridization probes. **A. Reed**, D. Nedorezova, N. Kikuchi, D. Kolpashchikov, Y. Gerasimova

9:30 BIOT 35. Polymeric acidoCEST MRI contrast agent for imaging tumor extracellular pH. **C.J. Kombala**, M.D. Pagel

9:50 Intermission.

10:10 BIOT 36. Approaches toward point-of-care molecular diagnostics of infectious diseases. **Y. Gerasimova**, R. Connelly, A. Reed, B.C. Dhar, K. Rohde, H. Choe

10:30 BIOT 37. Rapid detection of antibiotic resistant bacteria in blood. **M. Al-Adhami**, M. Patsy, A. Cross, G. Rao, I.V. Kostov

10:50 BIOT 38. Pharmacological evaluation of the neuromuscular junction in a human-based functional in vitro system. **S. Lindquist**, X. Guo, V. Smith, Y. Cai, M. Jackson, C. McAleer, J. Rumsey, C. Long, J. Hickman



TECHNICAL PROGRAM

11:10 BIOT 39. Immuno-nanoparticle PCR for ultrasensitive detection of proteins. **D. Chavan**, H. Chen, M. Crum, B. Vu, K. Kourentzi, R.C. Willson

SUNDAY AFTERNOON

Section A

Rosen Centre Hotel
Grand A

Spotlights on Research Areas

Upstream Processes

P. Peralta Yahya, A. Russo, C. T. Trinh, *Organizers*
K. Solomon, *Presiding*

2:00 BIOT 40. Keynote: Engineered autonomous control of metabolic pathways. **K.L. Jones Prather**

2:40 Rapid Fire Presentations.

3:20 Intermission.

3:40 Discussion.

4:00 BIOT 41. B&B Gaden Award: Engineering microbes for the production of isoprenoid compounds. **G. Stephanopoulos**

Section B

Rosen Centre Hotel
Grand B

Downstream Processing

Monitoring & Control of mAb Product-Related Variants/Mechanistic & Molecular-level Understanding in mAb Processes

S. Chollangi, M. Gruvegard, C. Heldt, *Organizers*
S. Ghose, A. C. Roque, J. Woo, *Presiding*

2:00 BIOT 42. Non-protein A purification platform for continuous processing of monoclonal antibody therapeutics. **A.S. Rathore**

2:20 BIOT 43. Mitigation for monoclonal antibody disulfide bond reduction in manufacturing: A case study. **S. Ozturk**, J. Yan, K. Baptista, R.B. Wollacott, G. Zhang, S. Nilapwar, J. Sinha, W. Wang, S. Singh, S. Gangloff



TECHNICAL PROGRAM

2:40 BIOT 44. Development and implementation of a harmonized purification platform for a modern, diverse pipeline. **T. Vetter**, T. Prouzeau, H. Hoffmann, B. Murray, M. Fischer, H. Picard, D. Boeth, C. Gay, K.P. Brower

3:00 BIOT 45. Optimization of a platform hydrophobic interaction chromatography step for robust aggregate removal in flow-through mode. **M. Dolan**, O. Bhate, H. Vo, B. Nguyen, R. Phatate, H. Takeuchi, L. Kurt, H. Han, O. Paley, N. Schuelke

3:20 Intermission.

3:40 BIOT 46. Investigating the effect of pH on mAb retention in multimodal chromatography. **J. Robinson**, D.J. Roush, S.M. Cramer

4:00 BIOT 47. Hydrophobicity of CEX resins and Its Impact on mAb aggregation. **C. Huang**, Y. Wang, J.J. Perry, J. Mills, X. Xu, S. Ghose

4:20 BIOT 48. Influence of ligand density on two-peak elution behavior of mAb charge variants in cation exchange chromatography. **G. Sanchez Reyes**, C. Stange, C. Frech

4:40 BIOT 49. Novel semi-preparative chromatographic method to enrich charge-variant species for extended characterization. **E.S. Schutsky**, K. Stone, L. Duhamel, Y. Song, J. Chen, R. Swanson, S. Ghose, Z. Li

Section C

Rosen Centre Hotel
Salon 4

Biomolecular Technologies

Protein Conjugates & Fusions

B. Hackel, B. F. Marques, *Organizers*
S. Parimal, J. B. Spangler, *Presiding*

2:20 BIOT 50. Effect of a long genetic fusion tag on the structure and stability of a pharmaceutical protein. S. Bandi, S. Singh, **K. Mallela**

2:40 BIOT 51. Engineering a blue light inducible spycatcher system (BLISS) as a tool for protein photopatterning and optogenetics. **E. Hartzell**, J. Terr, W. Chen

3:00 BIOT 52. Virus detection via osmolyte-induced aggregation of gold nanoparticles. **D.G. Turpeinen**, X. Mi, E. Lucier, S. Kriz, J. Kah, C. Heldt

3:20 Intermission.

3:40 BIOT 53. Expansion of genetically encoded amino acids containing a tetrazine functional group for fast protein conjugation. **I. Kwon**, S. Kim

4:00 BIOT 54. N and C terminal oriented protein conjugation onto nanoparticles using split intein technology. **J. Miozzi**, Y. Fan, D.W. Wood, A. Rampersaud, D. Albertson, I. Rampersaud



TECHNICAL PROGRAM

4:20 BIOT 55. Immobilization of enzyme fusions on superparamagnetic nanoparticles: Two case studies.. **R.M. Hughes**, J.L. Norris, W.M. Taylor

4:40 BIOT 56. Conjugation of cofactors using polymeric swing arms enables creation of cofactorless ping pong enzymes with predictable kinetics. **S. Banta**, H. Ozbakir, N. Massad

Section D

Rosen Centre Hotel
Salon 2

Biomedical Technologies

Precision Medicine: Biomarkers, Imaging & Diagnostics

R. D. Sheth, G. Thurber, M. Westoby, *Organizers*
K. Orcutt, S. L. Servoss, *Presiding*

2:00 BIOT 57. Discrimination of single nucleotide substitutions causing drug resistance in *Mycobacterium tuberculosis* using split deoxyribozyme sensors with visual readout. **B. Dhar**, R. Connelly, S. Mitra, Y. Gerasimova

2:20 BIOT 58. Detection of cathepsin B activity with caged melanin precursors for photoacoustic imaging. **S.D. Lokugama**, M.D. Pagel

2:40 BIOT 59. Identification of novel protein biomarkers using liquid chromatography/tandem mass spectrometry from pre and post-cryotherapy treated bones of osteosarcoma patients. **R. Madda**, J. Wang, C. Chen, P. Wu

3:00 BIOT 60. Engineering a bioluminescence-based protein kinase reporter for in vivo, longitudinal studies of receptor tyrosine kinase inhibitor response. **E. Day**, M. Lazzara

3:20 Intermission.

3:40 BIOT 61. Novel near-infrared fluorescence sensor for detection of platelet activation in vivo. **K. Ha**, X. Zheng, F. Jaffer, C. Kessinger, J.R. McCarthy

4:00 BIOT 62. Development of a PET/MRI contrast agent that measures tumor extracellular pH. **A.C. Pollard**, F. Pisaneschi, M.D. Pagel

4:20 BIOT 63. Quantitative imaging of protein phosphorylation and therapeutic efficacy in cancer. **L. Wang**, E. Schultz, A. Solanki, K. Tichauer, K.S. Samkoe, S.L. Gibbs

4:40 BIOT 64. Fluorescence detection of amyloids. K. Cao, J. Do, C. Sigurdson, **J.C. Yang**

SUNDAY EVENING

Section B



TECHNICAL PROGRAM

Rosen Centre Hotel
Grand B

General Biochemical Technology

BIOT Tank

N. Jacob, A. Kantardjieff, *Organizers, Presiding*

5:00 Introductory Remarks.

5:05 BIOT 65. Economic analysis of the biocoverion of biogas into bioproducts. **Q. Fei**, R. Fu, B. Liang

5:20 BIOT 66. Self-assembled, isoporous filtration technology platform for bioseparations. **R.M. Dorin**, Y. Gu, C. Crock, M. Siwak

5:35 BIOT 67. Wood microfluidic devices for point-of-care applications. **A. Andar**, E. Gutierrez, M. Al-Adhami, X. Ge, L.M. Tolosa, Y. Kostov, G. Rao

5:50 Concluding Remarks.

MONDAY MORNING

Section A

Rosen Centre Hotel
Grand A

Emerging Frontiers in BIOT

A Vision for the Next 25 Years

M. A. Blenner, C. A. Eckert, D. J. Roush, *Organizers*
V. Roy, P. Tessier, *Presiding*

8:30 BIOT 68. Next-generation protein therapeutics: Challenges and opportunities. **J. Cochran**

8:50 BIOT 69. GSKOs manufacturing technology roadmap for biopharmaceuticals: learnings and a look ahead. **D. Bhanushali**

9:10 BIOT 70. Continuous processing of biotech therapeutics & enabling case studies. **A.S. Rathore**

9:30 BIOT 71. Next generation bioprocess development: Let us breakdown the current barriers. **R.V. Venkat**

9:50 Intermission.



TECHNICAL PROGRAM

10:10 BIOT 72. Keynote: Smart agricultural systems: Designing plant-microbe communities. **C.A. Voigt**

10:50 BIOT 73. Big data driven biomanufacturing: Present state and future potential. **S.M. Cramer**

11:10 BIOT 74. Vectors of information flow between biology and microelectronics: Design principles and enabling technologies. **W.E. Bentley**

Section B

Rosen Centre Hotel
Grand B

Downstream Processing

Non-Chromatography Based Separation of Biomolecules

S. Chollangi, M. Gruvegard, C. Heldt, *Organizers*
E. Ayturk, A. Gupta, *Presiding*

8:30 BIOT 75. Contaminant removal from a purified protein stream. S. Bhattacharya, J. Keating, W. Xu, M. Sorci, **G. Belfort**

9:10 BIOT 76. Improving HCP reduction by depth filtration in an enzyme purification process. **F. Liu**, S. Kim, V. Ahuja, A. Phulgirkar, J. Ma

9:30 BIOT 77. Mechanistic understanding of viral clearance on depth filtration. **Y. Tao**, W. Luo, S. Langan

9:50 Intermission.

10:10 BIOT 78. Dirty harvest: overcoming high cell density depth filtration challenges using a scale-down sizing approach. **P. Liu**, J. Welsh, P. Rose, C. Furcht, C. Nieder, J. Pollard

10:30 BIOT 79. Effect of tangential flow filtration process parameters on antibody-drug conjugates. **K. Wilson**, M. Wendeler

10:50 BIOT 80. Mechanisms controlling protein fouling of virus filters. **F. Fallahianbijan**, S. Giglia, C.M. Carbrello, A.L. Zydney

11:10 BIOT 81. Unrevealing the plugging mechanisms during a combined tangential-flow and depth filtration process of a hollow fiber filter. **D. Zhang**, P. Patel, D. Strauss, S. Wickramasinghe, X. Qian

Section C

Rosen Centre Hotel
Salon 4

Upstream Processes



TECHNICAL PROGRAM

Microbial Metabolic Engineering

P. Peralta Yahya, A. Russo, C. T. Trinh, *Organizers*
Z. Rui, Z. Shao, K. Solomon, *Presiding*

8:30 BIOT 82. Engineering oleaginous yeast *Yarrowia lipolytica* for production of fuels and chemicals. **P. Xu**

8:50 BIOT 83. Improving ionic liquid tolerance in *Saccharomyces cerevisiae* through heterologous expression and directed evolution of the *ILT1* homolog from *Yarrowia lipolytica*. **K.B. Reed**, J.M. Wagner, S. d'Oelsnitz, J.M. Wiggers, H.S. Alper

9:10 BIOT 84. Medium chain fatty alcohol production via the reverse β -oxidation pathway. **D. Courtney**, C. Mehrer, J. Reed, B. Pflieger

9:30 BIOT 85. Biosynthesis of the hallucinogenic natural product psilocybin in *E. coli*. **J.A. Jones**, A.M. Adams, N.A. Kaplan, J. Brinton

9:50 Intermission.

10:10 BIOT 86. Deletion of four genes in *E. coli* enables preferential consumption of xylose and secretion of glucose as a valuable cross-fed nutrient in synthetic cocultures. **C. Diaz**, R.K. Bennett, E.T. Papoutsakis, M.R. Antoniewicz

10:30 BIOT 87. Quantifying photosynthetic carbon fluxes for limonene production in *Synechococcus* sp. PCC 7002. **C. Sake**, S. Becker, D. Newman, N. Boyle

10:50 BIOT 88. Transcriptional control through synthetic genetic regulation devices for. **N.R. Sandoval**, R.C. Joseph, N.M. Kim

11:10 BIOT 89. Cell-free prototyping tools for metabolic engineering. **A. Karim**, M.C. Jewett

Section D

Rosen Centre Hotel
Salon 2

End-to-End Biomanufacturing

Beyond the Platform: Non mAbs, Bispecifics , Fusion Proteins, ADCs

J. Bender, J. C. Love, V. Roy, *Organizers*
N. Bhokisham, A. E. Schmelzer, *Presiding*

8:30 BIOT 90. Process development for isolation of recombinant thioredoxin using mixed-mode resins: High throughput screening and scale up. **A. Ravi**, P. Heifetz, E. Foster, Z.L. Nikolov

8:50 BIOT 91. Exploration of a new affinity platform to address evolving diversity challenges. **J. Ohman**, **P. Lundback**, **S. Lindman**, **E. Lind**



TECHNICAL PROGRAM

9:10 BIOT 92. Chromatographic clarification: Early impurity removal in recombinant protein production. **K. Metzger**, S. De Groeve, K. Eyer, A. Voloshin, M. Maurer

9:30 BIOT 93. Continuous downstream processing of GCSF expressed as inclusion bodies using Cadence BioSMB PD system. **S.J. Narnaware**, N. Kateja, A. Tiwari, A.S. Rathore

9:50 Intermission.

10:10 BIOT 94. Development of a platform process for the rapid production and purification of single domain antibodies. **L. Crowell**, C.A. Goodwine, K.R. Love, S.M. Cramer, J.C. Love

10:30 BIOT 95. Development of a predictive model for Fab arm exchange of IgG1 and IgG4 bispecific mAbs: Implementation of QbD design space elements for bispecific abs. **A. Salehi**, J.D. Cohen, D. Bezila, R.G. Bertrand, R. Rao, W. Cressman, M. Chiu, P.J. Alfonso

10:50 BIOT 96. Integrated approach to understanding and controlling for scFv bispecific antibody aggregation during process development. **W. Chung**, C. Andrade, L. Arnold, M. Handlogten, D. Motabar, A. Matthew, A. Tang, T. Albanetti, N. Agarwal, A. Hunter

11:10 BIOT 97. Characterizing bioprocess samples with a high-throughput assay as a risk assessment tool for polysorbate degradation. **A. Chandrasekhara**

Section E

Rosen Centre Hotel
Salon 6

Biomedical Technologies

Development & Production of Gene & Cell Therapies

G. Thurber, M. Westoby, *Organizers*
A. Asokan, C. J. Morrison, S. Zolotukhin, *Presiding*

8:30 BIOT 98. Critical process parameters for baculovirus infection of a rAAV Sf9 manufacturing process and their impact on quality attributes. **K. Mathur**

8:50 BIOT 99. Efficiency, quality and traceability of PEIpro transfection reagent for clinical grade viral vector manufacturing. **M. Hellal**, M. Porte, F. Stock, Y. Philipson, V. Kedinger, C. Warteil-Weill, P. Belguise, P. Erbacher

9:10 BIOT 100. Enabling AAV production by suspension HeLa PCL cultivation at high cell densities through implementation and optimization of the inoculum processes while using proprietary chemically defined media. **J. Shupe**, T. Dobrowsky

9:30 BIOT 101. Quantitative characterization of the regulation of iron metabolism in glioblastoma stem-like cells using magnetophoresis. **J. Chalmers**, K. Park, M. Zborowski, J. Kim, M. Venere

9:50 Intermission.



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

10:10 BIOT 102. Platform approaches for downstream purification of viral vectors to advance manufacturing and commercialization of cell and gene therapies. **O. Terova**

10:30 BIOT 103. Optimization of an rAAV downstream purification process for increased robustness, simplification, and flexibility. **M. Luther**

10:50 BIOT 104. Development of a simple protocol of purifying rAAV vectors from endotoxin contamination. **L. Kondratova**, O. Kondratov, S. Zolotukhin

11:10 BIOT 105. Automated characterization of gene therapy viral vectors: Packaging, purity and integrity using transmission electron microscopy. **J. Royce**, M. Folea, M. Ryner, V. Carvalho, M. Colomb-Delsuc

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

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MONDAY AFTERNOON

Section A

Rosen Centre Hotel
Grand A

Spotlights on Research Areas

Biomolecular Technologies

B. Hackel, B. F. Marques, *Organizers*
I. R. Wheeldon, *Presiding*

2:00 BIOT 106. Keynote: Engineering immune cell and tissue function with biomaterials to improve immunotherapy. **C. Jewell**

2:40 Rapid Fire Presentations.

3:20 Intermission.

3:40 Discussion.

4:00 BIOT 107. BIOT YI Award: Engineering synthetic microbial consortia inspired by the herbivore rumen. **M.A. O'Malley**

Section B

Rosen Centre Hotel
Grand B



TECHNICAL PROGRAM

Downstream Processing

Chromatographic Separations of Novel Antibody Structures

S. Chollangi, M. Gruvegard, C. Heldt, *Organizers*
S. M. Cramer, S. T. Evans, J. Royce, *Presiding*

2:00 BIOT 108. Chromatographic behavior of bivalent bispecific antibodies on cation exchange columns. **L.K. Kimerer**, T. Pabst, A. Hunter, G. Carta

2:20 BIOT 109. Exploring options for the integration of bispecific Fab arm exchange reactions with standard downstream unit operations. **J. Newmark**, J. Woo, A. Ambrogelly, C. Emery, N. Sanaie

2:40 BIOT 110. Investigating selectivity trends of a bispecific antibody from key impurities on multimodal cation exchange systems. **S.S. Parasnvis**, J. Robinson, W. Chung, S.M. Cramer

3:00 BIOT 111. Development and optimization of a commercial scFv-IgG bispecific antibody manufacturing process. **W. Chung**, D. Motabar, A. Hunter

3:20 Intermission.

3:40 BIOT 112. Structural base analysis of production and purification of humanized anti-TAC monoclonal antibody. **Y.S. Ting**

4:00 BIOT 113. Integrated clarification and purification of biomolecules in semi-large process scale using magnetic bead technology. **O. Lind**, R. Palmgren, S. Häggblad Sahlberg, N. Norrman, K. Esfandiari, H. Ohrvik, B. Norén

4:20 BIOT 114. Application and adaptation of platform and alternative purification steps to two different Fc-Fusion Proteins. **N. Nicholes**, L. Wolfe, Y. Chang, S. Mostafa

4:40 BIOT 115. Development and scale-up of a Fab drug conjugate purification process. **A. Bill**

Section C

Rosen Centre Hotel
Salon 4

Upstream Processes

Engineering Microbial Communities & Non-Model Systems

P. Peralta Yahya, A. Russo, C. T. Trinh, *Organizers*
C. H. Collins, A. Guss, *Presiding*

2:00 BIOT 116. Fine carbohydrate structure sustains diversity in microbial consortia and governs competition at the strain level. T. Yao, M. Chen, Y. Tuncil, L.A. Libera, **S.R. Lindemann**



TECHNICAL PROGRAM

2:20 BIOT 117. Modeling and manipulation of microbial communities through the integration of machine learning and evolutionary algorithms. **R. Srivastava**, S. Lincoln, J. Benjamino, J. Graf

2:40 BIOT 118. Characterizing lignin-active enzymes in anaerobic fungi for biomass deconstruction. **T.S. Lankiewicz**, J. Henske, S. Gilmore, X. Peng, J. Brown, S. Wilken, M.A. O'Malley

3:00 BIOT 119. Targeting biofilm-forming pathogens using a microconsortium of engineered lactic acid bacteria (LAB). **T. Chappell**, N.U. Nair

3:20 Intermission.

3:40 BIOT 120. Co-Culture of Engineered *Escherichia coli* for Violacein Production from Hemicellulosic Sugars. **K. Gedeon**, M. Koffas, C.H. Collins

4:00 BIOT 121. Enabling engineering of *Cutaneotrichosporon oleaginosus*, a robust metabolizer of all components of lignocellulosic biomass-derived compounds for oleochemical production. **A. Yaguchi**, M. Spagnuolo, A. Robinson, N. Franaszek, M.A. Blenner

4:20 BIOT 122. Synthesis of polyketides from low cost substrates by the thermotolerant yeast *Kluyveromyces marxianus*. **T. McTaggart**, D. Bever, S. Bassett, N.A. Da Silva

4:40 BIOT 123. Tool development to manipulate early-branching anaerobic fungi as a platform for biotechnology. **K. Solomon**

Section D

Rosen Centre Hotel
Salon 2

End-to-End Biomanufacturing

Process Analysis & Control of Product Quality Attributes

J. Bender, J. C. Love, V. Roy, *Organizers*
T. D. Rau, N. Sanaie, *Presiding*

2:00 BIOT 124. Role of mechanistic modeling in optimization and control of bioseparation processes. **A.S. Rathore**

2:20 BIOT 125. Implement of flow cytometry in bioprocess monitoring. **X. Ji**, Y. Zhu, T.W. Eyster, J. Raley, R. Duvilla

2:40 BIOT 126. UF/DF monitoring and control by variable pathlength UV/Vis spectroscopy, light scattering and density measurements. **L. Rolinger**, M.R. Rüdts, J. Diehm, J. Hubbuch

3:00 BIOT 127. Using process analytical technology to accelerate process development. **J.M. West**, R. Swanson, S. Bhavsar, K. Trejo, H. Zhao, J. Ding, Z. Li

3:20 Intermission .



TECHNICAL PROGRAM

3:40 BIOT 128. Novel non-invasive sensor for real-time dissolved carbon dioxide (DCO₂) monitoring in shake flasks & in mini-bioreactors and its implications in bioprocess control. **V.R. Chopda**, J. Tyson, T. Holzberg, B. Folio, M. Tolosa, Y. Kostov, X. Ge, R. Adiga, L.M. Tolosa, G. Rao

4:00 BIOT 129. Using hydrogen peroxide and derivatives to prevent antibody disulfide bond reduction during manufacturing process. **C. Du**, Z. Tan, D. Choy, A.T. Lewandowski, S. Ghose

4:20 BIOT 130. You can't tuna fish, but can you tuna glycosylation?: Raman as a PAT tool for product quality control. **T.W. Eyster**, D.B. Ritz, J. Fernandez, S. Talwar, B. Wan, R. Allen, J. Hayes, S. Reidinger, S. Foster, D. Scheesley, X. Ji, C. Muste, Z. Ao, J. Aon, P. Patel

4:40 BIOT 131. Cell culture process optimization and scale up challenges for a late stage monoclonal antibody program. **B.M. Gupta**, L. Hoshan, M. Nelson, J.S. Bowers

Section E

Rosen Centre Hotel
Salon 6

Biomedical Technologies

Development & Production of Gene & Cell Therapies

R. D. Sheth, G. Thurber, M. Westoby, *Organizers*
L. Chan, W. J. Kelly, B. F. Marques, *Presiding*

2:00 BIOT 132. Viral vector manufacturing: History, technology and considerations for commercial readiness. **C. Murphy**

2:20 BIOT 133. Rapid development and characterization of a nuclease digestion step for multiple gene therapy viral vector manufacturing processes: A case study. **K.N. Kelly**, S. Wall, B. Coisman, A. Fulton, J. Xin, Y. Waghmare

2:40 BIOT 134. Synthetically facile stable and reversible cell-surface functionalization for cell based therapeutic applications. **J. Majumder**, **G. Chopra**

3:00 BIOT 135. Human pluripotent stem cell expansion as aggregates in Vertical-Wheel Bioreactors. **D.E. Nogueira**, C.A. Rodrigues, C.C. Miranda, Y. Hashimura, S. Jung, B. Lee, J.M. Cabral

3:20 Intermission.

3:40 BIOT 136. Quantitative analysis of lentiviral vector potency for gene therapy in hemoglobinopathies. **J.Y. Zhao**, C. Mintz, D. Bhattacharya, G. Payne, A. Lin, D. Schwalb, S. Duguay, K. MacLeod, J. Cram

4:00 BIOT 137. ERK activity-dependent suicide gene vector system for selective targeting of cancer cells. **E. Day**, B. Purow, M. Lazzara

4:20 BIOT 138. Immunometabolic reprogramming of natural killer cells as adoptive immunotherapies of solid tumors. J. Wang, A. Chambers, K. Lupo, **S. Matosevic**



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

4:40 BIOT 139. Imaging-based phenotypic screening for cell therapy manufacturing. J.C. Contreras-Naranjo, A. Hilaly, M.N. Karim, **V. Ugaz**

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

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Undergraduate Research Posters

Biotechnology

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MONDAY EVENING

Section A

Orange County Convention Center
West Hall C

Sci-Mix

J. Neville, B. Pflieger, *Organizers*

8:00 - 10:00

211, 213, 228, 246-247, 256, 259, 261, 263, 266, 300, 314, 319, 339, 351, 375, 430, 432, 486. See subsequent listings.

TUESDAY MORNING

Section A

Rosen Centre Hotel
Grand A



TECHNICAL PROGRAM

Spotlights on Research Areas

End-to-End Biomanufacturing

J. Bender, J. C. Love, V. Roy, *Organizers*
B. Pflieger, *Presiding*

8:30 BIOT 140. Keynote: Advances in gene therapy manufacturing. **C. Simpson**

9:10 BIOT 141. Study of surface chemistry to enhance viral bioprocessing. **C. Heldt**, X. Mi, P. Joshi, S. Kriz, E. Bromley

9:30 BIOT 142. From stillage to biogas: A year of waste from the Native Dextran factory takes the biogas bus around the globe! **A. Daniels**, A. Kokko, A. Stjernerhoff, E. Wall

9:50 Intermission.

10:10 Discussion.

10:30 BIOT 143. Johnson award: Past is new again. **K.H. Lee**

Section B

Rosen Centre Hotel
Grand B

Downstream Processing

Non-Chromatography Based Separation of Biomolecules

S. Chollangi, M. Gruvegard, C. Heldt, *Organizers*
B. V. Bhut, C. Gillespie, J. Lawler, *Presiding*

8:30 BIOT 144. Overcoming cell shear in mAb harvests with advanced clarification train technologies and design strategies. **A. Voloshin**, M. Nakamura, R. Warren

8:50 BIOT 145. Development of continuous ELP-Z-based affinity precipitation for the purification of monoclonal antibodies. **A. Mullerpatan**, M. Bhat, J. Chen, M. Holstein, P. Karande, S.M. Cramer

9:10 BIOT 146. Peptide immunofibers with modified protein A ligand for monoclonal antibody purification. **L. Lock**, Y. Li, J. Mills, H. Cui, X. Xu, S. Ghose

9:30 BIOT 147. Manufacturing scalability of isoelectric impurity precipitation during viral inactivation neutralization. **S.J. T aylor**, W. Jin, H. Hua, J. Guo, J. Lee, X. Xu, A.M. Lenhoff, S. Ghose

9:50 Intermission.



TECHNICAL PROGRAM

10:10 BIOT 148. Comparative Evaluation of TFF cassettes towards establishing a platform strategy for UFDF step. **A. Shirke**, D. Kanani, M. Jin

10:30 BIOT 149. Investigation of fouling mechanisms of virus filters during the filtration of protein solutions using a high throughput filtration screening device. **P. Kosiol**, M. Bieberbach, A. Seay, M. Bennecke, B. Hansmann, S. Hepbildikler, V. Thom

10:50 BIOT 150. Withdrawn

11:10 BIOT 151. Development of a method for the measurement of Interactions between protein molecules and the virus removal membrane surface: effects of immunoglobulin G adsorption on filter performance. **R. Hamamoto**, T. Hongo-Hirasaki, T. Hayashi

Section C

Rosen Centre Hotel
Salon 4

Upstream Processes

Systems Biology & Omics: Tools & Applications

P. Peralta Yahya, A. Russo, C. T. Trinh, *Organizers*
C. Chen, R. Saha, *Presiding*

8:30 BIOT 152. Constraint-based modeling and genome-scale metabolic models to understand metabolism of Chinese hamster ovary cells. Y. Chen, **M.J. Betenbaugh**

8:50 BIOT 153. Novel mechanistic insights towards precision control of n-glycosylation in CHO cell fed-batch cultures. **M. Sumit**, S. Dolatshahi, M.M. Chang, G. Jung, K. Cote, B. Tzvetkova, J.J. Scarcelli, J.K. Marshall, R.J. Cornell, R. Weiss, D.A. Lauffenburger, B. Figueroa, B.C. Mulukutla

9:10 BIOT 154. Multiscale modeling of antibody production and glycosylation for improved upstream process design. **Y. Luo**, J.V. Price, R.J. Lovelett, D. Radhakrishnan, K.A. Barnhouse, E.J. Schaefer, J. Cunningham, P. Hu, K.H. Lee, R. Shivappa, B. Ogunnaiké

9:30 BIOT 155. Elucidating fluxes in complex media: ¹³C metabolic flux analysis of *E. coli* grown in the presence of yeast extract. **B. McConnell**, M.R. Antoniewicz

9:50 Intermission.

10:10 BIOT 156. Systems-level analysis of metabolic flux responses to deletion of 50 core enzymes reveals flexibility and limits of *E. coli* metabolism. **M.R. Antoniewicz**, C.P. Long

10:30 BIOT 157. Elucidating and reverse engineering exceptional solvent tolerance in *Yarrowia lipolytica*. **C. Walker**, S. Ryu, C.T. Trinh

10:50 BIOT 158. Systems approaches for engineering microbial biocatalysts. **J. Reed**



TECHNICAL PROGRAM

11:10 BIOT 159. Optimizing heterologous gene dosage in eukaryotes informed by omic analysis of over 125 yeast strains. **J. Brady**, C.A. Whittaker, M.C. Tan, N.A. Colant, K.R. Love, J.C. Love

Section D

Rosen Centre Hotel
Salon 5

Biomolecular Technologies

Therapeutic Protein Discovery

B. Hackel, B. F. Marques, *Organizers*
J. Jardine, G. J. Rocklin, *Presiding*

8:30 BIOT 160. Design and evaluation of novel antibody libraries with drug-like specificity. **A.A. Desai**, C.G. Starr, G. Pornnoppadol, B. Berg, P.M. Tessier

8:50 BIOT 161. Development of deoxyribozyme DNA nanomachines for diagnostics and therapy. **D. Kolpashchikov**, D. Nedorezova, A.A. Spelkov, C. Roldan, C. Amanda

9:10 BIOT 162. Directed evolution of high affinity MDM2-binding ligands using stabilized bacterial peptide display. **T.A. Navaratna**, L. Atangcho, G. Thurber

9:30 BIOT 163. Novel LPS trap in cancer immunotherapy. **R. Liu**

9:50 Intermission.

10:10 BIOT 164. Developing and characterizing peptide bacteriocins as antimicrobial therapeutics. **V.D. Trivedi**, N.U. Nair

10:30 BIOT 165. Engineering hyperthermostable rcSso7d as a reporter molecule for *in vitro* diagnostic tests. **K. Sung**, E. Miller, H.D. Sikes

10:50 BIOT 166. Kinetics and characterization of non-enzymatic fragmentation of monoclonal antibody therapeutics. **A.S. Rathore**

11:10 BIOT 167. Redirected CAR T activity via CD19-ligand fusions engineered by deep mutational scanning. **J.R. Klesmith**, B. Hackel

Section E

Rosen Centre Hotel
Salon 6

Biomedical Technologies

New Strategies for the Delivery & Targeting of Therapeutics



TECHNICAL PROGRAM

R. D. Sheth, G. Thurber, M. Westoby, *Organizers*
A. C. Brown, A. Noyes, X. Qian, *Presiding*

8:30 BIOT 168. Tumor-targeted responsive nanocarriers for combined photothermo therapy and controlled drug release. **X. Pu**, X. Ju, L. Zhang, P. Hanyu, Z. Liu, W. Wang, R. Xie, L. Chu

8:50 BIOT 169. Integrated approach for tailoring chitosan hydrogels towards kinetically-tuned release of synergistic combinations of chemotherapeutics. J.D. Schneible, A. Singhal, R. Lilova, C.K. Hall, A. Grafmüller, **S. Menegatti**

9:10 BIOT 170. In situ-induced multivalent anticancer drug clusters in cancer cells for enhancing drug efficacy. **F. Lu**

9:30 BIOT 171. Materials for drug capture: An approach to mitigating the off-target toxicity of chemotherapy. **M.D. Schulz**, O. Wadsworth, M. Bardot, S. Oyola-Reynoso, S. Hetts

9:50 Intermission.

10:10 BIOT 172. 'Antimicrobial peptide'-functionalized catheter for efficacious antimicrobial protection. **S.S. Leong**

10:30 BIOT 173. Targeted siRNA delivery with modular hepatitis B virus-like particles. **D. Yur**, W. Chen, M.O. Sullivan

10:50 BIOT 174. Bacterial outer membrane vesicles as targeted antibiotic delivery devices. S. Collins, J.B. Nice, **A.C. Brown**

11:10 BIOT 175. Targeted breast cancer imaging and therapy enabled by tumor-targeting peptides. **C. Mao**

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TUESDAY AFTERNOON

Section A

Rosen Centre Hotel
Grand A

Spotlights on Research Areas



TECHNICAL PROGRAM

Biomedical Technologies

R. D. Sheth, G. Thurber, M. Westoby, *Organizers*
T. Mansell, *Presiding*

2:00 BIOT 176. Keynote: One language is not enough: Why biomedical innovation needs polyglots. **J.T. Beck**

2:40 Rapid Fire Presentations.

3:20 Intermission.

3:40 Discussion.

4:00 BIOT 177. Award Address (E. V. Murphree Award in Industrial and Engineering Chemistry sponsored by the ExxonMobil Research and Engineering Company). Tools for Systems Neurobiology. **H. Deligianni**

Section B

Rosen Centre Hotel
Grand B

Downstream Processing

Advancements in mAb platforms/Case-Studies & Applications in mAb Process Development

S. Chollangi, M. Gruvegard, C. Heldt, *Organizers*
S. Ghose, A. C. Roque, J. Woo, *Presiding*

2:00 BIOT 178. Where is Protein A affinity chromatography going? **H.J. Johansson**, M. Hicks, P. Gilbert

2:20 BIOT 179. Evaluation of next generation high capacity Protein A resins to improve productivity and maximize recovery of high titer processes. **A. Zubieta**, S. Wong, A. Keba

2:40 BIOT 180. Control strategies for removing difficult host cell proteins in monoclonal antibody processing. **J. Welsh**, I. Han, J. Pollard, D.J. Roush, N. Tugcu

3:00 BIOT 181. Utilizing mixed-mode cation exchanger in streamlined polishing step for mAb purification. A. Utturkar, **K. Gillette**, R. Quesenberry, M. Schofield

3:20 Intermission.

3:40 BIOT 182. Development of a polishing step for an atypical antibody using rapid purification techniques and particle size analysis. **H. Tjandra**, Y. Chang, D.S. Surendar, R. Zolyomi, A. Hesslein

4:00 BIOT 183. Evaluation of cost-effective viral surrogates for viral clearance studies for bioprocessing. **R. Dyer**, J. McGinnis, Y. Song, L. Jenkins, J. Chen, S. Sharma, S. Ghose, Z. Li



TECHNICAL PROGRAM

4:20 BIOT 184. Protein A on cellulose fibre takes bioprocess chromatography to a new level. **A. Graanberg**, S. Grönlund, M. Bergman, I. Scanlon, Z. Sexton, C. Morris, O. Hardick

4:40 BIOT 185. Toward a true Protein A mimetic: new peptide affinity ligand for IgG purification afford high HCP LRV. H. Reese, X. Xiao, C.K. Hall, **S. Menegatti**

Section C

Rosen Centre Hotel
Salon 4

Upstream Processes

Mammalian: Innovative Technologies

P. Peralta Yahya, A. Russo, C. T. Trinh, *Organizers*
L. Cella, N. S. Lewis, *Presiding*

2:00 BIOT 186. Quantification of reductase expression and correlations with cell growth and product quality. **M. Handlogten**, S. Ahuja

2:20 BIOT 187. Comparative analysis: An innovative siRNA-based technology versus traditional antibiotic-selection in the creation of stable expression of proteins/antibodies in CHO-K1 cells. **V. Muralidharan-Chari**, S. Sharfstein, Z. Wurz, N. St.John, E. Eveleth

2:40 BIOT 188. Implementation of the beacon nanofluidic platform into a manufacturing cell line development process. **K. Le**, J. Stevens, C. Tan, H. Le, J. Tat, E. Zasadzinska

3:00 BIOT 189. Genetic engineering of CHO host cell proteins: Approaches to improve product quality and production processes. **J. Mascarenhas**, V. Balassi, A. Kassim, T. Borgschulte

3:20 Intermission.

3:40 BIOT 190. Metabolic engineering of CHO cells for increased mAb production. **J. Young**, A.M. Pereira, S. Sacco, K. Smith, M.J. Betenbaugh

4:00 BIOT 191. Computational framework for mechanistic modeling and simulation of upstream bioprocesses. **W. Johnson**, M. Carcamo, P. Rolandi

4:20 BIOT 192. *Exploring the use of the human body as a novel source of raw materials for personalized medicine based on cell extracts.* **D. Burgenson**, X. Ge, I.V. Kostov, L.M. Tolosa, G. Rao

4:40 BIOT 193. Expansion of NOTCH^{high} and CD133^{high} GSC-enriched niche model using a small scale bioreactor. **J. Park**, Y. Kim

Section D

Rosen Centre Hotel
Salon 5



TECHNICAL PROGRAM

End-to-End Biomanufacturing

Beyond the Platform: Vaccines & Cell Therapies

J. Bender, J. C. Love, V. Roy, *Organizers*
K. Aggarwal, N. Agrawal, *Presiding*

2:00 BIOT 194. Scalable adenovirus production process, from cell culture to purified bulk. **A.M. McWhirter**, M. Bergman, E. Blanck, S. Häggblad Sahlberg, P. Sjöholm, M. Soultioti, S. Musunuri, E. Wallby, A. Akerblom, A. Lagerlof, M. Lundgren

2:20 BIOT 195. Viral vector platform development guidance based on process cost modeling. **D. Bohonak**, R. Patil

2:40 BIOT 196. Scaling up vaccine bioprocessing: envisioning continuous biopharmaceutical vaccine bioprocesses. **D.K. Roper**

3:00 BIOT 197. Transient transfection of HEK 293T cells to produce yellow fever VLPs. **G. Dekevic**, L. Tasto, J. Zitzmann, D. Salzig, P.M. Czermak

3:20 Intermission.

3:40 BIOT 198. Characterization of critical quality attributes of self-amplifying mRNA: A novel vaccine/therapeutic modality. **M. Xie**, G. Maruggi, D. Yu, N. Moniotte, K. Aggarwal

4:00 BIOT 199. Enabling large-scale ex vivo production of megakaryocytes and platelets from CD34+ cells using gas-permeable surfaces. **A. Martinez**, W.M. Miller

4:20 BIOT 200. Co-cultivation: A powerful tool for insulin-producing beta cell manufacturing. **F.S. Petry**, P.M. Czermak, D. Salzig

4:40 BIOT 201. Role of virus filtration in achieving pathogen safety of gene and cell therapy products. **D. Strauss**, S. Teitz, T. Sohka, N. Hiroto

Section E

Rosen Centre Hotel
Salon 6

Biomolecular Technologies

Engineering & Design

Cosponsored by BIOL[‡]
B. Hackel, B. F. Marques, *Organizers*
K. Brown, B. DeKosky, *Presiding*

2:00 BIOT 202. Structure-guided discovery of dual-recognition chemibodies. **A.C. Cheng**



TECHNICAL PROGRAM

2:20 BIOT 203. Generation of functional monoclonal antibodies inhibiting matrix metalloproteinases. **K. Lee**, Z. Dunn, T.J. Lopez, X. Ge

2:40 BIOT 204. Physicochemical determinants of drug-like monoclonal antibodies. **Y. Zhang**, L. Rabia, S. Ludwig, C.G. Starr, P. Gupta, M. Julian, P.M. Tessier

3:00 BIOT 205. Engineering the local environment for enhanced enzyme biocatalysis. **I.R. Wheeldon**

3:20 Intermission.

3:40 BIOT 206. Developing a branched-chain amino acid biosensor from bacterial periplasmic binding proteins for human diagnostics. **L. Wong**, C. Gurramkonda, G. Rao, L.M. Tolosa

4:00 BIOT 207. ROSETTA-informed design of structurally stabilized cyclic anti-amyloid peptides. **C. Est**, P. Mangrolia, R.M. Murphy

4:20 BIOT 208. Synthetic molecular evolution of antimicrobial peptides. C.G. Starr, J. Ghimire, S. Guha, **W.C. Wimley**

4:40 BIOT 209. Design of membrane-active peptides that assemble into macromolecular-size pores. **K.A. Hristova**, S.Y. Kim, A. Pittman, G. King

Exploring the Frontiers of Chemistry through NASA Research

Living There: Science for the Future of Manned Space Exploration

Sponsored by COMSCI, Cosponsored by ANYL, BIOL[‡], BIOT, CELL, COLL, ENFL[‡], I&EC[‡], INOR[‡], NUCL[‡], PHYS[‡], PMSE[‡] and POLY[‡]

Polymer Bioconjugates for a Changing World

Sponsored by POLY, Cosponsored by BIOT

TUESDAY EVENING

Section A

Orange County Convention Center
West Hall E2

Biomedical Technologies

Poster Session



TECHNICAL PROGRAM

R. D. Sheth, G. Thurber, M. Westoby, *Organizers*
K. Solomon, I. R. Wheeldon, *Presiding*

6:00 - 8:00

BIOT 210. Acoustic levitation as a screening method for spray drying thermally stable viral vector powders. **B. Morgan**, Z. Xing, M.R. Thompson, E.D. Cranston

BIOT 211. Structural basis for protein energy landscapes in a de novo designed proteome. **G.J. Rocklin**, S. Houlston, C. Arrowsmith, M. Guttman, D. Baker

BIOT 212. Cellular clocks in *Neurospora crassa* demonstrate synchronization. **J. Cheong**, B. Hull, J.R. Griffith, L. Mao, J. Arnold, H. Schuttler

BIOT 213. Spatial, temporal, and dose control of drug delivery using non-invasive magnetic stimulation. **C. Cheng**, W. Chen, J.I. Zink

BIOT 214. Improved antibacterial properties in titanium implants by acid etching and atomic layer deposition. **P. Ghannadian**, J. Moxley, T. Webster

BIOT 215. Electrical, optogenetic, and magnetic stimulation of myelination. **I. Yang**, A. Blasiak

BIOT 216. Ascorbic oxidase-like activity of cupric oxide nanoparticles and its antibacterial application. **Z. Quanquan**, **S. He**, W. Chen

BIOT 217. Patterned microwell compartments harbor hepatocyte spheroids for genotoxicity testing. **C. Chao**, L. Ngo, B.P. Engelward

BIOT 218. Drug cocktail-carrying Nanomedicine for the treatment of Cancer. **R. Bean**, S. Santra, T. Banerjee, L. Hadorn, S. Naz, S. Anant, Q. Austin

BIOT 219. Cathepsin B stimuli controlled drug delivery system. **K. Leatherman**, H. Pierce, K. Roth

BIOT 220. Microfluidic degasser for lab-on-chip devices. **M. Al-Adhami**, E. Gutierrez, A. Andar, G. Rao, I.V. Kostov

BIOT 221. Synthesis of fluorogenic activated platelet sensor and application in stent thrombosis imaging. **A. Trice**, E. Marris, K. Ha, F. Jaffer, X. Zheng, C. Kessinger, J. McCarthy

BIOT 222. In vivo-jetPEI, an alternative to viral vectors for nucleic acid-mediated therapies. **M. Hellal**, V. Moreau, F. Prémartin, T. Benchimol, V. Kedingler, P. Belguise, P. Erbacher

BIOT 223. Toward clinical translation of near-infrared nerve-specific fluorophores for fluorescence image-guided nerve sparing surgical procedures. **L. Wang**, C.W. Barth, V. Shah, A.W. Alani, A. Antaris, J. Sorger, S.L. Gibbs

BIOT 224. Diamagnetic CEST MRI contrast agent that can simultaneously detect extracellular tumor pH and enzyme activity. **C.J. Kombala**, M.D. Pagel

BIOT 225. Ratiometric pH imaging with a dendritic CEST MRI contrast agent. **C.J. Kombala**, M.D. Pagel



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- BIOT 226.** Development of functional magnetic relaxation nanosensors for the investigation of zika binding and fusion mechanism. **S. Darji**, T. Banerjee, S. Santra
- BIOT 227.** Responsive fluorophore aggregation provides contrast for lifetime imaging in cells. **K. Schleyer**, B. Datko, X. Ma, J.K. Grey, L. Cui
- BIOT 228.** Peptide bilayer capsules to peptide bilayer coated metallic nanoparticles- BAPCs through the decade! **P. Natarajan**, S. Whitaker, S. Fleming, J.M. Tomich
- BIOT 229.** Self-immobilizing NIR probe for imaging of cellular senescence *in vivo*. **J. Liu**, X. Ma, Y. Wang, C. Cui, P.R. Deenik, L. Cui
- BIOT 230.** In vitro evaluation of a reductively labile prodrug albumin-doxorubicin conjugate. **A. McGhee**, A. Patel, R.A. Petros
- BIOT 231.** Split deoxyribozyme sensor for detection of a highly structured highly modified nucleic acid: Transfer ribonucleic acid. **R. Paredes**, A. Reed, R. Sapia, C. Dowis, Y. Gerasimova
- BIOT 232.** Molecular logic gates for the detection of multiple single-nucleotide polymorphisms conferring antibiotic resistance. **R. Connelly**, S. Farnell, Y. Gerasimova
- BIOT 233.** Self-assembly of immune signals as a modular platform to direct TLR signaling for tolerance. **R.S. Oakes**, L.H. Tostanoski, C. Jewell
- BIOT 234.** ZIGIRs for the fluorescence imaging of Zn²⁺ in secretory granules. **E.H. Ghazvini Zadeh**, W. Li
- BIOT 235.** Using silica to stabilize flavivirus vaccines. **D. Demchenko**, K. Stedman, W. Messer, Z. Lyski
- BIOT 236.** Folic acid-conjugated cross-linked cytochrome c nanoparticles combining triggered release and active targeting for lung cancer therapy. **I. Dominguez Martinez**, K. Griebenow
- BIOT 237.** DNA nanoparticles condensed by pure metal ionics: Applications in nano-medical treatment. **L. Lin**, H. Zhao, L. Tian
- BIOT 238.** Novel piezoelectric microcantilever sensor for measurement of contracting muscle force generation. **E. Coln**, A. Colon, C. Long, N. Narasimhan, J.J. Hickman
- BIOT 239.** Developing a new sensing technology for detecting antibiotic resistance genes utilizing engineered zinc finger proteins and graphene oxide. D. Ha, **M. Kim**
- BIOT 240.** Stability of trans-retinol embedded in phosphatidylcholine multilayer vesicles. **Y. Chmykh**
- BIOT 241.** Isolation and characterization of the probiotic bacterium *Pediococcus acidilactici*. **K. Christopher**, V. Zambare
- BIOT 242.** Miniaturized wireless system for hepatitis C detection. **J.C. Costa**, W.B. Bastos, P.I. Costa, E. Longo, M.A. Zaghete, J.P. Carmo
- BIOT 243.** Evaluation of bare and functionalized reduced graphene oxide as a platform for organelle targeting. **M. Farell**, E. Gomez, M. Kumar



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

BIOT 244. Comparison of nanoparticle and nanoparticle-free formulations for the active delivery of cytochrome c by targeting folate receptors. **V.C. Barcelo Bovea**, I. Dominguez Martinez, F.M. Joaquin, L.A. Amador, E. Castro, A. McGoron, Y. Ferrer-Acosta, K. Griebenow

BIOT 245. Developing a facile system for synthetic engineering of advanced silk-based materials. J. Chen, C. Huang, R. Wang, J. Yang, T. Yang, **H. Wu**

BIOT 246. Intra-lymph node vaccine depots to promote selective tolerance in type 1 diabetes. **J. Gammon**, C. Jewell

BIOT 247. Engineering a calcium-responsive molecular recorder from *E. coli* DNA polymerase I. **A. Castinado**, A. De Paz, K.E. Tyo

BIOT 248. Gene screen reveals chromatin proteins influence abnormal nuclear morphology associated with breast cancer cell models. **A. Tamashunas**, V.J. Tocco, J. Matthews, Q. Zhang, S. Pathak, J. Licht, A.D. Stephens, H. Luesch, T.P. Lele

BIOT 249. Directed evolution of the tissue inhibitor of metalloproteinases-1 (TIMP-1) scaffold for developing selective therapeutic agents. **M. Raeeszadeh Sarmazdeh**, B. Sankaran, D. Radisky, E. Radisky

BIOT 250. Self-assembly of DNA-minocycline complexes by metal ions with controlled drug release. T. Zhang, J. Nong, N. Alzahrani, Y. Zhong, **J. Fu**

BIOT 251. DNA-crowded enzyme complexes with controlled spatial confinement and improved function. **J. Fu**

BIOT 252. Engineering microbial production of spider silks that fully replicate the primary mechanical properties of their natural counterparts. **C. Bowen**, F. Zhang

BIOT 253. Two-dimensional materials that enhance human embryonic stem cell-signal detection. **S. Chan**, Y. Tan, K. Wu, C. Cheung, D. Loke

BIOT 254. Developing of a DNA nanorobot with RNA sensing and cleaving functions. **T. Molden**, D. Kolpashchikov

Section A

Orange County Convention Center
West Hall E2

Biomolecular Technologies

Poster Session

B. Hackel, B. F. Marques, *Organizers*
K. Solomon, I. R. Wheeldon, *Presiding*

6:00 - 8:00

BIOT 255. Discovery of general amyloid inhibitors against the aggregation and toxicity of both amyloid- β and hIAPP. **B. Ren**, Y. Zhang, F. Yang, J. Zheng



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

BIOT 256. Transient expression of an anthrax decoy protein in *Nicotiana benthamiana*: The impacts of N-glycosylation on protein expression, stability and function. **Y. Xiong**, K. Karuppanan, Q. Li, A. Bernardi, V. Kommineni, C.B. Lebrilla, R. Faller, K. McDonald, S. Nandi

BIOT 257. Rapid detection of monoclonal antibodies and other biomolecules through functionalized nanoparticle crosslinking. **A. Swartz**, W. Chen

BIOT 258. Development and application of a continuous evolution system to program protein-protein interactions. **J. Zinkus-Boltz**, B.C. Dickinson

BIOT 259. Positive selection screens for DNA endonuclease activity. **M. Mechikoff**, K. Lee, P. Pandolfi, K. Solomon

BIOT 260. Polymerization and synthesis of biostyrene by engineering *E. coli* using iCREATE strategy. **L. Liang**, R. Liu, E. Freed, C.A. Eckert, R.T. Gill

BIOT 261. Optimizing key amino acids in CHO cell culture medium improves productivity and reduces waste byproducts for biologics manufacturing. **S.B. Khurana**, A. Deresiensk, G. Dong

BIOT 262. Scalable cell-free extract preparation and minimal genetic template methods for rapid protein prototyping. **J. Dopp**, N. Reuel

BIOT 263. Process development for production of a live biotherapeutic drug product for the treatment of Phenylketonuria. **P. Reeder**, C. Bergeron, M. Momin, V. Isabella, D. Lubkowitz, P. Miller, R. Schwartz, E. Antipov

BIOT 264. Characterization of chemically defined media variation on the level of secreted phospholipase-B like protein by recombinant CHO cell cultures. **J. Crawford**, W.J. Kelly, Z. Huang

BIOT 265. Micro-channel cantilever spotting (μ CS) and the immobilization of Cucurbit[7]uril complex for determination of sensitivity on analyte exposure. **A.V. Mora**, P. Avon, M. Hirtz, C. Wilson, A.E. Holmes

BIOT 266. Engineering stable anaerobic consortia by understanding the genomic basis for syntrophic interactions. **J. Brown**, X. Peng, S. Gilmore, J. Henske, M.A. Perisin, M.A. O'Malley

BIOT 267. Designing fatty acid-conjugated therapeutic proteins with a high molecular weight for the extended serum half-life. J. Cho, J. Park, **I. Kwon**

BIOT 268. Deamidation compromises antibody colloidal stability and solubility in a pH-dependent manner. **M.E. Alam**, G.V. Barnett, T.R. Slaney, T. Das, P.M. Tessier

BIOT 269. Improved expression of human tachykinin NK₂ receptor using a receptor-receptor chimera with the rat homologue. **A.R. Jain**, Z.T. Britton, A.S. Robinson

BIOT 270. Start with the end in sight: Developability & improved biopharmaceutical molecule quality. **R. Casey**

BIOT 271. Cost-effective construction of high quality diversity-containing sequences of variable length for protein libraries. **I. Dodevski**, C.A. Sarkar

BIOT 272. Designing vaccines that elicit broadly neutralizing antibodies. **A. Arsiwala**, S. Frey, A. Castro, C. Varner, T. Rosen, R.S. Kane



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- BIOT 273.** Using synthetic biology strategies for studying flux towards isobutanol in *Saccharomyces cerevisiae*. **F. Gambacorta**, B.F. Pflieger
- BIOT 274.** Artificial dual-functional enzyme constructed by combining an enzyme and an organometallic catalyst. **J. Cha**, Y. Jung, V. Ganesan, S. Yoon, I. Kwon
- BIOT 275.** Mechanically controlled thermodynamics of biorecognition events. H. Reese, M.A. Daniele, **S. Menegatti**
- BIOT 276.** Site-specific fatty acid-conjugation of therapeutic proteins for the extended serum half-life. **J. Cho**, I. Kwon
- BIOT 277.** Improving antifungal efficacy for the high mannose binding lectin Myxovirin. **J.L. Osier**, R.L. McFeeters
- BIOT 278.** Magnetic relaxation nanosensors (MRnS) for rapid detection and one-step differentiation between subtypes of influenza. **S.S. Ramanujam**, S. Santra, T. Banerjee
- BIOT 279.** TNF- α and sophorolipids: Combination approach for the treatment of prostate cancer. **Z. Shaw**, J. Kallu, J. Beach, T. Banerjee, R.A. Gross, S. Santra
- BIOT 280.** Expression of TALEs in plants and development of TALE arrays for diagnostic applications. **C.S. Jackson**, W. Cecil, K. Kim, K. Ko, M. Kim
- BIOT 281.** Engineered zinc finger proteins immobilized on the silane polymer surface for diagnostic probes to detect antibiotic resistance genes. **J. Shim**, M. Kim
- BIOT 282.** Single particle virus isoelectric point determination with chemical force microscopy. **X. Mi**, P. Joshi, E. Bromley, F. Long, C. Heldt
- BIOT 283.** Conformation and mechanism of ferritin early-step disassembly process at low pH. **Z. Li**, T. Ueno, D. Lu
- BIOT 284.** Withdrawn
- BIOT 285.** Effect of homodimer IgG4 bispecific antibody aggregates on controlled F_{ab}-Arm-Exchange (cFAE). **R. Rao**, R.G. Bertrand, P.J. Alfonso, R. Smith, M. Capaldi
- BIOT 286.** Competition study between wild type cyanobacteria *Synechococcus elongatus* PCC 7942 and plasmid transformant *Synechocystis* PCC 6803. **O. Sacko**, L.H. Greene, **J.W. Lee**
- BIOT 287.** Triple helix involved in genomic targeting. **N. Kikuchi**
- BIOT 288.** Characterization and development of a halogenase enzyme as a tool for synthesis. **S. Mori**, A. Pang, N. Thamban Chandrika, S. Garneau-Tsodikova, O.V. Tsodikov
- BIOT 289.** Zinc finger proteins for pathogen detection. **S. Petrucci**, H. Joda, D. Broyles, E. Dikici, S. Daunert, S.K. Deo
- BIOT 290.** Pilot purification of horse hemoglobin a1c. **T.M. McCaffrey**
- BIOT 291.** Assessing the stability and expression of transgenes in genetically engineered cyanobacteria for biofuel production. **C. Barnes**, **L.H. Greene**, **J.W. Lee**



TECHNICAL PROGRAM

BIOT 292. Developing a double-stranded DNA biosensor using engineered zinc finger proteins linked to a β -lactamase for detecting antibiotic resistance genes. **W.M. Cecil**, M. Kim

BIOT 293. Synthesis of nucleoside analogs for inhibition of HIV-1 RT. **B. Mueller-Mabry**, C.E. Ledezma, D. Kolpashchikov

BIOT 294. Impact of mobile phase conditions on multimodal ligand association on SAM surfaces. **M. Vats**, C. Bilodeau, S. Garde, S.M. Cramer

BIOT 295. Withdrawn

BIOT 296. Developability assessment of an IgG2 Monoclonal Antibody prior to commencement of process development. **C. Ramineni**, J. Xu

BIOT 297. Chemometrics approach in establishing functional comparability of biosimilars. **T.S. Savane**, R. Dash, N. Budholiya, A.S. Rathore

BIOT 298. Accelerating proton transport in a novel biological p-n junction for fabricating an artificial retina. **Y. Lv**, D. Liang, S. Lu, X. Yan

BIOT 299. Harnessing self-assembly to promote immune tolerance during autoimmune disease. **E. Froimchuk**, C. Jewell

BIOT 300. Computational optimization of a thioesterase for selective chain-length product distribution. **M.A. Jindra**, R. Chowdhury, B. Pflieger, C. Maranas

BIOT 301. Directed evolution of antibodies with high conformational specificity for glucagon amyloid fibrils. **S.D. Stimple**, S. Kalyoncu, A.A. Desai, J. Mogensen, L. Spang, D. Asgreen, A. Staby, P.M. Tessier

Section A

Orange County Convention Center
West Hall E2

Downstream Processing

Poster Session

S. Chollangi, M. Gruvegard, C. Heldt, *Organizers*
K. Solomon, I. R. Wheeldon, *Presiding*

6:00 - 8:00

BIOT 302. Tank cycling approach for continuous diafiltration process. **A. Gupta**, E.M. Goodrich, H. Lutz

BIOT 303. Real-time monitoring of antibody in Protein A column breakthrough. **U. Patil**, M. Crum, B. Vu, K. Kourentzi, R.C. Willson

BIOT 304. Mixed-mode peptide ligands for improved clearance of CHO host cell proteins. **A. Lavoie**, A. di Fazio, K. Blackburn, D.C. Muddiman, M.B. Goshe, R.G. Carbonell, S. Menegatti



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- BIOT 305.** Streamlining schistosomiasis vaccine development in collaboration with Texas Children's Hospital Center. **B. Fryszczyn**
- BIOT 306.** Purification of human milk oligosaccharides obtained from fermentative processes via crystallization from water or aqueous mixtures on industrial scale. **M. Baier, T. Seitz, A.R. Gräßle, S. Jennewein**
- BIOT 307.** Effect of column chromatography process on the permeability of virus filter. **A.D. Pilley, D. Strauss, H. Shirataki, S. Aoyama, Y. Matsumoto**
- BIOT 308.** Prediction of mass transfer coefficients in linear pH and salt gradient elution. **J. Hedrich, C. Frech**
- BIOT 309.** Application of mechanistic modeling to speed up purification process development of novel formats: A virus-like particle case study. **T. Hahn, M. Casals Peralvarez, T. Huuk, J. Wölfel, C. Niehus, N. Stempel**
- BIOT 310.** Single use centrifuge, uniFuge, in bioprocessing of mammalian cell. **D. Richardson**
- BIOT 311.** Using flocculating agents to increase depth filter throughput during cell harvesting. **E. Or, C. DiSpirito, T. Cheung, K. Zeleznik, S. McDonough, S. Ozturk**
- BIOT 312.** Purification development for robust removal of a challenging product related impurity for a hetero-mAb. **L. Rockwell, M. Iammarino, S. Kandula, N. Tugcu**
- BIOT 313.** Scale up and virus studies of a twin-column continuous capture process for monoclonal antibodies. **J.M. Angelo, S. Chollangi, J. Pagano, D. Baur, K. Mihlbachler, T. Müller-Späth, X. Xu, M. Morbidelli, S. Ghose**
- BIOT 314.** Intein-mediated affinity capture: A novel platform enabling rapid prototyping and characterization of discovery-phase biologics by single-column purification and integrated tag removal. **J. Taris, D.W. Wood, Y. Fan, A. Kiesewetter, O. Rammo**
- BIOT 315.** Novel adsorbent platform for antibody purification using small synthetic affinity ligands. **M. Matos, F. Trovão, A. Pina, J. Gonçalves, A.C. Roque**
- BIOT 316.** Understanding capacity loss during continuous counter-current tangential ion exchange chromatography. **J. Martin Bufajer, Y. Zhou, D.G. Bracewell**
- BIOT 317.** Competitive binding of monomer-dimer mAb mixtures and their separation by frontal analysis using ceramic hydroxyapatite. **Y. Wang, G. Carta**
- BIOT 318.** Process intensification in biomanufacturing – a case study – straight through processing via continuous capture with ilc. **S. Jain, R. Shi, S. Yanamadala, L. Grillberger, A. Shukla**
- BIOT 319.** Cell size variation-inclusive, tumor antigen-independent enrichment of viable circulating tumor cells. **Y. Liu, W. Zhao, L. Mao**
- BIOT 320.** Automated high throughput development of multimodal chromatography for capture step in non-mAb recombinant protein purification. **M. Zhu, J. Ma**
- BIOT 321.** Optimization of batch and continuous multi-column protein A chromatography with mechanistic model and experiments. **J. Guo, S. Zhang, D. Kanani, M. Jin**



TECHNICAL PROGRAM

BIOT 322. Micromixing in the salt precipitation of antibodies via batch and continuous processing. **M. Martinez**, M. Spitali, E.L. Norrant, D.G. Bracewell

BIOT 323. Leveraging surface diffusion to increase the dynamic binding capacity of ion exchange resins for monoclonal antibody. **O. Khanal**, V. Kumar, F. Schlegel, P. Rolandi, O. Kaltenbrunner, A.M. Lenhoff

BIOT 324. Rapid sanitization of Protein A resin in bioprocess columns with sporicidal agent. **J. Avallin**, A. Nilsson, H. Ingvarsson, A. Grönberg, P. Norrman, E. Blanck, M. Asplund, L. Persson, R. Pettersson, **R. Braaz**, J. Vinnemeier, P. Lester

BIOT 325. Modeling framework for simulation of transport, adsorption, and buffer equilibria in packed bed columns. **J. Diedrich**, S. Leweke, E. von Lieres

BIOT 326. Enabling high productivity processes with a stackable chromatography cassette: Synergy of device, resin and process design. **G. Platteau**, **G. Ströhlein**

BIOT 327. Virus removal by filtration: Comparison of batch and continuous operation - virus clearance validation and process scaling. **B. Hansmann**, B. Kleindienst, A. Manzke, P. Kosiol

BIOT 328. Isolation of monoclonal antibodies using mimotope-containing membranes. **H. Tan**, W. Liu, J. D. Berwanger, M.L. Bruening

BIOT 329. Continuous virus validation: Understanding fundamental mass transfer enables simplified virus validation. **M. Brown**, R. Orozco, J.L. Coffman

BIOT 330. Design of Protein A resins for continuous chromatography. **M. Hicks**

BIOT 331. Characterization of product related substances in high-throughput analytical environment during late-stage biologics commercial process development. **K. Stone**, E.S. Schutsky, Y. Song, L. Duhamel, N. Zvereva, X. Xu, Y. Gu, Y. Huang, R. Swanson, J. Ding

BIOT 332. Inline concentration of monoclonal antibody feed to increase the productivity of a continuous multi-column chromatography capture step. **T. Elich**, H. Lutz

BIOT 333. Efficient purification of a recombinant protein from *E. coli* fermentate with mixed-mode chromatography resins. **J.M. Sulzberger**, D. Frisch, H. Choi, W. Rushton

BIOT 334. High-capacity capture of a recombinant growth factor directly from refold solution using salt-tolerant cation exchange chromatography. **A. Stein**, A. Heinen-Kreuzig, A. Kiesewetter

BIOT 335. Control of beta-glucan levels in downstream processing by improved depth filtration wash. **D. Jang**, C. Urrea, L. Botta, W. Grimm, S. Sharma, M. Holstein, S. Ghose

BIOT 336. Flocculation optimization for a scalable cell-free harvest process. **K.A. Wessendorf-Rodriguez**, D. Kothari, B. Dransart

BIOT 337. Modeling of ion-exchange chromatography: Are we making the right assumptions? **T. Briskot**, T. Hahn, T. Huuk, F. Wittkopp, F. Stueckler, J. Hubbuch



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

BIOT 338. In-line Fourier-transform infrared spectroscopy as a PAT tool to monitor the integrated on-column PEGylation and purification of a protein. **A. Sanden**, S. Suhm, J. Hubbuch

BIOT 339. DNA impurity removal in the clarification stage is key to mAb process efficiency improvement. **J. Van de Velde**, A. Voloshin, K. Eyer

BIOT 340. Purification of recombinant monoclonal antibody – Rituximab Biosimilar – with alternate non-affinity based chromatographic processes. **A. Posch**, F. Kollmann, C. Pratt, L. Moriarty, P. Khandelwal, E. Dreskin

BIOT 341. Process Intensification: Case studies in downstream processing of monoclonal antibodies. **V. Yadav**, K. Jahagirdar, M. Chatterjee, D. Dongare, A. Kori, A. Puppala, S. Natarajan, C. Nirmalaraju

BIOT 342. Design of experiment approach to a mechanistic understanding of viral removal in anion exchange chromatography. **S. Lam, Z. Tan, J. Sheng, N. Chennamsetty, A.T. Lewandowski, S. Ghose, W. Qi, M. Lynch, Z. Li**

BIOT 343. Improving mAb purification process using a high capacity anion exchange resin coupled with buffer modulation. **Q. Zhang**, R. Mal, B. Thiyagarajan, N. Deorkar

BIOT 344. Effects of solution conditions on virus filtration of proteins: fouling behavior and clearance of minute virus of mice. **F. Namila**, D. Zhang, S.J. Traylor, T. Nguyen, S. Wickramasinghe, X. Qian

BIOT 345. Effects of substrate morphology on protein binding and elution for responsive hydrophobic interaction chromatography applications. **S. Chen**, S. Wickramasinghe, **X. Qian**

BIOT 346. Continuous, integrated biologics manufacturing. **D.C. Lourenco**, J. Welsh

BIOT 347. Rapid-filtration analysis of protein A and antibody affinity capture in membranes. **A. Nazem**, B. Vu, U. Patil, M. Crum, A. Goyal, R.C. Willson

BIOT 348. Using confocal microscopy to assess the effects of sterilizing grade filter morphology and experimental conditions on the filtration capacity of fluorescently tagged liposome, and in turn optimize filter selection for final drug manufacture. **K.R. Jones**, J. Welsh, N. Jackson, M. Hoare

BIOT 349. Novel applications of chromatofocusing for the purification of monoclonal antibodies. **Y. Liu**, S. Deldari, H. Guo, C.N. Rao, R. Bates, J. West, K. Trejo, R. Swanson, S. Ghose, Z. Li, D.D. Frey

BIOT 350. Effect of ligand structure, arrangement, and density on charge and hydrophobic characteristics of multimodal chromatographic surface. **C. Bilodeau**, E.Y. Lau, S. Garde, S.M. Cramer

BIOT 351. Ultrafiltration behavior of small RNA molecules: RNA size and ionic strength effect. **I. Manzano**, G. Vezeau, H. Salis, A.L. Zydney

BIOT 352. Process development of flow-through mAb polishing process. **J. Zhang**, M. Higson, J. Barna, M.W. Phillips

BIOT 353. Use of HPLC as an enabler of process analytical technology in process chromatography. **A. Tiwari**, N. Kateja, A.S. Rathore

BIOT 354. Precipitation of complex antibody solutions: Influence of contaminant composition and fermentation medium on the precipitation behavior. **S. Grosshans**, S. Suhm, J. Hubbuch



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- BIOT 355.** Visualization technique of protein bind and elute processes on a IEX membrane adsorber. **A. Ley**, D. Stein, J. Hubbuch, V. Thom
- BIOT 356.** Downstream processing and characterization of ranibizumab expressed in *E.coli*. **S.J. Narnaware**, N. Kateja, A. Tiwari, A.S. Rathore
- BIOT 357.** Recovery of valuable compounds from food industry side streams. **M. Moreno Gonzalez**, G. Ferreira, H. Wijngaard, M. Ottens
- BIOT 358.** Custom affinity chromatography for vaccine purification: A new PD paradigm. **R. Skudas**, R. Azevedo
- BIOT 359.** Impact of protein concentration on the size of PEGylated proteins and their adsorption in ion exchange chromatography. **J. Pagano**, Y. Song, H. Feroz, D. Yu, S. Ghose, Z. Li
- BIOT 360.** Purification of polysaccharide-protein conjugate vaccines using ultrafiltration/diafiltration processes. **P. Emami**, S. Motevalian, A.L. Zydney
- BIOT 361.** Modeling and prediction of excipient and pH drifts during ultrafiltration/diafiltration of monoclonal antibody drug substance for high concentration formulations. **V.S. Hebbi**, A. Shukla, S. Roy, A.S. Rathore
- BIOT 362.** Membrane filtration: Understanding particle intrusion through fundamental measurements and computational fluid dynamics. **M. Sorci**, C.C. Woodcock, J.L. Plawsky, G. Belfort
- BIOT 363.** Improve process efficiency in bioprocess streams by prefiltration optimization and bioburden reduction. **S. Liu**
- BIOT 364.** Nuvia IMAC: A metal affinity chromatography media for large-scale manufacturing of recombinant proteins under native and denaturing conditions. **L. Vang**, I. Chen, X. He
- BIOT 365.** Raw material evaluation of a novel chromatography resin. **J. Quang**
- BIOT 366.** Nuvia aPrime 4A: A new hydrophobic anion exchange resin for optimal target protein selectivity and recovery. **I. Chen**, L. Vang, X. He
- BIOT 367.** Accelerated resin lifetime methodology to de-risk resin cycling in commercial processes. **Y. Feng**
- BIOT 368.** Fabrication of a bio-functional porous nano active layer using the self-assembling characteristic of di-block copolymer PS-P4VP and lipase B from *Candida antarctica*. **J. Pazol**, A.S. Vazquez, E. Nicolau
- BIOT 369.** Assessment of automated high throughput chromatography techniques in vaccines process development. **S. Konstantinidis**, S. Wang, M. Wenger
- BIOT 370.** Building robust viral clearance studies: Implementing historical datasets to advance the early phase submission process. A.H. Schwartz, **R. Manzari**, C. Romanowski, D. Cipriano
- BIOT 371.** Robust viral clearance on virus removal filters using a targeted virus spiking approach. **V. Kaloudis**, E.B. Vyas, D. Strauss, P. Nemitz, J. Hughes, M. Burnham, N. Hiroto
- BIOT 372.** Design and implementation of a simple wireless data acquisition and remote control system for downstream process development activities. **M. Homsy**, M.A. Winters, J.G. Joyce, M.P. Watson



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- BIOT 373.** Understanding endotoxin control and protease degradation during scale-up and technology transfer for an HSA-fusion protein. **S. Parimal**, P. Gahr, A. Diener, Y. Feng, C. Gerberich, G. Tran, M.R. McGarrah, H. Ardesbna, A.C. Dumetz, G.J. Terfloth
- BIOT 374.** Development of a small-scale freeze thaw methodology using Blast Freezer 4002. **A. Alva**, A.C. Dumetz, S. Parimal
- BIOT 375.** Efficient purification of a recombinant bacterial DyP-peroxidase with a hydrophobic anion exchange resin. **N. Lončar**, N. Draškovića, N. Božić, M. Fraaije, Z. Vujčić, **P. Khandelwal**
- BIOT 376.** Process economy impact of using a highly alkaline-stable, high-capacity protein A chromatography resin. H. Blom, **M. Bergman**, D. Westman, J. Bolik
- BIOT 377.** Evaluation of sonic wave based separator for clarification of viruses from mammalian cells. **S. Krishnathu**, H. Ko
- BIOT 378.** Particle size evaluation for assessing harvest technologies and filtration performance. **J. Borrajo**
- BIOT 379.** Self-assembled isoporous nanofilters for high throughput viral clearance applications in bioprocessing. **Y. Gu**, C. Crock, J. Maslowski, J. Zhu, M. Siwak, **R. Dorin**
- BIOT 380.** High precision scaling procedure of sterilizing grade filtration. **J. Dippel**, M. Sommer, S. Handt, T. Loewe
- BIOT 381.** Increasing controllability for split intein mediated purification process. **Y. Fan**, D.W. Wood
- BIOT 382.** Mapping purified host cell proteins via high-throughput robotic screens. **L.A. Wong**, P. McKay, J. Franklin
- BIOT 383.** Virus filter optimization and transfer of bispecific antibody. **R. Alsop**, S. Dolan, S. Zhuo, W. Zhou, A. Mak
- BIOT 384.** High-throughput approach to developing and optimizing mixed-mode membrane chromatography for protein purification. **W. McKechnie**, J. Welsh, V. Thom, L. Kupracz, J. Pollard, S. Kandula, N. Tugcu
- BIOT 385.** Structural base analysis of production and purification of Human leukemia Interferon. **Y.S. Ting**
- BIOT 386.** Application of an anion exchange membrane adsorber in late-stage bioprocesses. T. Klimek, **C. Nieder**, **T. Parker**
- BIOT 387.** Challenging antibody purification process development: solving CEX peak splitting phenomenon. **A.M. Senczuk**, Z. Ma, G. Tietz, J. Ma, L. Grillberger
- BIOT 388.** Direct elution of purified monoclonal antibodies from ELP-Z-mAb precipitates. **M. Bhat**, A. Mullerpatan, J. Chen, S.M. Cramer
- BIOT 389.** Endotoxin removal using charged membranes. **A. Phulgirkar**, M. Zhu, J. Ma
- BIOT 390.** Increasing the efficiency of drug product development by automation of the tangential flow filtration system for early formulation screening. **D.L. Le**, C. Ren
- BIOT 391.** Mitigation of monoclonal antibody disulfide bond reduction by copper sulfate: Addition of copper sulfate during cell culture? **S. Ozturk**, J. Yan, R.B. Wollacott, K. Baptista, L. Hock, G. Zhang, S. Nilapwar, J. Sinha



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

BIOT 392. Application of novel multimodal anion-exchange membrane chromatography columns in a two-step mAb purification scheme: Aggregates and HCP removal. **A. Forsyth**, D. Henn, G. Temples, J. Zhou, S.M. Husson

BIOT 393. Robust design space for bispecific manufacturing using controlled fab-arm-exchange (cFAE): Implementing DSD and DOE designs. **R.G. Bertrand**, R. Rao, M. Capaldi, D. Bezila, R. Smith, P.J. Alfonso, W. Cressman, M.J. Sobkow

BIOT 394. Considerations for development of a platform Lentivirus harvest clarification process for cell and gene therapy. **L. Truong**, J. Taylor

BIOT 395. Examining the role of metals and surfaces on VLP cross-linking and the impact on VLP stability. **J. Konietzko**, E. Wen, J.G. Joyce, M. Kosinski

BIOT 396. Cation exchange as a single purification step alternative to reverse phase for conjugated peptides. **L. Rockwell**, H. Bao, I. Ikechukwu, S. Kandula, N. Tugcu

BIOT 397. Investigation of trisulfide variants and mitigation strategies to ensure product quality in an *E.Coli* expressed recombinant protein. **J.C. Castano**, A. Keefe, S. Tummala, J. Prien, J. Baniak, C. Barton, P. Salinas, J. Kaster, Y. Wang

BIOT 398. Using process modeling to quantify the benefits of an integrated mAb flow-through polishing solution. **J. Barna**, M.W. Phillips

BIOT 399. *In silico* evaluation of antibody developability: QSAR models to predict mAb solubility and viscosity. **X. Han**, J. Robinson, S.M. Cramer

BIOT 400. In situ analysis and imaging of aromatic amidine at varying ligand density on cellulose membranes. **A.J. Torres Rosado**, C.J. Ortiz-Hernandez, A. Santiago, I.J. Dmochowski, J. Sotero-Esteva, V. Bansal, **E. Fasoli**

BIOT 401. Effects of ligand density on protein binding capacity of affinity membranes. **E.J. Sanchez**, S. Aponte, E. Fasoli, **V. Bansal**

BIOT 402. Comparison of three tentacular strong cation exchange resins that have the same base bead. **M.T. Stone**, R. Skudas, P. Menstell, H. Graalfs

BIOT 403. Counterflow-centrifugation and depth filtration optimization: Systematic approach to develop CHO harvest process. **A. Thiefes**, **V. Thom**, G. Bremer, R. Petersen, E. Lam, H. Kaligotla

BIOT 404. Withdrawn

BIOT 405. Manufacturing strategies for Biosimilars: A case of continuous capture. **S.R. Hadpe**

BIOT 406. Enabling robust CHT purification: Implementation of a raw material specification for control of pyrophosphate impurity. **I. Stear**, K. Valente, E. Baragar

BIOT 407. Microscale chromatography toolkits for rapid screening and purification of therapeutic proteins. **E. Gutierrez**, A. Andar, S. Deldari, D. Burgenson, M. Al-Adhami, S. Borhani, C. Gurrakonda, L.M. Tolosa, Y. Kostov, D.D. Frey, G. Rao

BIOT 408. High-capacity multimodal anion-exchange membranes for purification of biologics. **J. Osofa**, A. Forsyth, J. Zhou, S.M. Husson



TECHNICAL PROGRAM

BIOT 409. New protein A membranes for the rapid isolation and purification of monoclonal antibodies. **G. Temples**, J. Zhou, D. Henn, A. Forsyth, S.M. Husson

BIOT 410. Evaluation of the donnan effect and a mitigation strategy in UFDF process development. **D. De Ghosh**, J. Woo, B. Kluck, C. Emery

BIOT 411. Development of an improved downstream process for enhanced monoclonal antibody purification. **J. Fura**, L. Fortin, J. Sumoski, S. McLinden, C. Cheah, J. Oh, Q. Zhang, R. Mal, B. Thiyagarajan, N. Deorkar

BIOT 412. Fc (igg1) binding to multimodal cation exchange surfaces: Effect of salt on preferred binding region. **R.B. Gudhka**, C. Bilodeau, S.A. McCallum, M. McCoy, D.J. Roush, S.M. Cramer

BIOT 413. Investigation of the adsorptive properties of depth filters in bioprocessing. **N. Nejatishahidein**, E. Espah Borujeni, D.J. Roush, A.L. Zydney

BIOT 414. Paper-based biosensors for glycan analysis. **F. Enam**, A. Alvarez-Acosta, T. Mansell

Section A

Orange County Convention Center
West Hall E2

End-to-End Biomanufacturing

Poster Session

J. Bender, J. C. Love, V. Roy, *Organizers*
K. Solomon, I. R. Wheeldon, *Presiding*

6:00 - 8:00

BIOT 415. Small scale end-to-end mAb platform with a continuous, integrated and compact process. **J. Gomis Fons**, N. Andersson, B. Nilsson, H. Schwarz, V. Chotteau

BIOT 416. Implementation of end-to-end disposable single use systems for rapid fermentation process design to GMP manufacturing. **E.M. Nordwald**, E. Raubach, V. Yu, A. Ridl, R. Todd, A. Pilling

BIOT 417. High throughput process development toolbox for rapid and reliable development and implementation of intensified processes for the flexible facilities of the future. **H. Kaligotla**, G. Zijlstra, T. Erdenberger, M. Monge, J. Matuszczyk

BIOT 418. Start with the end in sight: A holistic bioprocessing strategy for cell line selection: GSKs onestream approach. **W. Lewis**

BIOT 419. Use of single-use systems (SUS) to mitigate risks and enable flexibility in continuous bio-manufacturing facilities: Case studies in raw material handling to sampling. **P. Vengsarkar**, J. Oh, C. Cheah, T. Lee, N. Deorkar, T. Korwan

BIOT 420. Withdrawn



TECHNICAL PROGRAM

BIOT 421. Process-related impurity assessments in downstream development: A streamlined life-cycle approach. **A. Pearson**, M. Dempster, T. Hart, G. Whelan, R. Luo

BIOT 422. Implementing process analytical technology for production of recombinant proteins in *E.coli* using advanced controller scheme. **J. Kumar**, P. Dalal, J. Gomes, A.S. Rathore

BIOT 423. Implementing advanced control strategies to improve the bioprocess applications. **P. Priyanka**, S. Roy, V.R. Chopda, J. Gomes, A.S. Rathore

BIOT 424. Excessive protein aggregation in low pH viral inactivation/neutralization and mitigation strategy: A case study. **W. Jin**, Z. Xing, X. Xu, S. Ghose

BIOT 425. Continuous refolding of a biotech therapeutic in a novel coiled flow inverter reactor. **N. Kateja**, A.S. Rathore, H. Agarwal

Section A

Orange County Convention Center
West Hall E2

General Biochemical Technology

Poster Session

K. Solomon, I. R. Wheeldon, *Organizers, Presiding*

6:00 - 8:00

BIOT 426. Monitoring and controlling critical components in cell culture process using PAT Tool, Raman spectroscopy. **C. Rafferty**, K.M. Balss, **C. O'Mahony Hartnett**, F. Madden, B. McCarthy, E.J. Schaefer, K.A. Barnhouse, R. Rea, J. O'Mahony, R. Shivappa

BIOT 427. Transition analysis: Real-time column performance monitoring in commercial scale chromatography. **C. O'Mahony Hartnett**, C. Kiely, R. Hayes, B. McCarthy, E.J. Schaefer, P.R. Randolph

BIOT 428. Mapping the ultramorphological changes of SPION-induced cell death in Glioblastoma Multiforme. **M.A. Tovar**

BIOT 429. Eco-friendly extraction of sinapic acid from agro-industrial residue toward sustainable bio-based anti-UV and antioxidants. **A.L. Flourat**, E.C. Achinivu, G. Willig, F. Allais

BIOT 430. Withdrawn

BIOT 431. Process development of a precipitation-filtration unit for recombinant protein capture step II: Continuous counter-current washing and filtration. **Z. Li**, Q. Gu, J.L. Coffman, T.M. Przybycien, A.L. Zydney

BIOT 432. Cellulose-based biopolymers for controlled drug delivery: a mechanistic investigation. **K.L. O'Donnell**, G. Oporto, N. Comolli



TECHNICAL PROGRAM

- BIOT 433.** Process development of a precipitation-filtration unit for recombinant protein capture step. I: Characterizing protein solubility and precipitate morphology. **Q. Gu**, Z. Li, T.M. Przybycien, J.L. Coffman, A.L. Zydney
- BIOT 434.** Single use fermentation process design. **S. Fitzgibbon**
- BIOT 435.** Texture, particle, and rheometric analysis of precipitated polysaccharide. **C. Lowry**, C.J. Farrell, N. McFarlane, E. Wen
- BIOT 436.** Production of L-asparaginase free of glutaminase and urease: A kinetic model approach to the optimized production of the enzyme. **A. Ashok**, K. Doriya, S. Devarai
- BIOT 437.** Developing molecular tools for membrane protein expression in *Saccharomyces cerevisiae*. **R. Karki**, M.D. Rieth
- BIOT 438.** Expanding the substrate scope of serine palmitoyltransferase utilizing mutagenesis and high-throughput screening. **H. Choe**, M. Cha, J.D. Stewart
- BIOT 439.** Research of the detection for the ampicillin resistance gene by denaturation bubble-based strand exchange amplification technology. **H. Wang**, C. Ma
- BIOT 440.** Investigating the enantiocomplementary nature of old yellow enzymes utilizing non-conical amino acid mutagenesis. **R.R. Watkins**, S. Lenka, M.P. Buteler, J.D. Stewart
- BIOT 441.** High throughput development of a difficult to express protein. **P. Jones**
- BIOT 442.** Primary recovery & harvest processes for non-mAb recombinant proteins. **D. Chang**, N. Bubna, C. Philips, J. Hamlin, S. Mostafa
- BIOT 443.** Dual substrate/product colorimetric method for measuring the relative strength of inhibitors of bacterial choline kinase isoforms. **T. Zimmerman**, S.A. Ibrahim
- BIOT 444.** Development of a novel assay for Refsum disease utilizing phytanic acid isotopologues and liquid chromatography-high resolution mass spectrometry. **J. Smith**, D. von Trentini, A. Schwartz, N. Snyder, R. Broadrup
- BIOT 445.** Fluorescent biomarker: Detection of cysteine and cytosine in aqueous medium using thiophene based organic nanoparticles decorated with Au NPs. **C.A. Huerta-Aguilar**, P. Thangarasu
- BIOT 446.** Effect of gases on the expression of recombinant erythropoietin using CHO cell-free coupled *in vitro* transcription and translation system. A. Rao, **S. Borhani**, M. Tolosa, G. Rao, **C. Gurramkonda**
- BIOT 447.** Development of chimeric two-component system based on *paracoccus denitrificans* FlhS to sense methanol in recombinant *escherichia coli*. **S. Hong**
- BIOT 448.** Efficient gamma-aminobutyric acid production through co-localization of neurospora crassa OR74A glutamate decarboxylase with Escherichia coli GABA transporter using synthetic scaffold. **S. Hong**
- BIOT 449.** Desulfatation of glucosinolates using glucosinolate sulfatase from *xylostella plutella*. **T. Nguyen**, K. Hall, F. Allais, J.D. Stewart



TECHNICAL PROGRAM

BIOT 450. Using protein design to engineer a scaffold for regio-selective C-H functionalization. **M. Basilaia, T. Maisuradze, C. Rodriguez, A. Ramiez**, J.L. Gustafson, J.J. Love

BIOT 451. Evaluation of the influence of agitation and aeration on the production of green fluorescent protein (GFP) using recombinant *Escherichia coli* in conventional bioreactor. **A.C. Jesuino**, A.A. Sousa, M. Scontri, J.B. Pereira, M.O. Cerri

Section A

Orange County Convention Center
West Hall E2

Upstream Processes

Poster Session

P. Peralta Yahya, A. Russo, C. T. Trinh, *Organizers*
K. Solomon, I. R. Wheeldon, *Presiding*

6:00 - 8:00

BIOT 452. RAPS: Rapid annotation of photosynthetic systems. **A. Metcalf**, A. Nagygyor, N. Boyle

BIOT 453. Investigating the barriers to high ethanol titers in *Clostridium thermocellum*. **T. Korosh**, D. Amador-Noguez, D. Olson, L. Tian, S. Hon, L.R. Lynd

BIOT 454. *In vitro* – *in vivo* toxicity correlations via high-throughput three-dimensional primary hepatocyte culture. **D. Bruckner**, J.J. Connerney, J.S. Dordick

BIOT 455. 3d printed bioreactors: Enabling rapid proces optimization. **G.E. Barringer**, A. D'Ambruoso, T. Walvoort

BIOT 456. Transcriptomics study of recombinant *Escherichia coli* during recombinant protein production in micro-aerobic and aerobic condition at bio-reactor level. **A.S. Chauhan**, K. Pandi, A.S. Rathore

BIOT 457. *In vivo* thermodynamic analysis of *Zymomonas mobilis* metabolism using combined ²H and ¹³C metabolic flux analysis and metabolomics for renewable biofuel production. **P.A. Adamczyk**, T.B. Jacobson, J.L. Reed, D. Amador-Noguez

BIOT 458. Nanoscale optical sensors to characterize hydrolytic enzymes for health, agriculture, and industrial biotechnology. **N. Kallmyer**, R. Khor, M. Abdennadher, N. Roby, S. Agarwal, E. Peterson, N. Reuel

BIOT 459. Dynamic phosphoproteomic and transcriptomic study provides insights into cell wall integrity signaling network in *Aspergillus nidulans*. **C. Chelius**, W. Huso, A. Doan, S. Reese, R. Purohit, K. Lawson, R. Liliane, R. Srivastava, H. Steven, M. Marten

BIOT 460. Quantification of pyocanin-promoted *Pseudomonas aeruginosa* persister cells and the analysis of their growth in a microfluidic device. **A. Sutlief**, M. Perez, A. Fletcher, C. Marcelino, S. Sikich, A.E. Holmes

BIOT 461. Engineering bacterial systems to probe miRNAs secreted from mammalian cells. **C. Huang**, H. Wu, Y. Kung, Y. Chen



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- BIOT 462.** CHO cell-free coupled *in vitro* transcription and translation system for the production recombinant mAbs. **S. Borhani**, A. Rao, M. Mysore, B. Punshon-Smith, E. Gutierrez, A. Andar, R. Adiga, M. Tolosa, Y. Kostov, L.M. Tolosa, D.D. Frey, G. Rao, **C. Gurramkonda**
- BIOT 463.** Debottlenecking manufacturing capacity using high seed density production processes. **R. Ottman**, Y. Gowtham, S. Mostafa
- BIOT 464.** Microaerobic fermentation alters lactose metabolism enhancing recombinant proteins in *Escherichia coli*. **K. Pandi**, A.S. Chauhan, A.S. Rathore
- BIOT 465.** Novel strategy for developing cost-effective biosimilar in the microbial system. **P. Priyanka**, S. Singha, R. Patil, A.S. Rathore
- BIOT 466.** Effective bioreactor pH control using only sparging gases. **X. Zhang**, L. Hoshan, R. Jiang, J. Moroney, A. Bui, T. Hang, S. Xu
- BIOT 467.** Improvement of mammalian bioreactor simulation through variation in specific oxygen uptake rates. **J.D. Cohen**
- BIOT 468.** Upstream strategies to address process & quality challenges associated with molecules of new modality. **R. Pangule**, J. Moroney, P. Liu, E. Espah Borujeni, X. Li, J. Yang, S. Rios
- BIOT 469.** Metabolic cross-feeding interactions between adipocytes and hepatocytes in an engineered mammalian co-culture system. **E.H. Oates**, M.R. Antoniewicz
- BIOT 470.** Withdrawn
- BIOT 471.** Intensified fed-batch vs. fed-batch: Is high-density cell culture necessarily better? **K.M. Blocker**, H. Waoti, J. Rivera
- BIOT 472.** Compatibility characterization of a multi-use sterile to sterile connector with a mammalian cell culture perfusion process. **A. Wood**, A. Fournier, A. Dupont, K. Fouhy, M.A. Cunningham
- BIOT 473.** Process characterization strategy for implementing a high-density *n*-1 seed bioreactor step supported by ATF into a legacy CHO cell culture process. **D. Harrison**
- BIOT 474.** Engineering cooperation in nitrogen self-sufficient cocultures of *Azotobacter vinelandii* and *Escherichia coli*. **C. Diaz**, M.R. Antoniewicz
- BIOT 475.** High-throughput mini-bioreactor platform for optimizing production of anti-malarial precursor drug from an engineered yeast *Yarrowia lipolytica*. **V.R. Chopda**, S. Borhani, B. Folio, M. Tolosa, C. Gurramkonda, Y. Kostov, X. Ge, R. Adiga, L.M. Tolosa, G. Rao
- BIOT 476.** Optical control of exopolysaccharide production in *Sinorhizobium meliloti* in a synthetic soil microsystem. A. Pirhanov, Y. Guo, C. Bridges, R. Goodwin, J. Furrer, D. Gage, L.M. Shor, **Y. Cho**
- BIOT 477.** Novel stable isotope approaches to identify flux bottlenecks in photosynthetic microbes. **J. Young**, Y. Cheah, Y. Xu, C. Johnson



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- BIOT 478.** Genome-scale metabolic model of *Chromochloris*, an emerging model organism for sustainable fuel production. N. Boyle, **A.J. Metcalf**, A. Nagygyor, W. Prentice, S. Ramsey
- BIOT 479.** Deconvolution of fatty acid mass spectral patterns to determine the acetyl-CoA mass isotopomer distribution for ^{13}C metabolic flux analysis. **D. Lugar**, N. Boruah, A. Quinn, G. Sriram
- BIOT 480.** Bacterial production of ^{13}C -labeled cellulose for ^{13}C metabolic flux analysis of cellulose degradation. **M.R. Antoniewicz**
- BIOT 481.** Investigating nutrient cycling mechanisms in a filamentous cyanobacterium using advanced multi-scale multi-paradigm metabolic models. **J. Gardner**, B. Hodge, **N. Boyle**
- BIOT 482.** Implementing upstream platform upgrades across Janssen BioTherapeutics Development. **A.T. Levy**, A. Weith, J.V. Price, S. Berges, M. Weiss, J. Simons, C. Canova, S. Savage, J. Ruben, R. Shivappa
- BIOT 483.** 3D-printed human villi-on-a-chip with capillary system for drug screening and disease interrogation. **C. Chen**, W. Shang, G.F. Payne, R. Sochol, W.E. Bentley
- BIOT 484.** Impact of trace metal impurities from chemically defined media on process performance and product quality of an antibody produced in a CHO cell culture process.. **P.A. Laitala**
- BIOT 485.** Production bioreactor pH setpoint controls monoclonal antibody charged species distribution and aggregation characteristics. **B.F. Wolf**, L. Sager, X. Lu, J. Olsen, P. Huang
- BIOT 486.** Universal reference platform development for Chinese hamster ovary cell culture. V. Dhara, H. Naik, H. Dahodwala, J. Baik, D. Nmagu, C. Morris, D. Odenwelder, **M.J. Betenbaugh**, K.H. Lee, S. Yoon, S.W. Harcum, J.L. Coffman
- BIOT 487.** Enhance bioreactor control: Near-infrared spectroscopy for upstream applications. **H. Ohrvik**, L. Blomqvist, B. Immerdahl, R. Pettersson, M. Antti
- BIOT 488.** Withdrawn
- BIOT 489.** Improvements in isopentenol production using the IPP-bypass mevalonate pathway by fed batch fermentation. D. Mendez-Perez, A. Kang, **T. Lee**
- BIOT 490.** Engineering sulfate donor accumulation in *Escherichia coli*: Improved *in vitro* chondroitin sulfate biotransformation and a step towards *in vivo* microbial production. **A. Badri**, A. Williams, R.J. Linhardt, M. Koffas
- BIOT 491.** Bioprocess control: Deeper insights into LacI autoregulation and how to exploit it. **A. Schuller**, M. Cserjan, J. Jarmer, M. Wagenknecht, D. Reinisch, R. Grabherr, G. Striedner
- BIOT 492.** Production of antibody fragments with plasmid-based and genome integrated T7 *E. coli* expression systems – evaluation of systems performance in microtiter fed-batch like cultivations. **S. Vazulka**, M. Fink, J. Jarmer, M. Cserjan, G. Striedner
- BIOT 493.** Sustainable synthesis of natural 2-phenylethanol from biobased *L*-phenylalanine *via* five-steps artificial cascade biotransformation. **B. Lukito**, S. Wu, H. Saw, Z. Li



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- BIOT 494.** Utilization of probiotic *Bacillus coagulans* in the production of fructooligosaccharides (FOS): reduction of the glycemic index and formation of the endospores. R. Fan, **P.M. Czermak**
- BIOT 495.** Use an autosampler to improve efficiency in developing Raman-based calibration models for mammalian cell cultures. **R. Jiang**
- BIOT 496.** Developing chemoselective probes to label secondary metabolites in metabolome. **R. Wu**, W. Chang, T.A. Wang
- BIOT 497.** Engineering *Escherichia coli* for production of poly(3-hydroxyoctanoic acid) from glycerol. **K. Xu**, N. Hernandez Lozada, B. Pflieger
- BIOT 498.** Development of an alternating tangential flow based perfusion process for the production of therapeutic proteins with non-natural amino acids. **J. Reier**, M. Marelli, G. Roy
- BIOT 499.** Development of a high throughput screen to engineering a long chain acyl-CoA thioesterase for medium chain methyl ketone production in *Escherichia coli*. **T. Simmons**, M. Incha, N. Hernandez Lozada, C. Breckner, B. Pflieger
- BIOT 500.** Genetic engineering of *Pseudomonas putida* for the heterologous production of polyketides and nonribosomal peptides. **T.B. Cook**, B. Pflieger
- BIOT 501.** Development of Gibco™ Qp-CHO™ Medium through multi-omic analysis. **P. Gulde**, J. Smith, M. Reynolds, A. Pierce, A. Campbell
- BIOT 502.** Increased CHO cell lysis in intensified high-density perfusion processes with alternating tangential filtration (ATF) elucidated by a lactate dehydrogenase (LDH) activity assay. **A. Samadzoda**, V. Gnanavel, R. Chelikani
- BIOT 503.** Thwarting RNA decay in *Escherichia coli* and cyanobacteria: Better RNAs or a better understanding of the process? **M. Engstrom**, G. Gordon, J. Cameron, B. Pflieger
- BIOT 504.** Microbioreactors for high-cell density CHO perfusion scale-down and personalized T-cell manufacturing. K. Lee, **H. Lee**
- BIOT 505.** Electrochemically-tunable CRISPRa system through OxyR promoter in *Escherichia coli*. **S.P. Wang**, N. Bhokisham, E. VanArsdale, W.E. Bentley
- BIOT 506.** Applications of metabolic models during large molecule development life cycle. **J.V. Price**, J. Bucher, Y. Luo, K.A. Barnhouse, P. Hu, J. Cunningham, E.J. Schaefer, K.H. Lee, B. Ogunnaike, R. Shivappa
- BIOT 507.** Zinc enhances β -glucuronidase secretion from CHO cells by suppressing apoptosis. **R. Graham**, S.A. Ketcham, B. Ghosh, A. Mohammad, P.J. Faustino, M. Ashraf, C.n. Madhavarao
- BIOT 508.** Evaluation of raman spectroscopy as a tool for PAT in perfusion processes. **A. Nazempour**, D. Rank
- BIOT 509.** Scalability of novel geometry single-use bioreactors. **I. Wang**, S. Chilvers, J. Welsh, R. Gantier
- BIOT 510.** Evaluation of *Vibrio natriegens* as a suitable metabolic engineering platform for high-value chemical production. **J. Brinton**, J.A. Jones



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

BIOT 511. Clinical and commercial-launch process scalability in a single-use bioreactor platform. **N. Bubna**, J. Kim, C. Phillips, D. Chang, C. Norman, S. Mostafa

BIOT 512. Application of voronoi tessellated neural networks (VTNN) for bioprocess control. **P. Priyanka**, S. Roy, J. Gomes, A.S. Rathore

BIOT 513. Exploring bioreactor heterogeneities with wireless *in situ* 'smart marble' platform. **J.M. Stine**, L. Beardslee, R.M. Sathyam, **W.E. Bentley**, R. Ghodssi

BIOT 514. Minimally-invasive, continuous glucose monitoring approach. **V. Watson**, G. Rao, L.M. Tolosa

BIOT 515. Design of an electronic gene-expression control scheme with the capability to store and direct information flow. **E. VanArsdale**, N. Bhokisham, E. Kim, G.F. Payne, W.E. Bentley

BIOT 516. Tuning the dynamic range of 1-butanol-responsive transcription factor-based biosensor in *Escherichia coli*. **N.M. Kim**, N.R. Sandoval

BIOT 517. Improving vaccine production with a serum-free medium for MRC-5 cells. **A. Hachmann**, M. Pajak, N. DiNardo, A. Campbell

Polymer Bioconjugates for a Changing World

Posters

Sponsored by POLY, Cosponsored by BIOT

WEDNESDAY MORNING

Section A

Rosen Centre Hotel
Salon 10

Emerging Frontiers in BIOT

Beyond Earth: BIOT's Role in Space

Cosponsored by COMSCI
C. A. Eckert, D. J. Roush, *Organizers*
M. A. Blenner, *Organizer, Presiding*
M. Roberts, *Presiding*

8:30 BIOT 518. Merck microgravity crystallization experiments. **P. Reichert**

8:50 BIOT 519. Microfluidics and/or microgravity for protein crystallization. **S.L. Perry**

9:10 BIOT 520. Changes in vascular cell function under conditions of microgravity. M. Scotti, **J. Allen**



TECHNICAL PROGRAM

9:30 BIOT 521. Human emulation on the international space station: A platform for studying human biology in microgravity. **C. Hinojosa**

9:50 Intermission.

10:10 BIOT 522. Keynote: center for the utilization of biological engineering in space: Towards efficient biomanufacturing for deep space missions. **A.P. Arkin**

10:50 BIOT 523. Evaluating heterogeneity of protein expression from germinated *Bacillus subtilis* spores for shelf-stable cell factories in space. **D. Tamiev**

11:10 BIOT 524. Roadmap for the use of biotechnology in space exploration. **M.A. Blenner**

Section B

Rosen Centre Hotel
Grand B

Downstream Processing

Continuous & Integrated Downstream Bioprocessing

S. Chollangi, M. Gruvegard, C. Heldt, *Organizers*
T. Müller-Späth, L. W. Pampel, J. P. Pieracci, V. Warikoo, *Presiding*

8:30 BIOT 525. Gap analysis on downstream integrated processing. J.L. Coffman, **R. Orozco**

8:50 BIOT 526. Complexity of process development for continuous affinity chromatography of biopharmaceuticals. **A. Reeder**

9:10 BIOT 527. Gamma irradiated chromatography resins for functionally closed downstream processing. **C. Varner**, R. Patil, K. Brower

9:30 BIOT 528. At-scale demonstration of an integrated continuous multi-column chromatography process. **E. Gefroh**, T. Wanek, B. Barrios, L. Horton, R. Piper, M. Vandiver, M. Brower, N. Pinto

9:50 Intermission.

10:10 BIOT 529. Meeting cost and facility utilization targets through single-batch use of convective membranes for chromatographic capture steps. **V. Thom**, P. Adametz, A. Bluma, G. Zijlstra, H. Kaligotla, T. Erdenberger

10:30 BIOT 530. Small scale integrated downstream process with online analytics for realtime release. **B. Nilsson**, S. Tallvod, J. Gomis Fons, N. Andersson, L. Berghard

10:50 BIOT 531. Design of a periodic counter-current chromatography process for efficient oncolytic virus purification. **R. Silva**, J. Mendes, M. Berg, L. Mathiasson, M.J. Carrondo, C. Peixoto, P.M. Marques

11:10 BIOT 532. Virus clearance in continuous multicolumn chromatography. K. Boenning, **M. Pagkaliwangan**, M. Chiang, S. Lute, K. Mehta, D. Kole, G. Bolton, K.A. Brorson, M. Schofield



TECHNICAL PROGRAM

Section C

Rosen Centre Hotel
Salon 4

Upstream Processes

Mammalian: Media & Metabolism

P. Peralta Yahya, A. Russo, C. T. Trinh, *Organizers*
K. Haynes, H. Lin, *Presiding*

8:30 BIOT 533. Using OPLS regression with stoichiometric balances to optimize amino acid concentrations in chemically defined CHO cell culture medium. **T. Salim**, G. Chauhan, N. Templeton, W. Ling

8:50 BIOT 534. Enhancing chondrogenesis of adipose derived stem cells through temporal supplementation of dexamethasone, TGF- β 3, ascorbic acid and their combinations. **H. Abusharkh**, A. Mallah, M. Amr, A. Gozen, J. Mendenhall, N. Abu-Lail, B. Van Wie, V. Idone

9:10 BIOT 535. Evaluation of CHO cells metabolically engineered towards reduced biosynthesis and accumulation of growth inhibitory catabolic byproducts of branched chain amino acids in fed-batch cultures. **C. Harrington**, P. Geoffroy, J. Mitchell, L. Zhang, G. Hiller, B.C. Mulukutla

9:30 BIOT 536. Improved harvest robustness: Enabling process scale-up through media engineering and redox control. **S. Loebrich**, C. Williams, S.A. Kitchener, T.K. Ryll

9:50 Intermission.

10:10 BIOT 537. Utilizing ^{13}C metabolic flux analysis to quantify glucose and lactate dependent metabolic shifts in induced pluripotent stem cells. **D. Odenwelder**, S.W. Harcum

10:30 BIOT 538. Automated and high throughput ICP-MS sample prep platform to study the effect of trace metals in upstream manufacturing of therapeutic proteins. **A. Mohammad**, R. Graham, S.A. Ketcham, C.n. Madhavarao, C. Agarabi, P.J. Faustino

10:50 BIOT 539. Role of redox stress in modulating CQAs of recombinant antibody expressed in mammalian cell culture processes. **R. Kaur**

11:10 BIOT 540. Elucidating amino acid metabolism in CHO cells. **B. McConnell**, J. Gonzalez, M.R. Antoniewicz

Section D

Rosen Centre Hotel
Salon 5

Biomolecular Technologies

Engineering Cellular Interactions



TECHNICAL PROGRAM

B. Hackel, B. F. Marques, *Organizers*
J. Rhoden, L. Stern, *Presiding*

8:30 BIOT 541. Intra-lymph node delivery of tolerogenic microparticles reverses disease and prevents relapse in a relapsing-remitting model of multiple sclerosis. **E.A. Gosselin**, C. Jewell

8:50 BIOT 542. Engineering cellular-based selections for translatable ligand discovery. **P.S. Lown**, B. Hackel

9:10 BIOT 543. Chemical testing in a two-organ human-on-a-chip NAFLD model. **V. Slaughter**, R. Boone, D. Malik, J. Rumsey, C. Long, J.J. Hickman

9:30 BIOT 544. Engineered bispecific antibodies for targeted inhibition of cancer metastasis. **W. Wang**, J.B. Spangler

9:50 Intermission.

10:10 BIOT 545. Liposome-coated iron oxide nanoparticles (LIONS): A dynamic approach for the investigation of influenza fusion mechanisms. **T. Banerjee**, V. Jain, S. Santra

10:30 BIOT 546. Application of kinetic reaction modeling for process development of antibody-drug conjugates. **S. Andris**, J. Seidel, M. Wendeler, J. Hubbuch

10:50 BIOT 547. Single cell PK/PD of antibody-drug conjugates: Computational predictions and experimental validation to improve *in vivo* efficacy of targeted therapeutics. **E. Khera**, C. Cilliers, I. Nessler, G. Thurber

11:10 BIOT 548. Regulation of trafficking and transport of antibodies across the human blood-brain barrier. **J. Ruano-Salguero**, K.H. Lee

Section E

Rosen Centre Hotel
Salon 6

Biomedical Technologies

New Strategies for the Delivery & Targeting of Therapeutics

G. Thurber, M. Westoby, *Organizers*
A. C. Brown, A. Noyes, X. Qian, *Presiding*

8:30 BIOT 549. Synthetic molecular evolution of hybrid cell penetrating peptides. W. Kauffman, S. Guha, **W.C. Wimley**

8:50 BIOT 550. Quantitative biodistribution of multimodal macrophage-targeted probes by optical and nuclear imaging. **H. Deng**, C. Konopka, T. Liu, K. Swanson, L. Dobrucki, A. Smith

9:10 BIOT 551. Guided design of sustained release biopharmaceutical systems through model predictions. **S. Koshari**, D. Chang, I. Zarraga, K. Rajagopal, N.J. Wagner, A.M. Lenhoff



TECHNICAL PROGRAM

9:30 BIOT 552. Facile strategy enabling both high loading and high release amounts of the water-insoluble drug clofazimine using mesoporous silica nanoparticles. **W. Chen**, C. Cheng, B. Lee, D.L. Clemens, W. Huang, M.A. Horwitz, J.I. Zink

9:50 Intermission.

10:10 BIOT 553. Photodegradable hydrogels for protein delivery: Tuning degradation rates through cleavage bond chemistry. **P. LeValley**, A.M. Kloxin

10:30 BIOT 554. Cationic microemulsion-based soft contact lenses for the controlled delivery of poorly water-soluble drugs. **C. Torres**

10:50 BIOT 555. Evaluation of drug-to-excipient ratio effects on the drug release profile in drug coated balloons. M. Tran, S. Woolford, S.T. Yoda, B. Oktem, A. Nguyenpho, M.K. McDermott, **S.I. Wickramasekara**

11:10 BIOT 556. Development of a topical prodrug to treat burn scar contracture. **K. Murray**, S. MacNeil, S. Spain

Polymer Bioconjugates for a Changing World

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WEDNESDAY AFTERNOON

Section A

Rosen Centre Hotel
Salon 10

Spotlights on Research Areas

Downstream Processing

M. Gruvegard, *Organizer*
S. Chollangi, C. Heldt, *Organizers, Presiding*
M. Stork, *Presiding*

2:00 BIOT 557. Keynote: Take that, batches! **J.L. Coffman**, R. Orozco, J. Salm, D. Ogawa, R. Fahrner, J. Vogel

2:40 Rapid Fire Presentations.

3:20 Intermission.

3:40 Discussion.

4:00 BIOT 558. Michaels Award: Membranes in bioprocessing: From Alan Michaels to the present. **A.L. Zydney**



TECHNICAL PROGRAM

Section B

Rosen Centre Hotel
Grand B

End-to-End Biomanufacturing

Automated Technologies & High-Throughput Systems in Biologics Production

J. Bender, J. C. Love, V. Roy, *Organizers*
E. M. Goodrich, S. W. Harcum, *Presiding*

2:00 BIOT 559. Cell line development strategies using a high throughput automated platform. **A. Kumar**, X. Tang

2:20 BIOT 560. Reduced scale model qualification of 5L bioreactor & Ambr250 using multivariant visualization & Bayesian inferential methods. **C. Canova**, D. Banton, K. Clark, S. Naguib, E.J. Schaefer

2:40 BIOT 561. Development of a high throughput scale-down model to mitigate shear sensitivity risk in cell culture process scale-up. **B. Zedalis**, D. Tong, B.P. Doyle, Y. Bai

3:00 BIOT 562. Development of a high-throughput purification method to assess the impact of bioreactor conditions on rAAV empty/full capsid ratio. T. Townsend, S. Nadir, V. Wingate, S. Khan, E. Caraballo-Pagan, D. Koback, K. Olson, J. Schoborg, T. Wagner, A. Whalley, **M. Roach**, W. Kish, E. Hwang, T. Zekovic, S. Bhardwaj, J. Lightholder, J. Pavlicek, C. Chu, A. Berrill

3:20 Intermission.

3:40 BIOT 563. High-throughput and automated process development for accelerated biotherapeutic manufacturing. **D.M. Ryan**

4:00 BIOT 564. In-silico aided strategy for efficient and rapid design of integrated purification processes. **N. Vecchiarello**, S.M. Cramer

4:20 BIOT 565. System for making real-time loading decisions for protein A chromatography in continuous manufacturing. **G. Thakur**, A.S. Rathore

4:40 BIOT 566. Automated, high-throughput, and computational methods for construction and analysis of protein phase diagrams. **M. Klijn**, J. Hubbuch

Section C

Rosen Centre Hotel
Salon 4

Upstream Processes

Mammalian: Advances in Perfusion & Continuous Processing



TECHNICAL PROGRAM

P. Peralta Yahya, A. Russo, C. T. Trinh, *Organizers*
A. Castan, Y. Cho, *Presiding*

2:00 BIOT 567. DoE-supported perfusion medium optimization for maximum cell densities and efficient media consumption. **P. Mayrhofer**, L. Damjanovic, A. Castan, R. Kunert

2:20 BIOT 568. Withdrawn

2:40 BIOT 569. Multivariate methods for troubleshooting continuous bioreactor process. **M. Khurshid**, N. Chavez, E. Franco, J. Huang

3:00 BIOT 570. Assessment of ambr® 250 perfusion bioreactor system as a model for high-throughput perfusion process development. **M. Manahan**, W.N. Napoli, J. Huang

3:20 Intermission.

3:40 BIOT 571. Developing a continuous upstream platform: Ensuring process and product consistency by maximizing ATF sieving efficiency. **M. Choi**, C. Kwiatkowski, K. Wiltberger

4:00 BIOT 572. Media and process development for high cell density cryopreservation and N-1 perfusion. **M. Bausch**, C. Ströder, M. Feigenspan, D. Matheis, L. Ayala Solares, C. Schultheiss, J. Sieck

4:20 BIOT 573. Implementation of a manufacturing scale, fully single use perfusion process leveraging media concentrates. **W.N. Napoli**, M. Brower, N. Pinto, N. Tugcu, E. Gefroh, R. Piper, M. Vandiver, B. McCoy, C. Cable, A. Leonard, B. Dell

4:40 BIOT 574. Challenges with TFF N-1 Perfusion in large scale manufacturing operations. **A. Vaca**

Section D

Rosen Centre Hotel
Salon 5

Biomolecular Technologies

Engineering & Characterizing Protein Developability

B. Hackel, B. F. Marques, *Organizers*
M. E. Krause, J. W. Schneider, *Presiding*

2:00 BIOT 575. Screening yeast display libraries against magnetized yeast cell targets enables efficient isolation of membrane protein binders. **K. Bacon**, M. Burroughs, A. Blain, S. Menegatti, B. Rao

2:20 BIOT 576. Yeast as a model to study biased signaling of GPCRs. **A.R. Jain**, A.S. Robinson

2:40 BIOT 577. High-throughput computational pipeline for 3-D structure preparation and in silico protein surface property screening: A case study on HBcAg VLP surface charge. **P. Vormittag**, M. Klijn, N. Bluthardt, T. Klamp, J. Hubbuch



TECHNICAL PROGRAM

3:00 BIOT 578. Engineering quality and manufacturability of a trivalent protein subunit vaccine. **N. Dalvie**, J. Brady, M. Tracey, D. Kristensen, K.R. Love, J.C. Love

3:20 Intermission.

3:40 BIOT 579. Improved methods for high-throughput screening of antibody colloidal interactions. **C.G. Starr**, G. Pornnoppadol, J. Kingsbury, Y. Gokarn, P.M. Tessier

4:00 BIOT 580. Cell-based selections aid yeast-display discovery of genuine cell-binding ligands: Targeting oncology vascular biomarker CD276. **L. Stern**, P.S. Lown, A. Kobe, L. Abou-Elkacem, R. Bam, J. Willmann, B. Hackel

4:20 BIOT 581. Characterization of the activity of glucuronyl C5-epimerase. **D. Vaidyanathan**, X. Ke, R.J. Linhardt, J.S. Dordick

4:40 BIOT 582. Co-ordinated enzyme catalysis: Designing a cell-free system. **M. Wong**, J. Zha, M. Sorci, M. Gupta, K. Jawed, M. Belfort, M. Koffas, G. Belfort

Section E

Rosen Centre Hotel
Salon 6

Biomedical Technologies

Cellular & Microbiome Engineering

R. D. Sheth, G. Thurber, M. Westoby, *Organizers*
P. Miller, N. U. Nair, *Presiding*

2:00 BIOT 583. Engineering bacteria to program animal behavior and lipid metabolism. **B. Gao**, Q. Sun

2:20 BIOT 584. Elucidating interspecies interactions as a key ecological driver of microbiome structure and function: microdroplet co-cultivation technology and its applications. **X.N. Lin**

2:40 BIOT 585. Engineering “sticky” probiotics. **Z.J. Mays**, N.U. Nair

3:00 BIOT 586. Prebiotic control of engineered probiotics. F. Enam, **T. Mansell**

3:20 Intermission.

3:40 BIOT 587. Protein engineering and metabolic engineering strategies for animal-free chondroitin sulfate production. **A. Williams**, W. He, M. Koffas, R.J. Linhardt

4:00 BIOT 588. Screening diffusive, antagonistic bacterial interactions using photoreleasable hydrogels. **N. Fattahi**, P. Guzman, T. Platt, R. Hansen

4:20 BIOT 589. Development of a RNA-sensing spatiotemporal gene regulation program for mammalian systems. **V.M. Hunt**, K.H. Lee, W. Chen



TECHNICAL PROGRAM

4:40 BIOT 590. Programming bacterial consortia: Platforms for user or autonomously regulated population compositions. **K. Stephens**, M. Pozo, C. Tsao, P. Hauk, W.E. Bentley

Polymer Bioconjugates for a Changing World

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THURSDAY MORNING

Section A

Rosen Centre Hotel
Grand A

Emerging Frontiers in BIOT

Frontiers in Sustainable Production

M. A. Blenner, C. A. Eckert, D. J. Roush, *Organizers*
K. A. Brown, J. Gavin, *Presiding*

8:30 BIOT 591. Keynote: Optimizing biopharma for a sustainable future. **K. Budzinski**

9:10 BIOT 592. Science-based sustainability: Further LCA studies in single-use biomanufacturing. **W.G. Whitford**

9:30 BIOT 593. Recycling biopharma single-use plastics: Overcoming the challenges and lessons learned. **J. Ignacio**

9:50 Intermission.

10:10 BIOT 594. Applying PMI (process mass intensity) to compare the environmental footprints of biologics manufacturing processes: Case studies for monoclonal antibodies, nanobodies and vaccines. **S. Madabhushi**, J. Gavin, X. Sen

10:30 BIOT 595. Economic impact of PMI on downstream improvement strategies. **A. Cataldo**, P. Satzer, A. Jungbauer

10:50 BIOT 596. Sustainability metrics: Driving environmental impact reduction for biopharmaceutical manufacturing activities. **P.R. Smith**, A. Adams, D.L. DAquila

11:10 BIOT 597. Environmental sustainability assessment of a biological active pharmaceutical ingredient manufacturing process. **A. Renteria Gamiz**, W. De Soete, B. Heirman, P. Dahlin, S. De Meester, J. Dewulf

Section B

Rosen Centre Hotel
Grand B



TECHNICAL PROGRAM

Downstream Processing

Continuous & Integrated Downstream Bioprocessing

S. Chollangi, M. Gruvegard, C. Heldt, *Organizers*
T. Müller-Späth, L. W. Pampel, J. P. Pieracci, V. Warikoo, *Presiding*

8:30 BIOT 598. Continuous recovery of mAb from the bleed line of a perfusion reactor using Acoustic Wave Separation. **M. Collins**

8:50 BIOT 599. Complexities of designing and automating a continuous virus inactivation unit operation. **N. Thite**

9:10 BIOT 600. Custom Protein A resin design and purification for column-free mAb capture - increased productivity with continuous countercurrent tangential chromatography. **A. Joshi**, C.L. Mason, D. Fedorenko, O. Shinkazh, P. Gilbert, H.J. Johansson, J. Aucamp

9:30 BIOT 601. Continuous formulation / buffer exchange using staged diafiltration or countercurrent dialysis. **M. Jabra**, C. Yehl, A.L. Zydney

9:50 Intermission.

10:10 BIOT 602. Fully connected flow-through polishing for monoclonal antibody purification. **T. Ito**, T. Ichihara

10:30 BIOT 603. Exploring overloading and productivity in continuous chromatography. **M. Bergman**, H. Blom, M. Berg

10:50 BIOT 604. Development and integration of continuous viral filtration, ultrafiltration, and diafiltration at pilot scale. **M.J. Coolbaugh**, T. Vetter, B. Bouchard, C. Varner, E. Davenport, K. Brower

11:10 BIOT 605. Challenges of implementing virus filtration into continuous manufacturing. **J. Kozaili**, S. Johnson, S. Lute, K.A. Brorson, D. Strauss

Section C

Rosen Centre Hotel
Salon 4

Upstream Processes

Synthetic Biology & Genome Engineering

Cosponsored by BIOL[†]
P. Peralta Yahya, A. Russo, C. T. Trinh, *Organizers*
C. A. Eckert, *Presiding*

8:30 BIOT 606. User-defined chemical genetic systems for plants. **T. Whitehead**, I.R. Wheeldon, S. Cutler

8:30 BIOT 607. Molecular drivers and epigenetic modifiers of complex heritability revealed by a natural genotype-to-phenotype map. **C. Jakobson**, J. Aguilar-Rodríguez, D.F. Jarosz



TECHNICAL PROGRAM

8:30 BIOT 608. Functional characterization of 3-hydroxyacyl ACP:CoA transferase for production of medium-chain-length oleochemicals. **Q. Yan**, B. Pflieger

8:30 BIOT 609. Developing a high affinity, dynamic scaffold toolkit for intracellular spatial organization of proteins. **A. Mitkas**, W. Chen

8:30 Intermission.

8:30 BIOT 610. Next generation industrial biotechnology based on halophiles. **G. Chen**

8:30 BIOT 611. Development of a synthetic biology toolbox for *Acinetobacter baylyi* (ADP1), a host for lignin-based metabolic engineering. **B.W. Biggs**, E. Arvay, S. Huang, H. Subramanian, E.L. Neidle, K.E. Tyo

8:30 BIOT 612. Light-based control of metabolic flux through assembly of synthetic organelles. **E.M. Zhao**, J.L. Avalos

8:30 BIOT 613. Evonetix D towards scalable and high-fidelity gene synthesis. **N.N. Khanizeman**, T. Brears, M. Hayes, S. Crosby

Section D

Rosen Centre Hotel
Salon 5

End-to-End Biomanufacturing

Design My Process: Big Data & Data Mining

J. Bender, J. C. Love, V. Roy, *Organizers*
J. Chartron, S. Rameez, *Presiding*

8:30 BIOT 614. End to end, data driven approach to unlock new science, improved efficiency, and project acceleration for biopharmaceutical upstream processing. **R.W. Muthard**, K. Love, S. Bamber

8:50 BIOT 615. Picking winners: Predictive modeling for cell line selection. Y. Xie, **J. Tat**

9:10 BIOT 616. Process analytical technology (PAT) based control of protein refolding: Granulocyte colony stimulating factor (GCSF) as a case study. **V.S. Hebbsi**, G. Thakur, A.S. Rathore

9:50 Intermission.

10:10 BIOT 617. Biopharmaceutical manufacturing: Getting to the cool stuff requires a new paradigm. **S.R. Hass**, M. Lipa, M. Hollenbeck

10:30 BIOT 618. Multivariate data analysis for biotech processes: Industrial case studies. **A.S. Rathore**

10:50 BIOT 619. Machine learning and real time data visualization for formulation applications. **B. Partopour**, M. Boggara, C. Ren, N. Rathore



TECHNICAL PROGRAM

11:10 Panel Discussion.

Section E

Rosen Centre Hotel
Salon 6

Biomolecular Technologies

Protein Structure, Function, & Interactions

B. Hackel, B. F. Marques, *Organizers*
P. A. Romero, J. Swain, *Presiding*

8:30 BIOT 620. Minimally disruptive optical control of protein tyrosine phosphatases. A. Hongdusit, P. Zwart, B. Sankaran, **J.M. Fox**

8:50 BIOT 621. Receptor heterodimerization modulates endocytic uptake through both collaborative and competitive mechanisms. **C. Zhao**, A. DeGroot, H. Ali, M. LaMonica, C. Hayden, J. Stachowiak

9:10 BIOT 622. Visualization and modulation of EF-G power stroke in ribosomal translocation. **H. Yin**, S. Xu, Y. Wang

9:30 BIOT 623. Improving protein crystallization outcomes using surface energy modified substrates. **A.H. Bond**, K.A. Nordquist, T.L. Kinnibrugh, K.M. Schaab, J.L. Johnson, Y. Kim, G. Babnigg

9:50 Intermission.

10:10 BIOT 624. Rapid mapping of glycoprotein structure-activity relationships by glycomutagenesis. **X. Zheng**, M. Li, M. DeLisa

10:30 BIOT 625. Structure and dynamics of the thyroid hormone-activating and deactivating iodothyronine deiodinases. **C.A. Bayse**

10:50 BIOT 626. Structural elucidation of engineered tissue inhibitor of metalloproteinase-1 (TIMP-1) variants with improved binding affinity toward matrix metalloproteinase-3 (MMP-3). **M. Raeszadeh Sarmazdeh**, B. Sankaran, D. Radisky, E. Radisky

11:10 BIOT 627. Structure-guided development of a biocatalyst for late-stage halogenation. **A.E. Fraley**, M. Garcia-Borràs, A. Cernijenko, J.L. Smith, H. Malik, K.N. Houk, D.H. Sherman

Polymer Bioconjugates for a Changing World

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THURSDAY AFTERNOON



TECHNICAL PROGRAM

Section A

Rosen Centre Hotel
Grand A

Emerging Frontiers in BIOT

E₂E Machine Learning

M. A. Blenner, C. A. Eckert, *Organizers*
D. J. Roush, *Organizer, Presiding*
D. Shukla, *Presiding*

2:00 BIOT 628. Characterizing protein hydration to inform its interactions. N. Rego, **A. Patel**

2:20 BIOT 629. Markov state model framework for exploring the effects of cosolvents on protein thermodynamics and kinetics. D. Shukla, **A.S. Moffett**

2:40 BIOT 630. Deep learning bioactivation: The metabolism and subsequent toxicity of drugs. **S. Swamidass**, T. Hughes, L. Dang, M. Matlock

3:00 BIOT 631. Unsupervised latent variable models for improved understanding of high-dimensional process data in early bioprocess development. **N. Afanador**, T. Salim, R. Baumgartner, D. Feng

3:20 Intermission.

3:40 BIOT 632. Artificial intelligence aided biopharmaceutical process development. **M. Ottens**

4:00 BIOT 633. Machine learning classification and fault detection using real-time chromatography data fusion. **B. Punshon-Smith**, I.V. Kostov, G. Rao, R. Adiga

4:20 BIOT 634. Chemical imaging coupled to machine learning for digital cancer diagnosis. **S. Mittal**, K. Yeh, A.K. Balla, R. Bhargava

4:40 Panel Discussion.

Section B

Rosen Centre Hotel
Grand B

Downstream Processing

High-Throughput Screening & Automation of Downstream Purification

S. Chollangi, M. Gruvegard, C. Heldt, *Organizers*
M. Ottens, J. Pollard, M. Stork, *Presiding*



TECHNICAL PROGRAM

2:00 BIOT 635. Multi-component model for prediction of elution of monoclonal antibody in ion exchange chromatography: Parameter estimation and peak shape analysis. **V. Kumar**, F. Schlegel, P. Rolandi, O. Kaltenbrunner, A.M. Lenhoff

2:20 BIOT 636. Enablers for QbD implementation: Mechanistic modeling of liquid chromatography. **A. Tiwari**, V. Kumar, L. Kanwar, A.S. Rathore

2:40 BIOT 637. Using knowledge for downstream process design. R. Khalaf, **A.T. Hanke**, L.W. Pampel

3:00 BIOT 638. Risk-based scale-up of high-throughput chromatography systems using Bayesian statistics and mechanistic modeling. **T. Briskot**, **F. Stueckler**, K. Doninger, F. Wittkopp, J. Yang, T. Hahn, T. Huuk, J. Hubbuch

3:20 Intermission.

3:40 BIOT 639. Integrated upstream and centrifugation scale-down framework for enhanced predictability of product heterogeneity, antibody reduction and filter sizing. **M. Sebastian**, S. Goldrick, A. Charles, A. Eswar, R. Turner

4:00 BIOT 640. Using high throughput screening to enable the development of an activated carbon filtration step for removal of host cell proteins in downstream processes. **A. Slocum**, S. Santora, J. Zhang

4:20 BIOT 641. Aggregate removal in polishing mAb process step with membrane chromatography by determining binding capacity and displacement effects in a HTS robotic set-up. **D. Stein**, J. Hubbuch, V. Thom

4:40 BIOT 642. High throughput strategies for ultrafiltration process development. **J. Pollard**, L. Fernandez Cerezo, E. Espah Borujeni, I. Han, N. Tugcu

Section C

Rosen Centre Hotel
Salon 4

Upstream Processes

Synthetic Biology & Genome Engineering

Cosponsored by BIOL‡
P. Peralta Yahya, A. Russo, C. T. Trinh, *Organizers*
H. S. Alper, T. Lee, *Presiding*

2:00 BIOT 643. Rapid optogenetic inverter circuits for yeast metabolic engineering. **E.M. Zhao**, J.L. Avalos

2:20 BIOT 644. Development of a quorum-sensing circuit for multiplexed metabolic flux control in engineered bacteria. **C.V. Dinh**, K.L. Jones Prather

2:40 BIOT 645. Design of an electronically regulated gene expression system for CRISPR-Cas9 activation and interference applications. **N. Bhokisham**, E. VanArsdale, W.E. Bentley

3:00 BIOT 646. Parallel integration and chromosomal expansion of metabolic pathways. **G. Goyal**, N. Hillson, T. Lee, H. Garcia Martin

3:20 Intermission.



TECHNICAL PROGRAM

3:40 BIOT 647. multiplex navigation of global regulatory networks for complex traits. **R. Liu**, L. Liang, E. Freed, C.A. Eckert, R.T. Gill

4:00 BIOT 648. Characterization of a mesophilic prokaryotic Argonaute for gene-editing. **K. Lee**, A. Kikla, A. Liu, F. Gimble, K. Solomon

4:20 BIOT 649. Storing temporal data with minutes resolution into DNA. **N.J. Bhan**, J. Strutz, R. Kalhor, J. Glaser, K. Kording, G. Church, K.E. Tyo

4:40 BIOT 650. Transcriptomics informs simplified CRISPR/Cas9 genome editing in *Pichia pastoris*. **N. Dalvie**, J. Leal, J.C. Love

Section D

Rosen Centre Hotel
Salon 5

End-to-End Biomanufacturing

Continuous & Agile Manufacturing

J. Bender, J. C. Love, V. Roy, *Organizers*
A. Brown, S. Farid, *Presiding*

2:00 BIOT 651. Process80 BioSMB Evaluation and Scale up Assessment. **L. Arnold**

2:20 BIOT 652. Model assisted process characterization and validation for a continuous two-column protein A capture process. D. Baur, J.M. Angelo, S. Chollangi, T. Müller-Späth, X. Xu, S. Ghose, **M. Morbidelli**

2:40 BIOT 653. Quality by design principles applied to characterization of a continuous downstream mAb purification process. **K. Gillette**, A. Utturkar, K. Boenning, R. Quesenberry, M. Bisschops, R. Gantier, M. Schofield

3:00 BIOT 654. Optimized continuous multicolumn chromatography enables increased productivities and cost savings by employing more columns. **M. Pagkaliwangan**, J. Hummel, X. Gjoka, M. Bisschops, M. Schofield

3:20 Intermission.

3:40 BIOT 655. Cost modelling of continuous and hybrid end-to-end bioprocesses for mAb production. S. Farid, **H. Mahal**

4:00 BIOT 656. Does process intensification add value in light of cost and facility planning. **P. Gupta**, M. Monge, N. Chopra

4:20 BIOT 657. Opportunities, challenges, and economic drivers for start-to-finish continuous biomanufacturing. **A. Vermunt**, A. Castan, O. Hardick, M. Bergman, H. Blom, G. Jagschies

4:40 BIOT 658. Rapid, end-to-end manufacturing of biologics enabled by a universal starter process for purification of proteins produced in *Pichia pastoris*. **L. Crowell**, N. Vecchiarello, K.R. Love, S.M. Cramer, C.J. Love



TECHNICAL PROGRAM

Polymer Bioconjugates for a Changing World

Sponsored by POLY, Cosponsored by BIOT

BIOL

Division of Biological Chemistry

P. Bevilacqua, *Program Chair*

SUNDAY MORNING

Section A

Orange County Convention Center
Room W240AB

Targeting RNA with Drugs

P. Bevilacqua, *Organizer*
M. D. Disney, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 BIOL 1. Inforna: A general and sequence-based approach to provide bioactive small molecules targeting RNA. **M.D. Disney**

9:05 BIOL 2. Riboswitches as models for studying small molecule-RNA interactions. **M. Hammond**

9:35 BIOL 3. Targeting RNA by small molecules: A perspective from nature. **R. Batey**

10:05 Intermission.

10:20 BIOL 4. Chemical tools to study the oncogenic activity of the MALAT1 triple helix. **A.E. Hargrove**

10:50 BIOL 5. Folding the druggable RNA structurome. **W. Moss**, C. O'Leary, R. Andrews

11:20 BIOL 6. Chemical approaches for analyzing RNA structure inside cells. **R. Spitale**

Section B

Orange County Convention Center
Room W240C



TECHNICAL PROGRAM

Graduate Student & Postdoctoral Fellow Symposium

P. Bevilacqua, *Organizer*
M. D. Distefano, *Organizer, Presiding*

8:00 BIOL 7. O⁶-(5-Pyridylmethyl)guanine derivatives as substrates for the self-labeling enzyme SNAP-tag. **M. Macias-Contreras**, L. Zhu

8:15 BIOL 8. Metals as mediators in the cross-talk between drug and fungal pathogen. **E.W. Hunsaker**, K.J. Franz

8:30 BIOL 9. Entropic contribution to enhanced thermal stability in the thermostable P450 CYP119. **Z. Liu**, S. Lemmonds, J. Huang, M. Tyagi, L. Hong, N. Jain

8:45 BIOL 10. Chemical profiling, antioxidant and antimicrobial activities of the stem and fruit peel crude extracts of *citrus jambhiri*. **O.E. Ogunjinmi**, N.O. Olawore, A.A. Aliyu

9:00 BIOL 11. Near-infrared photoactivatable nitric oxide donors with integrated photoacoustic monitoring. **E. Zhou**, H.J. Knox, C.J. Reinhardt, G. Partipilo, M. Nilges, J. Chan

9:15 BIOL 12. Redefining the protein kinase conformational space with machine learning. **R. Rahman**, P.M. Ung, A. Schlessinger

9:30 BIOL 13. Directed evolution of bioluminescent probes enables ultrasensitive live-animal imaging and multiplexed bioassay. **H. Yeh**, H. Ai

9:45 BIOL 14. Effect of Li⁺ Binding on secondary and tertiary structure, hydrophobicity, thermodynamics, and interactions with interacting partners of DREAM. **S. Azam**, J. Miksovská

10:00 BIOL 15. Realization of unnatural codon translation in mammalian cells. **A.X. Zhou**, F.E. Romesberg

10:15 BIOL 16. Development of split RNAP biosensors for directed evolution of protein-protein interactions. **J. Zinkus-Boltz**, B.C. Dickinson

10:30 BIOL 17. Structural characterization of hemoglobin adducts with hydroxylamines. **S. Powell**, V.E. Herrera, K.Y. Prather, N.T. Nguyen, G.B. Richter-Addo

10:45 BIOL 18. Robust method for the purification and characterization of human histone H1 variants. **A. Osunsade**, N.A. Prescott, J.M. Hebert, D.M. Ray, Y. David

11:00 BIOL 19. Surveillance of cancer stem cell plasticity using an isoform-selective fluorescent probe for aldehyde dehydrogenase 1A1. **C. Anorma**, J. Hedhli, T. Bearrood, N.W. Pino, S. Gardner, H. Inaba, P. Zhang, Y. Li, D. Feng, S. Dibrell, K.A. Kilian, L. Dobrucki, T. Fan, J. Chan

11:15 BIOL 20. Dual anti-nitration and antioxidant activity of boronate-based prochelators: Kinetic and mechanistic aspects. **S. Oehm**, J. Zielonka, F. Kielar, A. Sikora, K.J. Franz, B. Kalyanaraman

11:30 BIOL 21. Do supramolecular catalysts mimic enzymes? **V. Vaissier**



TECHNICAL PROGRAM

Interdisciplinary Chemistry for New Frontiers in Biology and Medicine

NanoBio

Sponsored by ANYL, Cosponsored by BIOL, COLL, MPPG, PHYS and PMSE‡

Bio-Based Materials for Energy Conversion & Storage Applications

Electrolyte & Separators for Battery Applications

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Bio-Based Materials for Energy Conversion & Storage Applications

Electrodes for Battery Applications

Sponsored by CELL, Cosponsored by ANYL and BIOL

Interplay of Cellulose & Other Biopolymers in Biological & Designed Materials Systems

Interactions of Plant Polymers in Model Systems

Sponsored by CELL, Cosponsored by ANYL, BIOL and CARB

SUNDAY AFTERNOON

Section A

Orange County Convention Center
Room W240AB

Murray Goodman Award: Symposium in honor of David Beratan

P. Bevilacqua, H. Crichton, *Organizers*
D. N. Beratan, *Presiding*

1:00 Introductory Remarks.

1:05 BIOL 22. Radicals: Your life is in their hands. J. Stubbe, D.G. Nocera, M. Bennati, C. Tommos, D. Britt, C.L. Drennan

1:30 BIOL 23. Electric fields and enzyme catalysis. S.G. Boxer



TECHNICAL PROGRAM

1:55 BIOL 24. Conformational motions and electrostatics facilitate proton-coupled electron transfer in BLUF photoreceptor proteins. **S. Hammes-Schiffer**

2:20 BIOL 25. Electron transport and spin selectivity in nucleic acids and peptides. **D.H. Waldeck**

2:45 Intermission.

3:00 BIOL 26. Exploring the energy landscape for protein folding and function: The convergences of structural models and sequence coevolution information. **J.N. Onuchic**

3:25 BIOL 27. *De novo* protein design. **W.F. Degrado**

3:50 BIOL 28. Hole hopping through tryptophan and tyrosine chains in proteins. **H.B. Gray**

4:15 BIOL 29. Electron transfer pathways in biology. **D.N. Beratan**

Section B

Orange County Convention Center
Room W240C

Early Career Investigators in Biological Chemistry

M. D. Distefano, *Organizer*
P. Bevilacqua, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 BIOL 30. Light-activatable probes for cancer biology. **A. Beharry**

1:30 BIOL 31. Manipulation of redox signaling in mitochondria with trialkylphosphine chemical probes. **P. Rivera-Fuentes**

1:55 BIOL 32. Biogenic metallic nanoparticles. A nanometric Trojan horse approach. **D. Medina Cruz**, A. Vernet Crua, T.J. Webster

2:20 BIOL 33. Molecular basis of off-target effects in CRISPR-Cas9. **G. Palermo**, C. Gravina Ricci, J.S. Chen, Y. Miao, M. Jinek, J.A. Doudna, J.A. McCammon

2:45 Intermission.

3:00 BIOL 34. Understanding oxygen tolerant [Fe-Fe] hydrogenase. **A. Silakov**, P.S. Corrigan

3:25 BIOL 35. Further investigation of the antibacterial activity of 2-hexadecynoic acid analogs against multi-drug resistant bacteria. **D.J. Sanabria Rios**, C. Morales-Guzman, J.W. Mooney Garozzo, X. Torres, D. Diaz, N.M. Carballeira

3:50 BIOL 36. Synthesis of novel organometallic scaffolds as target oriented anticancer drug for glioma. **A.P. P K**

4:15 BIOL 37. Atomically precise hybrid nanoparticles with multivalent capabilities. **A.M. Spokoyny**



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

Interdisciplinary Chemistry for New Frontiers in Biology and Medicine

Microbia

Sponsored by ANYL, Cosponsored by BIOL, COLL, MPPG, PHYS and PMSE‡

Bio-Based Materials for Energy Conversion & Storage Applications

Lignin-Based Materials for Supercapacitor & other Applications

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Bio-Based Materials for Energy Conversion & Storage Applications

Electroconductive Hydrogels

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Interplay of Cellulose & Other Biopolymers in Biological & Designed Materials Systems

Structure & Mechanics of Plant Cell Walls

Sponsored by CELL, Cosponsored by ANYL, BIOL and CARB

SUNDAY EVENING

Section A

Orange County Convention Center
West Hall C

Current Topics

P. Bevilacqua, M. D. Distefano, *Organizers*

7:00 - 9:00

BIOL 38. Logic of non-elongation module in *trans*-acyltransferase polyketide synthases. **R. Al-Dhelaan**, P. Russo, S. Padden, A. Amaya, Y. You



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- BIOL 39.** Structural factors controlling orientation of kras G-domain membrane binding. **A. Trifan**, E. Tajkhorshid
- BIOL 40.** Design of bivalent nucleic acid ligands for recognition of RNA-repeated expansion associated with Huntington's disease. **J. Perera**, S.A. Thadke, R.R. Gil, A. Mukherjee, C. Thornton, D.H. Ly
- BIOL 41.** Shape selective bifacial recognition of double helical DNA. **S.A. Thadke**, V.M. Hridya, J. Perera, R.R. Gil, A. Mukherjee, D.H. Ly
- BIOL 42.** Peptide-assisted supramolecular polymerization of the anionic porphyrin meso-tetra(4-sulfonatophenyl)porphine. **E.M. Kohn**, D. Shirly, **C.J. Fry**, G.A. Caputo
- BIOL 43.** Role of RecO in the DNA double-strand break repair mechanisms of Mycobacteria. **R. Gupta**
- BIOL 44.** Withdrawn
- BIOL 45.** Oxidative DNA damage prevention via tyrosine and tryptophan in a peptide model system. **P. Perez**, J. Ordenana, E.D. Stemp
- BIOL 46.** Understanding proteome dependent cellular zinc trafficking to form native Zn-proteins. **A.A. Mahim**, D.H. Petering
- BIOL 47.** Chemically activated crosslinking with bioorthogonal cyclopropanones. **A.J. Ferreira**, S. Nguyen, D. Row, J.A. Prescher
- BIOL 48.** Inhibitor of nonhomologous end joining (NHEJ): Implications in DNA double-strand break repair and cancer progression. **F. John**, S. Poopadi, J. George, U. Ray, S. Raghavan
- BIOL 49.** Isolation of a novel complex between human NER proteins XPC and XPA. **S.M. Shell**, I. Holyfield, M. Kvaratskhelia, F.A. Beckford
- BIOL 50.** Selective N-terminal peptide modification and development of glucose-responsive insulin. **D. Chen**
- BIOL 51.** Novel class of chemicals that react with abasic sites in DNA and specifically kill B cell cancers. **M. Watuthanthrige Perera**, S. Wei, A. Bhagwat
- BIOL 52.** Analysis of the effects of vegetation on CH₄ emission in landfill cover soils: Combined effects of root architectures, radial oxygen loss, root-water uptake and plant-mediated CH₄ transportation. **B. Rongxing**, X. Chai
- BIOL 53.** Investigating interactions of short-chain menaquinones in Langmuir monolayers. **C. Van Cleave**, B.J. Peters, A. Haase, K.R. Werst, J.T. Koehn, D.C. Crick, D.C. Crans
- BIOL 54.** Mutation of residues in CD loop and distal pocket impact protein stability of human neuroglobin. **R. Lei**, D. Butcher, S. Bernad, V. Derrien, J. Miksovska
- BIOL 55.** Examination of *neurod4* in retinogenesis. **A. Saunders**, T. Bailey
- BIOL 56.** Investigating penicillin-binding proteins using chemical probes. **B.A. Bogin**, S. Sharifzadeh, E.E. Carlson
- BIOL 57.** Intracellular assembly for enhancing drug efficacy and combating resistance. **C. Yanyan**, S. Wang



TECHNICAL PROGRAM

- BIOL 58.** Characterization of NADPH oxidase 5 and dual oxidase by fluorescence and calorimetry. **E. Fabry**, L.A. Lloyd, C. Wei
- BIOL 59.** Self-assemble of γ -conjugated polymer and polypeptide and control of gene expression in living cells. **L. Liu**
- BIOL 60.** Osmotic and load-bearing properties of cartilage on microscopic and macroscopic levels. **F. Horkay**, E.K. Dimitriadis, I. Horkayne-Szakaly, P.J. Basser
- BIOL 61.** Engineering melting temperatures of carbohydrate binding modules through site-directed mutagenesis. **A. Jablunovsky**
- BIOL 62.** Novel 5-cyanopyrimidine derivatives induces apoptosis in THP-1 and A549 cancer cell lines. **P. Melnikov**, M. Kravtsova, D. Khochenkov, A.S. Bunev
- BIOL 63.** Evaluation of nitrate, metformin and/or AMPK inhibitor dorsomorphin on primary and cancer bladder cells. **T. Phan**
- BIOL 64.** Site-specific modification of recombinant thrombomodulin with retention of bioactivity and stability. **X. Liu, X. Sun**
- BIOL 65.** Quantitative determination of abiotic AHL hydrolysis by ^1H NMR. **E.W. Ziegler**, N. Nesnas, A.B. Brown, A.G. Palmer
- BIOL 66.** Importance of the leader peptide in recognition by NosK. **S. Marshall**, B. Wang, S. Booker
- BIOL 67.** Light-induced cell death in response to a novel porphyrin derivative. **T.E. Hayes**, A. Podguzov, A. Abbott, H. Brandon, J.E. Bradshaw
- BIOL 68.** Inhibitory effect of green tea catechins on recombinant human angiogenin. **A. Panda**, S. Dasgupta
- BIOL 69.** *In Vitro* effects of pentamidine isethionate on fibrinolysis and coagulation. **R.A. Al-Horani**, D.K. Afosah, M. Mottamal
- BIOL 70.** Biochemical study of human PRMT5 and its structure-based designer small molecule inhibitors for potential cancer therapeutics. **W. Zhou**, X. Yang, C. Li
- BIOL 71.** Effect of acidosis on the mechanism of cell death under hypoxia induced by cobalt chloride in dopaminergic MN9D cells. **A. Tabatabai**, V. Le
- BIOL 72.** Limited proteolysis analysis of Rok1p- Δ NTD. **K.R. Perroz**, M. Arnold, I. Garcia
- BIOL 73.** *N-Amino peptide inhibitors of $A\beta_{1-42}$ aggregation.* **K. Tillett**, J.R. Del Valle
- BIOL 74.** Small Angle X-Ray Scattering study of conformational changes in steroid responsive activator (SRA) RNA upon binding repressor protein (SHARP). **D. Diatta**, T. Leeper
- BIOL 75.** Electrochemical and nanogravimetric immunosensors for the detection of exosomes isolated from glioblastoma. **M. Stobiecka**, K. Ratajczak, S. Jakiela



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- BIOL 76.** Chinese herb extracts may exert chemopreventive effects through inhibition of cytochrome P450 1A1 and 1B1. N. Leon, C. Palacio, M. San Angelo, R. Isovitsch, **D.S. limoto**
- BIOL 77.** Identification of 4-hydroxy-isoleucine in human breastmilk using UHPLC-MS. **S.A. Nelson**, J. Thompson, T. Johnson
- BIOL 78.** Characterization of 4-hydroxy-isoleucine in complex mixtures by UHPLC-MS. **J. Thompson**, S.A. Nelson, T. Johnson
- BIOL 79.** Evaluation of the antiproliferation effects of glucosinolates against human MCF-7 cells. **M.A. Anderson**, **E. Ronning**, **A.A. Snyder**, J.R. Mays
- BIOL 80.** Efficient solubilization and purification of highly insoluble membrane proteins expressed as inclusion bodies using perfluorooctanoic acid. **K.T. Root**
- BIOL 81.** Molecular structure of bovine leukemia virus gag polyprotein determined by SAXS and computational modeling. **S. Cooper**, D.F. Qualley, E. Olson, K. Musier-Forsyth
- BIOL 82.** Ester-protected ethambutol derivatives as a screen for mycobacterial esterase activity. **R. Johnson**, E.K. Kile
- BIOL 83.** Kinetic analysis of ATP dissociation from a variation of rok1p: A DEAD-box protein. **K. Sutter**, A. DiLoreto, L. Yoder, Z. Iezzi, I. Garcia
- BIOL 84.** Investigating calcitonin aggregation through oxidation of the disulfide bond and inhibition with small molecules. **R. Lantz**, D. Du
- BIOL 85.** Kinetic analysis of ATP dissociation from wt-Rok1p. **A. DiLoreto**, K. Sutter, L. Yoder, Z. Iezzi, I. Garcia
- BIOL 86.** Exploring the effects of macromolecular crowding on conformational change in *escherichia coli* prolyl-tRNA synthetase using intrinsic tryptophan fluorescence. **K. Weeks**, J. Liebau, M. Weinzetl, S. Bhattacharyay, S. Hati
- BIOL 87.** O⁶- Methylguanine DNA methyltransferase activatable photosensitizers for cancer therapeutics. **M. Walker**, A. Beharry
- BIOL 88.** Characterization of the PLP-dependent functions of CISD proteins. C. Kunk, J. Kruger, M. Menze, **M. Konkle**
- BIOL 89.** Oligomerization affects the ability of human cyclase associated proteins 1 and 2 (CAP1 and CAP2) to promote actin severing by cofilins. **V. Purde**, D. Kudryashov
- BIOL 90.** Molecular cages for protein encapsulation and delivery. **M.Z. Alyami**, S. Alsaiari, N.M. Khashab
- BIOL 91.** Validation of ephrinB1 binding partners. **P. Sanchez**, P.L. Colbert, M. Madeo, P.D. Vermeer
- BIOL 92.** Application of biologically synthesized silver nanoparticles on callus growth of *vigna radiata* (Mung Bean) and accumulation of secondary metabolites. **A. Bhat**, P. Bhat
- BIOL 93.** Catalytic properties of RNA-cleaving deoxyribozymes with peptide cofactors. **R. Sapia**, Y. Gerasimova
- BIOL 94.** Investigating structure and function in VOC family dioxygenases: The structure of L-DOPA dioxygenase from *Streptomyces sclerotialis*. **Y. Fu**, Y. Wang, I. Shin, A.D. Horwitz, A. Liu, **K.L. Colabroy**



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- BIOL 95.** Synthesis, characterization and cytotoxicity studies of copper-based nanoparticles. **M.M. Hossain**, S. Yarabarla
- BIOL 96.** Developing methyltransferase activity probes for cancer diagnostics. **A.M. Rotaru**, A. Beharry
- BIOL 97.** Effects of anthocyanin rich extracts on the human gut microbiota. **P.J. Iles**, J. Al-Haddad, M. Nelson, K. Slessor, A. Pabon, R.V. Valcarce, L.D. Giddings
- BIOL 98.** Molecular mechanisms in pH dependency of isocitrate dehydrogenase I (idh1) activity. **M.e. Scott**, E. Vasquez-Hidalgo, L. Luna, J.E. Fonbon, D.D. Sohl, P. Katira
- BIOL 99.** Diving into the Pacific fish microbiome: Exploration of antibiotics in a unique ecosystem. **M. Austin**, P.E. Mandelare, S. Loesgen
- BIOL 100.** Occurrence, behavior and fate of polycyclic aromatic hydrocarbons in vermifiltration for domestic wastewater treatment. **X. Ma**, Y. Wang
- BIOL 101.** Study of DNA damage repair in *Aedes aegypti* larvae in response to oxidative stress. **M.d. Mota**, R.D. Mesquita
- BIOL 102.** Probing metal and hypoxia response elements in the promoter of human metallothionein-3. S.R. Lubin, A.M. Pinsky, J. Sanchez, C. Kaseke, J. Bousleiman, **M.J. Sever**
- BIOL 103.** Synthesizing building blocks for bioactive lipids: Biocatalytic approach using 5-aminolevulinic acid synthase. **A. Kim**
- BIOL 104.** VT-REELI experience in agricultural sciences: Gene mapping of soybeans and biochemical responses to stress in potato. **H. Aliff**, M.A. Saghai-Marroof, R. Arancibia, R. Biyashev, E. Clevinger
- BIOL 105.** Binding and inhibition of NRAS mRNA with drug like small molecules. **Z. Torrey**, D. Calabrese, C. Connelly, J.S. Schneekloth
- BIOL 106.** Attenuation of G-wire self-assembly using G-quadruplex ligands. **E. Kinfu**, T.C. Marsh
- BIOL 107.** Bio-production of isoprene precursor using engineered *E. coli*. **K.C. Vogt**, Y. Wu, K. Zhang
- BIOL 108.** Development of an assay for antimicrobial susceptibility testing of *Coxiella burnetii*. **M. Khan**, C.N. Miller, M.L. Hale
- BIOL 109.** Synthesis, purification, and testing of next generation vWF inhibitors. **G.M. Barreto**, **C.M. Kouba**, D. Guarracino
- BIOL 110.** Evaluation of amyloid- β protein as an antimicrobial peptide in Alzheimer's disease. **C. Hunter**, A. Fanni, D. Brown, E.Y. Chi
- BIOL 111.** Constructing farnesylated anti-EpCAM CSANs for cancer immunotherapy. **H. Tarbox**, Y. Wang, M.D. Distefano
- BIOL 112.** *In vivo* genotoxicity evaluation of efavirenz, lamivudine, tenofovir DF and their combinations using two mice bioassays. **K.M. Akinseye**, B.A. Dauda



TECHNICAL PROGRAM

BIOL 113. Acyclic identification of aptamers (AIA): Rapid identification of DNA and 2'-OMe RNA aptamers for human alpha-thrombin. **C. Miller**, M.P. McPike, P.N. Borer

BIOL 114. Effect of dimerization on the activity of two antimicrobial peptides. **E.M. Harcourt**, A. Austin, A. Germakovski

BIOL 115. Synthesis and evaluation of MazE truncation peptides to probe inhibition of MazF activity. **R. Schneider**, D. Allen, W.E. Shaw, R. Loris, **M.S. Blackledge**

BIOL 116. Statin treatment of cells prior to metabolic labeling with isoprenoid analogues results in cell line-dependent changes in probe incorporation. **P. Thao**, K.F. Suazo, M.D. Distefano

BIOL 117. DNA-mediated proximity assembly circuit for biochemical sensing. **S. Oh**, T. Zhang, A. Pereira, A. Lane, J. Fu

BIOL 118. Development of FRET based assay to observe binding of RNA modification enzyme RsmG to 16S ribosomal RNA. **C.M. Hawkins**, S. Abeysirigunawardena

BIOL 119. Understanding how osmolytes affect protein stability: Comparison of thermophilic and mesophilic DNA photolyases. **A. Wildeman**, W. Ramos, A. Daghestini, Y.M. Gindt

BIOL 120. Site-specific local environmental changes and membrane-peptide interactions of an Alzheimer's disease peptide. **T.W. Kent**, D. Du

BIOL 121. Study on RNA detection based on constant temperature amplification. **J. Chen**, Y. Shi

BIOL 122. Identification of ssDNA aptamer specific to an oral anticoagulant. M. Roueifar, N. Trunzo, K. Masters, **K.L. Hong**

BIOL 123. Theoretical study on hydrolysis of β -lactam antibiotics and their structures with β -lactamases. **Y. Ceylan**, T.R. Cundari

BIOL 124. Protein kinase C regulation by Ca^{2+} binding: A computational study. **Y. Eken**, A.K. Wilson

BIOL 125. Neuronal calcium sensor DREAM interactions with insulinotropic agent repaglinide. **M.D. Santiago**, M.D. Santiago, J. Miksovskaja

BIOL 126. Biochemical changes in the shikimate and phenylpropanoid pathways in the bioenergy crop, shrub willow, due to nitrogen stress. **J.R. Holowko**, M. Serapiglia

BIOL 127. Investigation of the molecular basis of substrate selectivity in SULT1A1 and SULT1A3. **M.A. Hill**, C. Cochrane, M.L. Cafiero, L.W. Peterson

BIOL 128. Engineering substrate plasticity of serine hydrolase enzyme TM0077. **M. Albers**, M.R. Macbeth, R. Johnson, G.C. Hoops

BIOL 129. Flexible loop is the likely allosteric site of inhibition of Rv0045c serine hydrolase by +2 metal cations. **G.C. Hoops**, E.K. Lawson, I.E. Bowles, R. Johnson, M.R. Macbeth

BIOL 130. Decavanadate is a more potent growth inhibitor of two mycobacteria strains than other oxovanadates. **Z.k. Arhouma**, N. Samart, S. Kumar, H. Murakami, D.C. Crick, D.C. Crans



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- BIOL 131.** S-loop of human glutathione synthetase: Links between substrate binding, active site structure and allostery. **T.R. Cundari**, B. Shrestha, B.L. Ingle, M. De Jesus, H. Conrad-Webb, M.E. Anderson
- BIOL 132.** Use of M-methyl mesoporphyrin as a parallel G-DNA structure probe for G-wire assembly intermediates. **D. Su**, T.C. Marsh
- BIOL 133.** Optimization and qualification of a droplet digital polymerase chain reaction assay for quantiation of an aav2 viral vector. **T. Joseph**
- BIOL 134.** Longitudinal stability studies of peptoid nanosheets in various conditions. **A. Kost**
- BIOL 135.** Biochemical and structural analyses of mycobacterial L,D-transpeptidases. T. Zandi, P.K. Stateler, R.L. Marshburn, **L. Basta**
- BIOL 136.** Protein-protein interactions and the investigation of cooperative binding in the SloR-DNA complex. **S.G. Bender**, A. Glasfeld, G. Spatafora, J.Z. Chen
- BIOL 137.** Targeting Tet1 to improve long-term memory in a model of intellectual disability. **A.H. Howard**, X. Zhang, A.R. Boitnott, C.P. Gettens, K.E. Zengeler, H. Smith, B.G. Malachowsky, A. Kennedy
- BIOL 138.** Withdrawn
- BIOL 139.** Ellagic acid as a neuroprotectant against Amyloid beta in Parkinson's and Alzheimer's disease. **A. Gomez**, L. Mendez, G. Henriquez, M. Narayan
- BIOL 140.** Acetylation at lysine residues modulates A β 42 aggregates structure and cytotoxicity. **R. Adhikari**
- BIOL 141.** Delivery of cardiolipin to the mitochondria for Barth syndrome. **M. Kamran**, A. Kalathil, S. Dhar
- BIOL 142.** Exploring the dimerization of H3-H4. **V.M. Neumann**
- BIOL 143.** Purification of palmitoyl protein thioesterase and acyl protein thioesterase for use in in vitro depalmitoylation reactions. **J. Erickson**, D. Esoe, M.J. Hamann
- BIOL 144.** Effect of the cell penetrating peptide Pep-1 on vesicles containing lipid rafts. **B.M. Almarwani**, A. Sunda-Meya, N. Phambu
- BIOL 145.** Elucidating the biosynthesis of microviridins: A structural approach. **K. Patel**, G. Li, S. Bruner
- BIOL 146.** Pulmonary fibroblasts influence epithelial cells response to air pollution. **N. Aponte**, E. Vitucci, N. Mallek, S.D. McCullough
- BIOL 147.** Colorimetric sensor array for the characterization of the transcriptional coactivators Med25-AcID and CBP-KIX. **C.A. Azaldegui**, C.J. Regan, J.M. Garlick, N. Foster, R.M. Burks, A.K. Mapp
- BIOL 148.** Fragment based drug discovery targeting *P. aeruginosa* inhibitor of vertebrate lysozyme. **A. Schultz**, E. Cureau, S. Thomas, T.C. Leeper
- BIOL 149.** Targeted delivery of antioxidant coenzyme Q₁₀ to mitochondria for atherosclerosis. **M. Banerjee**, S. Dhar



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

BIOL 150. Spatially organized pattern recognition receptor tri-agonists: NOD2 agonist in combination with two tlr agonists. **N. Naorem**, S. Manna, A. Esser-Kahn

BIOL 151. Inhibition of fatty acid oxidation results in reduced stemness of glioma stem cells. **S. Sarkar**, S. Dhar

BIOL 152. Identification of *tet(62)*, a novel tetracycline resistance gene, through functional metagenomics. **J. Donato**, B. McGivern, R. McDonnell, T. LaPara

BIOL 153. Withdrawn

BIOL 154. Antimicrobial peptides (AMPs) in the American lobster, *Homarus americanus*: Changes to hemocytes and AMPs as a function of molt status. **T. Yoder**, D. Do, P.S. Dickinson, A. Christie, E.A. Stemmler

BIOL 155. Human glutathione synthetase: Negative cooperativity and binding studies. **M.E. Anderson**, A.R. Stopper, L. Haynes

BIOL 156. ANS binding of *Halobacterium salinarum* cysteinyl-tRNA synthetase. **S. Li**, C.M. Evilia

BIOL 157. Designing a fast enzyme 101: D101H mutation of *E. coli* alkaline phosphatase. **M. Walz**, K. Johansen, S. Chamberlin

BIOL 158. Withdrawn

BIOL 159. Withdrawn

BIOL 160. Modulation of activity for *B. subtilis* oxalate decarboxylase by the assembly of a π -stacked tryptophan residue pair. **A.J. Pastore**, M. Burg, U. Twahir, J.S. Italia, A. Chatterjee, S. Bruner, K.B. Green, M. Kamat, A. Angerhofer

BIOL 161. Using FRET to elucidate the lipid trafficking mechanism of SP-Bc terminal peptide in comparison with KL4. **A. Page**

BIOL 162. Withdrawn

BIOL 163. Kinky evolution of the alkaline phosphatase active site yields increased catalytic efficiency and promiscuity. **K. Johansen**, M. Walz, A. Wagner, S. Chamberlin

BIOL 164. Altering a hydrophobic platform in the *Escherichia coli* alkaline phosphatase active site. **T. Vu**, E. Plender, S. Chamberlin

BIOL 165. Cancer cell specific RNA labeling with orthogonal nucleoside probes. **S. Beasley**, R. Spitale

BIOL 166. Encoded self-assembling chemical (ESAC) libraries: A powerful technology for ligands discovery and affinity maturation. **E. Etienne**, F. Samain, M. Bigatti, J. Scheuermann, D. Neri

BIOL 167. The recovery of DNA-tagged ligands: Impact of different experimental parameters through affinity selections. **A. Sannino**, F. Samain, D. Neri

BIOL 168. Withdrawn



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

BIOL 169. EPR monitored studies of noncuboidal clusters present in heterodisulfide reductase. **C.B. Engel**, E.C. Duin, G. Martinez, J.G. Ferry

BIOL 170. Restoration of bone defects using modified heterogeneous deproteinized bone seeded with bone marrow mesenchymal stem cells. **J. Li**

MONDAY MORNING

Section A

Orange County Convention Center
Room W240AB

Chemical Signaling in Plants

Cosponsored by AGFD and AGRO
P. Bevilacqua, *Organizer*
K. Torii, *Organizer, Presiding*

9:00 Introductory Remarks.

9:05 BIOL 171. Signaling by 1-aminocyclopropane-1-carboxylic acid (ACC): the case for a novel plant hormone. **C. Chang**

9:45 BIOL 172. Unravel strigolactone signaling and controlling parasitic plant behaviors. **Y. Tsuchiya**

10:25 Intermission.

10:45 BIOL 173. Chemical biology in plant membrane trafficking and cell growth. **C. Zhang**

11:25 BIOL 174. Harnessing synthetic chemistry to hijack auxin signaling in plants. **K. Torii**

Section B

Orange County Convention Center
Room W240CD

Protein Folding & Aggregation

P. Bevilacqua, *Organizer*
X. Zhang, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 BIOL 175. Chaperoning in vitro and inside cells. **M. Gruebele**



TECHNICAL PROGRAM

8:45 BIOL 176. Controlling protein folding via *de novo* design of small molecules. **S.R. McAlpine**

9:20 BIOL 177. Elucidating binding sites in amyloid- β using photoactive rhenium(I) dipyridophenazine complexes. B. Jiang, A. Aliyan, T.J. Paul, C. Pennington, G. Sharma, R. Prabhakar, **A.A. Marti**

9:55 Intermission.

10:15 BIOL 178. Detecting protein aggregation in live cells with turn-on fluorescence using chemically modulated fluorescent protein chromophores. **X. Zhang**, Y. Liu, C. Wolstenholme

10:50 BIOL 179. Atomic structures of infectious amyloid assemblies. **J.A. Rodriguez**

11:25 BIOL 180. Amyloids in disease and biology. D.N. Dean, J.D. Flynn, R.P. McGlinchey, M.D. Watson, **J.C. Lee**

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Sponsored by PROF, Cosponsored by AGFD, ANYL, BIOL, BIOT, CARB, CELL, CHED, CMA, COLL, COMP, ENVR, GEOC, I&EC, MEDI, MPPG, NUCL, ORGN, PHYS, PMSE, POLY, PRES, WCC and YCC

Interdisciplinary Chemistry for New Frontiers in Biology and Medicine

Biomarker Discovery

Sponsored by ANYL, Cosponsored by BIOL, COLL, MPPG, PHYS and PMSE \ddagger

Nucleic Acids-Based Therapeutics

Sponsored by CARB, Cosponsored by BIOL and MEDI

Interplay of Cellulose & Other Biopolymers in Biological & Designed Materials Systems

Xylan & Lignin Interactions with Cellulose

Sponsored by CELL, Cosponsored by ANYL, BIOL and CARB

MONDAY AFTERNOON

Section A

Orange County Convention Center
Room W240AB



TECHNICAL PROGRAM

Chemical Signaling Between Organisms

P. Bevilacqua, *Organizer*
R. A. Butcher, *Organizer, Presiding*
S. Loesgen, *Presiding*

1:00 BIOL 181. Unveiling hidden signaling small molecules in pathogenic bacteria. **W. Zhang**

1:40 BIOL 182. Decoding the chemical signals of the worm. **R.A. Butcher**

2:20 Intermission.

2:40 BIOL 183. Talking with molecules: Marine bacteria and microalgae. **M. Seyedsayamdost**

3:20 BIOL 184. Sex, drugs, and genetics: Gene activation strategies to access silent fungal metabolites. P.E. Mandelare, G.F. Neuhaus, D.A. Adpressa, **S. Loesgen**

Section B

Orange County Convention Center
Room W240CD

Advances in Metabolic Labeling & Profiling

P. Bevilacqua, *Organizer*
M. D. Distefano, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 BIOL 185. Orthogonal enzyme/substrate engineering to profile biological substrates of glycosyltransferases. **C.R. Bertozzi**

1:45 BIOL 186. Redefining druggability using chemoproteomic platforms. **D. Nomura**

2:25 BIOL 187. Enzymatic labeling of bacterial proteins for live-cell super-resolution imaging. **S. Ho**, D.A. Tirrell

3:05 Intermission.

3:20 BIOL 188. Cell-specific bio-orthogonal metabolic labeling of RNA. **R. Spitale**

4:00 BIOL 189. Applications of metabolic labeling and profiling of prenylated proteins in chemistry and biology. **M.D. Distefano**

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

Sponsored by PROF, Cosponsored by AGFD, ANYL, BIOL, BIOT, CARB, CELL, CHED, CMA, COLL, COMP, ENVR, GEOC, I&EC, MEDI, MPPG, NUCL, ORGN, PHYS, PMSE, POLY, PRES, WCC and YCC

Interdisciplinary Chemistry for New Frontiers in Biology and Medicine

DNA/RNA & Disease Diagnosis

Sponsored by ANYL, Cosponsored by BIOL, COLL, PHYS and PMSE

Nucleic Acids-Based Therapeutics

Sponsored by CARB, Cosponsored by BIOL and MEDI

Fluorescence Techniques Applied to Lignocellulose Characterization

Sponsored by CELL, Cosponsored by ANYL and BIOL

Undergraduate Research Posters

Biochemistry

Sponsored by CHED, Cosponsored by BIOL and SOCED

MONDAY EVENING

Section A

Orange County Convention Center
West Hall C

Sci-Mix

P. Bevilacqua, *Organizer*

8:00 - 10:00

8, 13, 38, 51, 56, 66, 70, 75, 83, 88, 93, 105, 109-110, 120, 137, 165. See previous listings.

BIOL 190. Discovery and diversification of tiancimycin (TMN) natural products for Antibody Drug Conjugates (ADCs). **C. Teijaro**, A. Adhikari, X. Yan, T. Annaval, I. Crnovcic, C. Chang, C. Rader, B. Shen



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

230, 234. See subsequent listings.

TUESDAY MORNING

Section A

Orange County Convention Center
Room W240AB

ACS Chemical Biology Award Symposium

P. Bevilacqua, A. Weidmann, *Organizers*
L. L. Kiessling, *Organizer, Presiding*

9:00 Introductory Remarks.

9:05 BIOL 191. Attenuating oncogenic transcription with small molecules. **A.N. Koehler**

9:35 BIOL 192. Chemical tools to probe signaling by dynamic protein lipidation. **B.C. Dickinson**

10:05 BIOL 193. Using old antibiotics to uncover new ones. **M. Seyedsayamdost**

10:35 BIOL 194. Deciphering patterns in selective small molecule: RNA interactions. **A.E. Hargrove**

11:05 Introduction of Awardee.

11:10 BIOL 195. RNA methylation in gene expression regulation. **C. He**

Exploring the Frontiers of Chemistry through NASA Research

Getting There: Advanced Materials for Space Travel

Sponsored by COMSCI, Cosponsored by ANYL, BIOL, BIOT, CELL, COLL, ENFL, I&EC, INOR, NUCL, PHYS, PMSE and POLY

MEDI Awards Symposium

Sponsored by MEDI, Cosponsored by BIOL

Interdisciplinary Chemistry for New Frontiers in Biology and Medicine



TECHNICAL PROGRAM

Structure, Imaging & Sensing

Sponsored by ANYL, Cosponsored by BIOL, COLL, PHYS and PMSE‡

Advanced Chemistry of "Non-Traditional" Polysaccharides

Sponsored by CELL, Cosponsored by AGFD, ANYL, BIOL and CARB

TUESDAY AFTERNOON

Section A

Orange County Convention Center
Room W240AB

ACS National Awards: Breslow & Nakanishi

P. Bevilacqua, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 BIOL 196. Award Address (Nakanishi Prize sponsored by the Nakanishi Prize Endowment). Solution NMR spectroscopy: Why Bother? **L. Kay**

2:05 BIOL 197. Light receptive molecules and their precise control of the brain, infections, and more. **N. Nesnas**

2:20 Introductory Remarks.

2:25 BIOL 198. Award Address (Ronald Breslow Award for Achievement in Biomimetic Chemistry sponsored by the Ronald Breslow Award Endowment). Reinterpreting the Genetic Code: Non-Canonical Amino Acids in Protein Science and Engineering. **D.A. Tirrell**

Exploring the Frontiers of Chemistry through NASA Research

Living There: Science for the Future of Manned Space Exploration

Sponsored by COMSCI, Cosponsored by ANYL, BIOL‡, BIOT, CELL, COLL, ENFL‡, I&EC‡, INOR‡, NUCL‡, PHYS‡, PMSE‡ and POLY‡

Exploring the Frontiers of Chemistry through NASA Research

Living There: Science for the Future of Manned Space Exploration



TECHNICAL PROGRAM

Sponsored by COMSCI, Cosponsored by ANYL, BIOL[‡], BIOT, CELL, COLL, ENFL[‡], I&EC[‡], INOR[‡], NUCL[‡], PHYS[‡], PMSE[‡] and POLY[‡]

Advanced Chemistry of "Non-Traditional" Polysaccharides

Sponsored by CELL, Cosponsored by AGFD, ANYL, BIOL and CARB

Biomolecular Technologies

Engineering & Design

Sponsored by BIOT, Cosponsored by BIOL[‡]

WEDNESDAY MORNING

Section A

Orange County Convention Center
Room W240AB

DNA Instability & Repair

P. Bevilacqua, *Organizer*
K. Dalby, *Organizer, Presiding*

9:00 BIOL 199. Investigation of the function of maternal embryonic leucine zipper kinase (MELK) in response to chemotherapeutic DNA-damaging agents in triple negative breast cancer. **K. Dalby**, K.M. Vasquez

9:25 BIOL 200. Structural and biochemical studies to assess protein interactions and classify VUSs. **A. Prakash**

9:50 BIOL 201. New players in DNA damage-induced protein modification cascades. **G. Liszczak**, T.W. Muir, K. Diehl

10:15 BIOL 202. Phosphorylation control of homologous recombination. **M.S. Smolka**

10:40 BIOL 203. Novel mechanisms of genetic instability in cancer. **K.M. Vasquez**

Section B

Orange County Convention Center
Room W240C

Mid-Career Investigators in Biological Chemistry



TECHNICAL PROGRAM

P. Bevilacqua, M. D. Distefano, *Organizers*
M. M. Pires, *Presiding*

8:00 Introductory Remarks.

8:05 BIOL 204. L,D-transpeptidase specific cell wall probes. **M.M. Pires**

8:35 BIOL 205. Promutagenic replication across the major oxidative adenine lesion 7,8-dihydro-8-oxoadenine. **S. Lee**, H. Jung

9:05 BIOL 206. Identification of translational recoding signals for an improved quadruplet codon decoding. Y. Chen, X. He, W. Niu, **J. Guo**

9:35 Intermission.

9:50 BIOL 207. Applications of a synthetic base-triple motif in nucleic acid structure-function, diagnostics and delivery. **D. Bong**

10:20 BIOL 208. Sustainable catalysis of a conjugated polymer by a protein enzyme. **T. Leeper**, D. Morris, C.J. Ziegler

Nanocellulose: From Fundamentals to Function

Sponsored by CELL, Cosponsored by AGFD, ANYL and BIOL

Bioactive Delivery: Frontiers in Biomaterials

Sponsored by CELL, Cosponsored by ANYL, BIOL and CARB

Bio-Based Gels & Porous Materials

3D printing & Rheology of Cellulose & Nanocellulose

Sponsored by CELL, Cosponsored by ANYL, BIOL and COLL

WEDNESDAY AFTERNOON

Section A

Orange County Convention Center
Room W240AB

Graduate Student & Postdoctoral Fellow Symposium



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

M. D. Distefano, *Organizer*
P. Bevilacqua, *Organizer, Presiding*

1:00 BIOL 209. Unusual heme properties of a bifunctional O₂-dependent globin coupled sensor. **D.C. Patterson**, E.E. Weinert

1:15 BIOL 210. Inhibition of the epithelial-mesenchymal transition: Targeting FOXC2. **M. Castaneda**, L. Jiyong

1:30 BIOL 211. Biological evaluation of molecules of the azaBINOL class as antiviral agents reveals specific inhibition of HIV-1 RNase H activity. **R. Overacker**, S. Banerjee, G.F. Neuhaus, S. Sephton, A. Herrmann, J. Strother, R. Brack-Werner, P.R. Blakemore, S. Loesgen

1:45 BIOL 212. New class of red absorbing activatable PDT drugs. **T. Almammadov**, G. Atakan, G. Gunaydin, G.E. Gunbas, S. Kolemen

2:00 BIOL 213. Overcoming the hydrophobic barrier of the membrane: The role of COQ9 in promoting coenzyme Q biosynthesis. **D. Aydin**, D.C. Lohman, D.J. Pagliarini, M. Dal Peraro

2:15 BIOL 214. hNQO1-activatable photosensitizer for cancer-selective photodynamic therapy. **E.M. Digby**, A. Beharry

2:30 BIOL 215. Rationally designed peptidyl virus-like particles enable targeted delivery of genetic cargo. **J. Kong**

2:45 BIOL 216. Exploiting the cellular redox control system for activatable Photodynamic Therapy. **N. Gharibi**, K. Kailass, A. Beharry

3:00 BIOL 217. Improved synthesis of the dinitroindolinyI cage (CDNI) and its application in neuroscience and beyond. **C. Guruge**, Y.P. Ouedraogo, R.L. Comitz, J. Ma, A.B. Pabarue, A. Losonczy, N. Nesnas

3:15 BIOL 218. Restoring activity to oxygen-damaged glycyI radical enzymes: Spare parts for proteins. **M.C. Andorfer**, L. Backman, S.E. Bowman, R. Bjork, P. Li, S. Yori, C.L. Drennan

3:30 BIOL 219. Identification and exploration of RNA-privileged small molecule chemical space. **S. Wicks**, B. Morgan, A.E. Hargrove

3:45 BIOL 220. "Geometric Mutation" for decoupling receptor signaling crosstalk between Dectin-1 and Toll-like Receptor 2 at phagosome membranes. **W. Li**, J. Yan, Y. Yu

4:00 BIOL 221. Mild oxidation of *N*-phenylglycinyI peptides for bioconjugation reactions. **Q. Guthrie**, C. Proulx

4:15 BIOL 222. Photoactivation of inhibitors of anti-cancer therapy. **R. Bodagh**, A. Beharry

4:30 BIOL 223. Bacteriophage lysozyme catalyzed synthesis of 2-ethynylpyridine conjugated polymer. **S. Thomas**, C.J. Ziegler, T. Leeper

4:45 BIOL 224. Kinetic modeling of H₂O₂ dynamics in mammalian mitochondria. **K.T. Stein**, H.D. Sikes

Section B



TECHNICAL PROGRAM

Orange County Convention Center
Room W240C

Mid-Career Investigators in Biological Chemistry

P. Bevilacqua, M. D. Distefano, *Organizers*
D. A. Harki, *Presiding*

1:00 Introductory Remarks.

1:05 **BIOL 225.** Role of the N-terminal charge-rich region of amyloid- β in amyloidogenesis and interaction with lipid membrane. **D. Du**

1:35 **BIOL 226.** Traceless-cleavage of protein-biotin conjugates under biologically-compatible conditions. **M.J. Hall**

2:05 **BIOL 227.** Chemical modulation of APOBEC-catalyzed mutation. **D.A. Harki**

2:35 Intermission.

2:50 **BIOL 228.** Non-canonical substrate recognition and processivity define serine protease HtrA2 and antiapoptotic Pea15 interaction. **K. Bose**

3:20 **BIOL 229.** Role of AT hook flanking sequence on DNA affinity and global structure. **K.L. Buchmueller**

Nanocellulose: From Fundamentals to Function

Sponsored by CELL, Cosponsored by AGFD, ANYL and BIOL

Bioactive Delivery: Frontiers in Biomaterials

Sponsored by CELL, Cosponsored by ANYL, BIOL and CARB

Bio-Based Gels & Porous Materials

Gels in Medical Applications

Sponsored by CELL, Cosponsored by ANYL, BIOL and COLL

THURSDAY MORNING

Section A



TECHNICAL PROGRAM

Orange County Convention Center
Room W240AB

Graduate Student & Postdoctoral Fellow Symposium

M. D. Distefano, *Organizer*
P. Bevilacqua, *Organizer, Presiding*

8:00 BIOL 230. Mechanistic study of glycyl radical enzyme. **Z. Yang**, L. Backman, Y.Y. Huang, L. Rajakovich, E.P. Balskus, C.L. Drennan, H.J. Kulik

8:15 BIOL 231. Ratiometric fluorescent chemosensing of carboxylesterase 2 activity in patient-derived xenografts. **K. Kailass**, A. Beharry

8:30 BIOL 232. Exploring the roles of 2',3'-cyclic nucleotide monophosphates in bacterial signaling. **Y. Duggal**, B. Fontaine, E.E. Weinert

8:45 BIOL 233. Development of an eosin-based probe activated by carboxylesterase 2 (CES2) for fluorescence-guided photodynamic therapy. **A. Kwan**, K. Kailass, A. Beharry

9:00 BIOL 234. Eneidyne functionalization by a cofactor-promiscuous methyltransferase. **A. Adhikari**

9:15 BIOL 235. Acid-induced folding of caspase-activated Par-4 tumor suppressor. **A. Clark**, K. Ponniah, M. Warden, E. Raitt, A. Yawn, S. Pascal

9:30 BIOL 236. Lipoxazolidinone A and analogs as lead compounds for novel antibiotics. **K.R. Robinson**, J.G. Pierce

9:45 BIOL 237. Synthesis and biological evaluation of the morpholinone fragment of the monanchocidin family of marine natural products. **C. Martinez-Brokaw**, J.G. Pierce

10:00 BIOL 238. Designer dendrons to modulate innate immune signaling. **S. Manna**, W.J. Howitz, N.J. Oldenhuis, S. Maiti, W. Du, Z. Guan, A.P. Esser-Kahn

10:15 BIOL 239. Effect of dimerization and halogen bonding on substrate binding to the thyroid hormone-activating and -deactivating iodothyronine deiodinases. **E.S. Marsan**, C.A. Bayse

10:30 BIOL 240. High-resolution orthogonal imaging with diverse bioluminescent substrates. **C. Brennan**, Z. Yao, B.S. Zhang, J.A. Prescher

10:45 BIOL 241. Effects of isotopic labeling in formate dehydrogenase. **C.U. Ranasinghe**, P.L. Pagano, A. Kohen, C.M. Cheatum

11:00 BIOL 242. Viperin: A S-adenosyl-L-methionine-dependent regulation of viral protein NS5A. **S. Ghosh**, A.B. Dumbrepatil, A. Patel, K. Zegalia, R. Kennedy, E.G. Marsh

11:15 BIOL 243. Theoretical investigation of biologically-relevant 1-hydroxyethyl radical: Preferential formation of cyclic hydrogen bonding networks versus electrostatic interaction maximization. **A.E. Williams**, N. Hammer, S.R. Davis



TECHNICAL PROGRAM

11:30 BIOL 244. Understanding recognition mechanism of contact allergen and evaluation of its usage as novel adjuvants. **S. Kim**, A. Esser-Kahn

Section B

Orange County Convention Center
Room W240C

Early Career Investigators in Biological Chemistry

P. Bevilacqua, M. D. Distefano, *Organizers*
M. S. Blackledge, *Presiding*

8:00 Introductory Remarks.

8:05 BIOL 245. Protein and small molecule engineering towards an orthogonal chromatin landscape. **K. Islam**

8:30 BIOL 246. Unlocking complex barrier transport via chaperone-like small molecules: A new platform for gram-negative bacteria and blood-brain barrier penetration. **R. Rafferty**

8:55 BIOL 247. Macropinosome organizes sorting and recycling of IgG from the surface of nanoparticles in macrophages. **G.J. Opoku-Kusi**, N. Gitanjali, J. Kerkvliet, A. Hoppe

9:20 Intermission.

9:35 BIOL 248. Breaking bad bugs with repurposed drugs: Evaluating FDA-approved drugs to target biofilm formation and antibiotic resistance in pathogenic bacteria. **M.S. Blackledge**

10:00 BIOL 249. Understanding the pH modulation in the *E. coli* mechanosensitive channel of small conductance (MscS). H.M. Dickinson, B.L. Miller, **H.R. Malcolm**

10:25 BIOL 250. Direct comparison of paralogous PB1 domains with disparate roles in regulation. R. Garner, S. Johnston, K. Piemonte, M. Chiriboga, **J.P. Ellis**

10:50 BIOL 251. Expanding the imaging tool box with photoacoustic probes for noninvasive in vivo imaging. **J. Chan**

Nanocellulose: From Fundamentals to Function

Sponsored by CELL, Cosponsored by AGFD, ANYL and BIOL

Additive Manufacturing of Bio-based & Renewable Materials

Sponsored by CELL, Cosponsored by AGRO, ANYL and BIOL



TECHNICAL PROGRAM

Bio-Based Gels & Porous Materials

Nanostructuration of Gels & Aerogels & their Use as Sensors

Sponsored by CELL, Cosponsored by ANYL, BIOL and COLL

Upstream Processes

Synthetic Biology & Genome Engineering

Sponsored by BIOT, Cosponsored by BIOL‡

THURSDAY AFTERNOON

Nanocellulose: From Fundamentals to Function

Sponsored by CELL, Cosponsored by AGFD, ANYL and BIOL

Additive Manufacturing of Bio-based & Renewable Materials

Sponsored by CELL, Cosponsored by AGRO, ANYL and BIOL

Bio-Based Gels & Porous Materials

Gels, Aerogels & Carbogels

Sponsored by CELL, Cosponsored by ANYL, BIOL and COLL

Upstream Processes

Synthetic Biology & Genome Engineering

Sponsored by BIOT, Cosponsored by BIOL‡

BMGT



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

Division of Business Development and Management

A. DeMasi and J. Bryant, *Program Chairs*

SUNDAY AFTERNOON

Section A

Hilton Orlando
Lake George B

Chemical Angel Network

Chemists Investing in Chemical Companies-Invited, Oral

Cosponsored by PROF and SCHB[‡]
Financially supported by CIEC
J. L. Bryant, J. C. Giordan, *Organizers*
M. Vreeke, *Presiding*

1:30 Introductory Remarks.

1:35 BMGT 1. Updates and news from the Chemical Angel Network (CaN) and its sixth year of supporting chemists and chemistry-based company creation. **S.S. White**, M. Vreeke, J.C. Giordan

2:00 Company Presentations.

3:00 Investment Discussion.

3:30 Open Forum.

4:00 Concluding Remarks.

MONDAY AFTERNOON

Section A

Hilton Orlando
Lake George B

ACS – A Place to Do Business

Cosponsored by SCHB[‡]
A. S. DeMasi, D. Mason, *Organizers*



TECHNICAL PROGRAM

1:30 Introductory Remarks.

1:40 **BMGT 2.** Innovation models with incubators and accelerators. **W.D. Provine**

2:00 **BMGT 3.** Chemical Angel Network chemists and chemical engineers investing in chemical businesses. **S.S. White,**
M. Vreeke, J.C. Giordan

2:20 **BMGT 4.** Stay relevant and play bigger - How to reinvent your company to succeed. **N.A. LaFranzo,** J. Armstrong, J.
Glasscock, D. Messina

2:40 Break.

2:50 **BMGT 5.** Citrus fractions 101. **C. Stone**

3:10 **BMGT 6.** Chemistry, engineering and business....can you marry the three? **G.M. Adjabeng**

3:30 **BMGT 7.** Being a woman entrepreneur in chemical science; Challenges and opportunities in developing new water
friendly catalysts for green manufacturing. **A. Mehta**

3:50 Get a leg up in business with industry coverage and tools from C&EN and ACS.

4:10 Moderated Panel/Meet Greet.

Kathryn C. Hach Award for Entrepreneurial Success

Sponsored by SCHB, Cosponsored by ANYL, BMGT and PROF

Beyond the Bench: Non-Traditional Careers in Chemistry

Sponsored by CHAL, Cosponsored by BMGT, PROF and YCC

Chemistry in Space: Future Directions

Sponsored by YCC, Cosponsored by AGFD, ANYL, BIOT, BMGT, CHAS, ENVR, FLUO, GEOC, HIST, I&EC, MEDI,
POLY and PROF

CARB

Division of Carbohydrate Chemistry

S. Sucheck, *Program Chair*



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

SUNDAY MORNING

Section A

Orange County Convention Center
Room W221B

Wolfrom Award

Cosponsored by CELL, MEDI, ORGN and PROF
Financially supported by Alectos Therapeutics
E. Rozners, *Organizer, Presiding*

9:00 Introductory Remarks.

9:05 **CARB 1.** Recent advance in design of a glycopeptide-based HIV vaccine. **L. Wang**

9:30 Discussion.

9:35 **CARB 2.** Synthetic oligosaccharides self-assemble to form novel materials. **P.H. Seeberger**

10:00 Discussion.

Section A

Orange County Convention Center
Room W221B

Horton Award

Cosponsored by CELL, MEDI, ORGN and PROF
Financially supported by Alectos Therapeutics
E. Rozners, *Organizer*
J. H. Lauterbach, *Presiding*

10:20 Introductory Remarks.

10:35 **CARB 3.** Reinventing oligonucleotide synthesis. **P.S. Baran**

11:00 Discussion.

11:05 **CARB 4.** Carbohydrate-based drug discovery and development. **F. Fang**

11:30 Discussion.



TECHNICAL PROGRAM

Advances in Renewable Materials

Sponsored by CELL, Cosponsored by ANYL and CARB

Opportunities & Challenges in Carbohydrates

Sponsored by ORGN, Cosponsored by CARB†

Interplay of Cellulose & Other Biopolymers in Biological & Designed Materials Systems

Interactions of Plant Polymers in Model Systems

Sponsored by CELL, Cosponsored by ANYL, BIOL and CARB

SUNDAY AFTERNOON

Section A

Orange County Convention Center
Room W221B

Hudson Award

Cosponsored by CELL, MEDI, ORGN and PROF
Financially supported by Alectos Therapeutics
E. Rozners, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 **CARB 5.** Mechanistic investigations of the radical SAM enzyme, DesII. **M.W. Ruszczycky**

2:00 Discussion.

2:05 **CARB 6.** Exploring the biosynthetic pathways to unusual sugars found in nature. **H. Liu**

2:30 Discussion.

Section A

Orange County Convention Center
Room W221B

Isabell Award



TECHNICAL PROGRAM

Cosponsored by CELL, MEDI, ORGN and PROF
Financially supported by Alectos Therapeutics
E. Rozners, *Organizer, Presiding*

2:50 Introductory Remarks.

2:55 CARB 7. Stereospecific and site-selective glycosylation reactions catalyzed by bis-thioureas. **E.N. Jacobsen**

3:20 Discussion.

3:25 CARB 8. Organoboron catalysts and reagents for site-selective transformations of carbohydrate derivatives. **M.S. Taylor**

3:50 Discussion.

Section A

Orange County Convention Center
Room W221B

Gin New Investigator Award

Cosponsored by CELL, MEDI, ORGN and PROF
Financially supported by Alectos Therapeutics
E. Rozners, *Organizer, Presiding*

4:10 Introductory Remarks.

4:15 CARB 9. Glyco-immune modulation in the tumor microenvironment. **C.R. Bertozzi**

4:40 Discussion.

4:45 CARB 10. Specificity, function, and regulation of protein O-GlcNAc modification. **J. Jiang**

5:10 Discussion.

Opportunities & Challenges in Carbohydrates

Sponsored by ORGN, Cosponsored by CARB[†]

Advances in Renewable Materials

Sponsored by CELL, Cosponsored by ANYL and CARB



TECHNICAL PROGRAM

Interplay of Cellulose & Other Biopolymers in Biological & Designed Materials Systems

Structure & Mechanics of Plant Cell Walls

Sponsored by CELL, Cosponsored by ANYL, BIOL and CARB

SUNDAY EVENING

Section A

Orange County Convention Center
West Hall C

General Posters

Cosponsored by CELL
S. J. Sucheck, *Organizer*

7:00 - 9:00

CARB 11. Stereoselective β -Mannosylation via Cs_2CO_3 -mediated anomeric O-alkylation: Mechanistic investigations and syntheses of complex carbohydrate molecules. **X. Li**, S. Meng, B. Bhetuwal, H.P. Nguyen, J. Zhu

CARB 12. Novel enzymatic thiogalactolipides owing revelant hydrogelation and cosmetic properties. **C. Peyrot**, L. Guillotin, P. Lafite, L. Landemare, L. Lemiègre, R. Daniellou

CARB 13. Chemoenzymatic glycan remodeling of therapeutic monoclonal antibody by *Streptococcus pyogenes* endoglycosidases S and S2. **X. Tong**, L. Wang

CARB 14. Phosphorylation of monosaccharides using inorganic phosphates. **M. Perez-Remirez**, B. Otoo

CARB 15. Synthesis and anti-proliferative evaluation of various 2-deoxy-D-glucobenzotriazoles and novel carbohydrate-fused heterocyclic compounds. **M. De Castro**

CARB 16. C-Galactosyl oxime cyclizations onto pendant alkenes. E.G. Nolen, **E. Hornik**, **J.M. Bennett**, K. Jeans

CARB 17. Targeting glioma progression: Non-anticoagulant heparinoids and the blood-brain-barrier transcytosis. **S. Nadji**

CARB 18. Concise total synthesis of Bradyrhizose from D-glucose. **P. Ngoje**, D. Crich

CARB 19. Interfering with the biosynthesis of *Helicobacter pylori*'s glycans. **D.A. Williams**, K. Pradhan, A. Paul, S.S. Kulkarni, D.H. Dube

CARB 20. Comparison of covalent delivery methods and their effects for immune-mediated killing of *Helicobacter pylori*. **H. Lee**, D.H. Dube

CARB 21. Novel sugar-based inhibitors of *Helicobacter pylori*. **T. Epstein**, B. Wu, M. Yan, D.H. Dube

CARB 22. Examining the glycosylation pathway in *Helicobacter pylori* using mass spectrometry. **C. Liu**, D.H. Dube



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- CARB 23.** Interplay of protecting groups and side chain conformation in glycopyranosides and azasugars as models for glycosylation reactions. S. Dharuman, H. Amarasekara, **P. Rajasekaran**, D. Crich
- CARB 24.** Synthesis and self-assembling property of a series of D-galactose and D-glucose triazole derivatives. **P. Sharma**, A. Chen, D. Wang, G. Wang
- CARB 25.** Synthesis of higher carbon sugars thio-functionalized with heterocycles. D. Kim, **Z.J. Witczak**, R. Bielski, D.E. Mencer, S. Jarosz, M. Cieplak
- CARB 26.** Hybrid conversion of D-fructose to 5-acetoxymethylfurfural. **N.T. Huynh**, J. Cho
- CARB 27.** Optimizing polysaccharides and cyclodextrin blends for electrospinning: Sustainable biomaterials for active packaging. **D. Poudel**, S.F. Okeefe, C. Fernandez Fraguas
- CARB 28.** Synthesis of neoglycoproteins as potential diagnostic tools for cutaneous leishmaniasis. **A.L. Montoya**, K.S. Subramaniam, V. Austin, A. Acosta-Serrano, K. Michael
- CARB 29.** Synthesis of neoglycoproteins as potential biomarkers and vaccines for Chagas disease. **E. Garcia Carvajal**, S. Portillo, F. Avci, I. Almeida, K. Michael
- CARB 30.** Synthesis and self-assembling properties of cationic glycolipids. **J. Morris**, G. Wang
- CARB 31.** Boron-catalyzed site-selective reduction and cyclization of carbohydrate-derivatives with catecholborane. **J. Lowe**, Y. Seo, M.R. Gagne
- CARB 32.** Development of 4,2'-pyridine-2-mercaptopyrimidine glycosides. **T.L. Nolkemper**, **E.A. Lind**, S.J. Hasty
- CARB 33.** Leaving group based hydrogen bonding influencing stereoselective outcome in carbohydrates. **S.R. Easley**, **S.D. Rivero**, S.J. Hasty
- CARB 34.** Towards the development of self-adjuvanting carbohydrate conjugate vaccines against cancer using monophosphoryl lipid A. **B. Smith**, Z. Guo
- CARB 35.** Formation of unexpected chromane heterocycle from dihydrolevoglucosenone. C. Hager, **Z.J. Witczak**, R. Bielski, D.E. Mencer
- CARB 36.** Topology and life: Golden ratio on pentagon surface. **C. Mitan**, E. Bartha, C. Draghici, M. Caproiu, P. Filip, R. Moriarty
- CARB 37.** Euler-Hückel approach in prediction of the conformational parameters. **C. Mitan**, E. Bartha, C. Draghici, M. Caproiu, P. Filip, R. Moriarty
- CARB 38.** Synthesis and Testing of monopicoloylated thiosialosides. **A. Behm**, S. Geringer, M. Lohman, S. Escopy, C. De Meo
- CARB 39.** Hopf fibration and Hückel theories on torsional angles. **C. Mitan**, E. Bartha, C. Draghici, M. Caproiu, P. Filip, R.M. Moriarty
- CARB 40.** Synthesis and Testing of dipicoloylated thiosialosides. **C. Dean**, B. Jones, M. Shadrick, C. De Meo



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

CARB 41. Synthesis of carbohydrate phthalocyanine conjugates for photodynamic therapy. **J.L. Bost**, S.L. Cooper, G. Cambronerio, K.W. Graepel, J.V. Ruppel, **N.L. Snyder**

CARB 42. Charge-complementary co-assembling tags as building blocks for peptide nanofibers bearing diverse N-linked glycans. **D.T. Seroski**, L. Astrab, T. Roland, G. Hudalla

CARB 43. Synthesis of hyaluronic acid mimetics for targeting CD44. **G. Alvarez**, **A. Sizemore**, **N. Minanov**, M.A. Vencil, M.L. Regan, D.G. Dennis, E. Xu, **N.L. Snyder**, J.V. Ruppel

CARB 44. Comparison of fructose-1,6-bisphosphate (fbp) aldolase inhibitors by structure and K_i to evaluate neokestose-1,6-di-phosphate as a potential inhibitor of fbp aldolase. J. Christus, **M.A. Madson**

General Posters

Sponsored by CELL, Cosponsored by ANYL and CARB

MONDAY MORNING

Section A

Orange County Convention Center
Room W224GH

Chemical Biology of Glycoproteins

O-Linked Glycosylation

Cosponsored by CELL
Financially supported by Advop Company, Limited, China
L. Wang, *Organizer*
Z. Tan, *Organizer, Presiding*

9:00 Introductory Remarks.

9:05 CARB 45. Synthesis of GPI-anchored glycoproteins. **P.H. Seeberger**

9:35 CARB 46. Uncovering the roles of O-GlcNAc in neurodegeneration using synthetic protein chemistry. **M. Pratt**

10:05 CARB 47. O-GlcNAc: A sweetheart of the cell cycle. **J. Li**

10:35 Intermission.

10:45 CARB 48. Effects of O-linked glycans on protein properties. **Z. Tan**

11:15 CARB 49. Efficient synthesis and structure-activity relationship studies of Lewis X / Y class antigens. **Q. Li**, W. Jiang, J. Guo, Z. Guo



TECHNICAL PROGRAM

11:35 CARB 50. Fighting cancer with a sweet bullet: rational design of mucin-1 based anticancer vaccines. **X. Wu**, X. Huang

Section B

Orange County Convention Center
Room W230D

Nucleic Acids-Based Therapeutics

Cosponsored by BIOL and MEDI
M. J. Damha, M. Manoharan, *Organizers*
Y. Tor, *Presiding*

9:00 CARB 51. Expanding the chemist's toolbox with the new, the old, and not so ugly nucleic acid analogues. **M.J. Damha**

9:25 Discussion.

9:30 CARB 52. Amide-modified RNA: Synthesis, structure, and RNAi activity. **E. Rozners**

9:55 Discussion.

10:00 CARB 53. Biomimetic chemistry of RNAi therapeutics. **M. Manoharan**

10:25 Discussion.

10:30 Intermission.

10:45 CARB 54. Structure-assisted discovery and optimization of next generation small interfering RNAs. **M. Egli**, J. Harp, L. Lei, P.S. Pallan, M. Seo

11:10 Discussion.

11:15 CARB 55. Bump/hole approach to oligonucleotide-directed RNA editing. **P.A. Beal**

11:40 Discussion.

11:45 CARB 56. Azobenzene-containing photoresponsive siRNAs. **J. Desaulniers**, M. Hammill

12:10 Discussion.

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Sponsored by PROF, Cosponsored by AGFD, ANYL, BIOL, BIOT, CARB, CELL, CHED, CMA, COLL, COMP, ENVR, GEOC, I&EC, MEDI, MPPG, NUCL, ORGN, PHYS, PMSE, POLY, PRES, WCC and YCC



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

Advances in Renewable Materials

Sponsored by CELL, Cosponsored by ANYL and CARB

Interplay of Cellulose & Other Biopolymers in Biological & Designed Materials Systems

Xylan & Lignin Interactions with Cellulose

Sponsored by CELL, Cosponsored by ANYL, BIOL and CARB

MONDAY AFTERNOON

Section A

Orange County Convention Center
Room W224GH

Chemical Biology of Glycoproteins

N-Linked Glycosylation

Cosponsored by CELL
Financially supported by Advop Company, Limited, China
Z. Tan, *Organizer*
L. Wang, *Organizer, Presiding*

2:00 Introductory Remarks.

2:05 CARB 57. Streamlining the chemoenzymatic synthesis of complex *N*-glycans by a stop-and-go strategy. **G. Boons**

2:35 CARB 58. Machine-driven chemoenzymatic synthesis of oligosaccharides and glycopeptides by a peptide synthesizer. **P.G. Wang**

3:05 CARB 59. Directed evolution of HIV vaccine glycopeptide antigens templated on the PGT128 antibody. **I.J. Krauss**

3:35 Intermission.

3:45 CARB 60. Studies towards human interleukin-17A: Chemical synthesis and investigation of *N*-glycan functions. **S. Dong**

4:15 CARB 61. Development of peptidyl coupling strategy at sterically hinderance peptide ligation sites. **Q. Zhang**

4:45 CARB 62. HPAE-PAD analysis of N-linked oligosaccharides from glycoproteins using dual eluent generation cartridge mode. **B. Huang, J. Rohrer**



TECHNICAL PROGRAM

Section B

Orange County Convention Center
Room W230D

Nucleic Acids-Based Therapeutics

Cosponsored by BIOL and MEDI
M. J. Damha, M. Manoharan, *Organizers*
E. Rozners, *Presiding*

2:00 CARB 63. Controlling chirality of phosphorothioate linkages in the DNA gap does not enhance potency of gapmer antisense oligonucleotides (ASO) in the liver or CNS. **W.B. Wan**, K. Ling, F.W. Rigo, W.J. Drury, P.P. Seth, E.E. Swayze

2:25 Discussion.

2:30 CARB 64. Designing and implementing isomorphous, isofunctional, fluorescent nucleosides and nucleotides. **Y. Tor**

2:55 Discussion.

3:00 CARB 65. Janus PNAs: PNA Analogues for simultaneous recognition of two complementary DNA/RNA strands for programmable supramolecular assemblies. M. Gupta, D. Datta, **K. Ganesh**

3:25 Discussion.

3:30 CARB 66. Overview of dinucleotide mRNA cap analogues: Design, synthesis, and biological evolution towards mRNA therapeutics. **A. Kore**

3:55 Discussion.

4:00 Intermission.

4:15 CARB 67. Rationally designed anti-CRISPR nucleic acid inhibitors of CRISPR-Cas9. **K.T. Gagnon**

4:40 Discussion.

4:45 CARB 68. Conception of mur ligase analogues for antibacterial activity. **V.O. Hervin**, L. Agrofoglio, C. Hoarau, V. Roy, U. Bajpai

5:00 Discussion.

5:05 CARB 69. DNA-based precision glycoalyx engineering. **S. Purcell**, N. Marroquin, T. MacCulloch, N. Stephanopoulos, K. Godula

5:20 Discussion.

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

Sponsored by PROF, Cosponsored by AGFD, ANYL, BIOL, BIOT, CARB, CELL, CHED, CMA, COLL, COMP, ENVR, GEOC, I&EC, MEDI, MPPG, NUCL, ORGN, PHYS, PMSE, POLY, PRES, WCC and YCC

Ionic-Liquids Processing of Polysaccharides

Sponsored by CELL, Cosponsored by ANYL and CARB

MONDAY EVENING

Section A

Orange County Convention Center
West Hall C

Sci-Mix

S. J. Sucheck, *Organizer*

8:00 - 10:00

11-17, 20, 23, 26, 28-31, 33-34, 41-43, 62. See previous listings.

TUESDAY MORNING

Section A

Orange County Convention Center
Room W240D

Exploration of Carbohydrate/Protein Interactions/Recognition: The Latest Techniques & Achievements

Cosponsored by CELL
P. G. Wang, *Organizer, Presiding*

8:30 Introductory Remarks.

8:40 CARB 70. Investigating antibody-carbohydrate recognition with the aid of carbohydrate microarrays. **J. Gildersleeve**

9:05 CARB 71. Defining the specificity of carbohydrate–protein interactions by quantifying functional group contributions. A. Sood, O.O. Gerlits, Y. Ji, N.V. Bovin, L. Coates, **R.J. Woods**

9:30 CARB 72. Fast and high-throughput detection of glycan-binding proteins. **P.G. Wang**

9:55 Intermission.



TECHNICAL PROGRAM

10:25 CARB 73. Drug candidate may slow metastasis in oral cancer by affecting *N*-linked glycosylation on the epidermal growth factor receptor (EGFR). K.B. Chandler, K. Alamoud, V.L. Stahl, K. Sadykov, S. Monti, M.A. Kukuruzinska, **C.E. Costello**

10:50 CARB 74. Modulating antibody-Fc receptor interactions through modifications of core fucosylation. **L. Wang**

11:15 CARB 75. Synthetic carbohydrate receptors with potent anti-Zika virus activity. **A.B. Braunschweig**, k. Palanichamy, H. Garg, A. Joshi

11:40 CARB 76. Sweet way to boost the efficacy of NK cell-based immunotherapy. **P. Wu**

Section B

Orange County Convention Center
Room W240C

Opportunities and Challenges in Carbohydrate Synthesis B

Cosponsored by CELL and ORGN
H. M. Nguyen, *Organizer*
S. J. Sucheck, *Presiding*

8:00 CARB 77. Synthesis of heparan sulfate oligosaccharides and glycopeptides. **X. Huang**, W. Yang, J. Gao, Y. Xu, J. Liu

8:30 CARB 78. Chemical synthesis of glucooligosaccharides directly from glucose as potential prebiotics. N. Li, Z. Wang, T. Qu, J. Oh, J. van Pijkeren, G.W. Huber, **X. Pan**

9:00 CARB 79. Total synthesis of bacterial polysaccharide PS A1 with alternating charges on adjacent monosaccharides. **P.R. Andreana**

9:30 CARB 80. Challenges and opportunities in the synthesis of trehalose-based macromolecules. **N.L. Snyder**

10:00 Intermission.

10:15 CARB 81. Solution and polymer-supported methods for the synthesis of oligosaccharide components of vaccines. **S.J. Sucheck**

10:45 CARB 82. Expanding the picoloyl effect in sialylations. **C. De Meo**

11:15 CARB 83. Stereocontrolled glycosylations in the absence of directing groups. **C. Bennett**

Advanced Chemistry of "Non-Traditional" Polysaccharides

Sponsored by CELL, Cosponsored by AGFD, ANYL, BIOL and CARB

TUESDAY AFTERNOON



TECHNICAL PROGRAM

Section A

Orange County Convention Center
Room W240D

Exploration of Carbohydrate/Protein Interactions/Recognition: The Latest Techniques & Achievements

Cosponsored by CELL
P. G. Wang, *Organizer*
R. R. Drake, *Presiding*

1:30 CARB 84. Adapting N-glycan MALDI imaging mass spectrometry workflows to create new chemo-enzymatic glycan profiling strategies for tissues, cells, and slide arrays. **R.R. Drake**

1:55 CARB 85. Genetically encoding bioreactive unnatural amino acids. **L. Wang**

2:20 CARB 86. Polysaccharide-lipid interactions. A theoretical study using molecular dynamics simulations and quantum chemical ^{13}C NMR spectra computation. **F. Jolibois**, A. Schahl, V. Réat

2:45 Intermission.

3:15 CARB 87. Dissecting multivalent protein-carbohydrate interactions using polyvalent multifunctional glycan-nanoparticles. Y. Guo, E. Poole, C. Sakonsinsiri, B. Turnbull, **D. Zhou**

3:40 CARB 88. Nanotechnology-based glycan analysis: Application in glycomics and diagnostics. **J. Tkac**, T. Bertok, L. Lorencova, M. Hires, E. Jane, E. Chocholova, F. Kveton, A. Blsakova

4:05 CARB 89. Carbohydrate-functionalized conductive polymer biointerface: Fabrication, characterization, and application for protein analysis. **X. Zeng**

4:30 CARB 90. 3D-printing model for ECM morphogenesis: Dual roles of a GPI-anchored structural organizer in the formation and layering of the complex ECM. D. Kim, A. Almishaal, **S. Park**

Section B

Orange County Convention Center
Room W240C

Opportunities and Challenges in Carbohydrate Synthesis B

Cosponsored by CELL and ORGN
H. M. Nguyen, *Organizer*
C. Bennett, *Presiding*

1:30 CARB 91. Catalytic stereoselective synthesis of glycosides: Old catalysts, new tricks. **M. Galan**

2:00 CARB 92. Catalytic site-selective acylation and alkylation of carbohydrates. **W. Tang**

2:30 CARB 93. Highly stereo-selective glycosylation. **F. Yu**



TECHNICAL PROGRAM

3:00 Intermission.

3:20 **CARB 94.** Stereoselective synthesis of oligosaccharides and glycoconjugates bearing β -mannopyranosides and β -mannosamines by anomeric O-alkylation. **J. Zhu**

3:50 **CARB 95.** Exploring cycloaddition reactions of glycals. **C.E. Marzabadi**, A. Abdullahi, A. Altamura

4:20 **CARB 96.** Synthesis of a cyclopropyl-containing mechanism-based glycoside hydrolase inhibitor. **S. Kapil**, S.J. Suheck

4:50 **CARB 97.** From stereocontrolled glycosylation to automated oligosaccharide synthesis. **A. Demchenko**

Ionic-Liquids Processing of Polysaccharides

Sponsored by CELL, Cosponsored by ANYL and CARB

Advanced Chemistry of "Non-Traditional" Polysaccharides

Sponsored by CELL, Cosponsored by AGFD, ANYL, BIOL and CARB

WEDNESDAY MORNING

Section A

Orange County Convention Center
Room W240D

Exploration of Carbohydrate/Protein Interactions/Recognition: The Latest Techniques & Achievements

Cosponsored by CELL
P. G. Wang, *Organizer*
L. Wang, *Presiding*

8:30 **CARB 98.** Multivalent inhibitors of protein carbohydrate interactions. **R.J. Pieters**

8:55 **CARB 99.** Mutant cell library for systematic analysis of heparan sulfate structure-function relationships. **L. Wang**

9:20 **CARB 100.** Investigation of pore-forming bacterial toxin-GPI interactions using synthetic GPIs. **Z. Guo**

9:45 Intermission.

10:15 **CARB 101.** Chemical approaches to exploration of protein-glycan interactions of natural glycans. **X. Song**

10:40 **CARB 102.** Synthesis and development of peptidoglycan fragment microarray and probes to investigate innate immune signaling. **J. Zhou**, K. Lazor, C.L. Grimes



TECHNICAL PROGRAM

11:05 CARB 103. Automated identification of gradations in determinant fine-specificities from glycan array data. Z. Klamer, **B. Haab**

11:30 CARB 104. Elucidating global glycan-protein interactions in native cellular environments. **M. Huang**

Bioactive Delivery: Frontiers in Biomaterials

Sponsored by CELL, Cosponsored by ANYL, BIOL and CARB

WEDNESDAY AFTERNOON

Section A

Orange County Convention Center
Room W240D

Exploration of Carbohydrate/Protein Interactions/Recognition: The Latest Techniques & Achievements

Cosponsored by CELL
P. G. Wang, *Organizer*
K. J. Yarema, *Presiding*

2:00 CARB 105. Control of protein recognition through modulation of amino sugar metabolism. C.T. Saeui, M.P. Mathew, S.R. Shaw, M. Martinez, R. Bhattacharya, A. Quinones-Hinojosa, N.E. Zachara, **K.J. Yarema**

2:25 CARB 106. Lectin microarrays for intact cell analysis. **S. TAO**

2:50 CARB 107. Glycan substructures specific for influenza cell and host tropisms. F. Wen, L. Li, L. Liu, Y. Lang, L. Li, P.G. Wang, **X.H. Wan**

3:15 Intermission.

3:45 CARB 108. Characterizing plant glycosyltransferases in high throughput using azido-functionalized sugar nucleotides on glycan arrays. C. Ruprecht, M.P. Bartetzko, D. Senf, A. Lakhina, M.J. Soto, P.J. Smith, B. Urbanowicz, **F. Pfrengle**

4:10 CARB 109. Development of high-affinity glycan analog ligands of siglecs and galectins. **C. Nycholat**, S. Duan, S. Willis, E. Wamhoff, C. Arthur, R. McBride, C. Rademacher, S. Stowell, J.C. Paulson

4:35 CARB 110. Bacterial derived peptidoglycans and their role in the regulation of immune responses in the human microbiome. **S. Mashayekh**, J. Burch, W. Drake, D. Wykoff, C.L. Grimes

Bioactive Delivery: Frontiers in Biomaterials



TECHNICAL PROGRAM

Sponsored by CELL, Cosponsored by ANYL, BIOL and CARB

CATL

Division of Catalysis Science & Technology

A. Savara, *Program Chair*

SUNDAY MORNING

Section A

Orange County Convention Center
Room W306A

Ipatieff Prize: Symposium in Honor of Ivo Hermans

C. A. Carrero, *Organizer*
L. Grabow, D. Rosenfeld, *Organizers, Presiding*

8:00 CATL 1. Methane challenge: C–H bond activation and C–C coupling. **H. Schwarz**, C. Geng, J. Li, X. Sun, L. Yue, S. Zhou

8:30 CATL 2. Selective hydrogenation using dilute PdAu alloys: Understanding catalyst evolution during reaction. **C.M. Friend**, M. Luneau, T. Shirman, R. Madix, J. Aizenberg, M. Aizenberg, W. Chen

9:00 CATL 3. Quantum mechanics based reaction mechanisms for heterogeneous catalysis: Selective oxidation and ammoxidation of alkanes and NH₃ synthesis. **W.A. Goddard**

9:30 CATL 4. Catalytic consequences of oxygen chemical potential on light alkane activation. **Y. Chin**, R. Yao

10:00 Intermission .

10:10 CATL 5. Models for strong metal support interaction (SMSI): from structure (geometric and electronic) to reactivity. **H. Freund**

10:40 CATL 6. Dynamic phase diagram for the catalytic surface of hexagonal boron nitride in conditions of oxidative dehydrogenation of propane. Z. Zhang, **A. Alexandrova**

11:10 CATL 7. Atomistic understanding of supported transition metal oxide catalysts in dehydrogenation reactions of methanol and propane. **J. Sauer**

11:40 CATL 8. Butene dimerization over cobalt oxide on N-doped carbon. Z. Xu, J. Chada, D. Zhao, C.A. Carrero, J. Rogers, I. Hermans, G.W. Huber, **D. Rosenfeld**



TECHNICAL PROGRAM

Section B

Orange County Convention Center
Room W306B

Mechano- & Tribochemistry & Catalysis

Cosponsored by I&EC
J. Mack, *Organizer*
R. G. Blair, *Organizer, Presiding*

8:00 Introductory Remarks.

8:10 CATL 9. Synthesis of polyaromatic hydrocarbons via mechanochemistry. **C. Wang**, J. Mack

8:30 CATL 10. Mechanochemical C–H-bond functionalization. **C. Bolm**, J.G. Hernandez

8:50 CATL 11. Mechanochemical routes for the synthesis of Schiff base ligands and coordination compounds relevant to catalysis. **T. Jurca**

9:10 CATL 12. Mechanochemical mélange: Milling and its consequences for catalyst generation. R.F. Koby, **T.P. Hanusa**

9:30 Intermission.

9:50 CATL 13. Thousand ways of monitoring mechanochemical reactions. **T. Friscic**

10:30 CATL 14. Ion pair reactions in the high speed ball mill. **L.N. Trankina**, J. Crain, C. Williams III, J. Mack

10:50 CATL 15. Tuning the potential: Stainless steel as an effective reducing agent for mechanochemical reactions. **R.A. Haley**, T. Estier, H. Guan, J. Mack

11:10 CATL 16. Additive manufacturing of catalytically active devices. J.S. Manzano, H. Wang, **I.I. Slowing**

11:30 CATL 17. 3D printed fixed-bed catalytic monolith for continuous chemistry. **B. Clark**, S. Smith, T. McIntosh, M. Dooley, J.K. Ferri, F. Gupton

Section C

Orange County Convention Center
Room W309A

Symposium in Honor of Chuck Peden's Research Career: Catalysis for Energy & the Environment

Cosponsored by ENFL, ENVR, I&EC and PHYS
F. Gao, J. Szanyi, *Organizers*
Y. Wang, *Organizer, Presiding*
C. Mims, *Presiding*

8:00 CATL 18. Kinetic isotope effects in catalysis. **C.T. Campbell**, Z. Mao



TECHNICAL PROGRAM

8:30 CATL 19. SiO₂/Al₂O₃ ratio and Cu-loading effects on the NH₃-SCR activity of Cu-Chabazite catalysts. R. Villamaina, I. Nova, E. Tronconi, M. Ruggeri, J. Collier, A. York, D. Thompsett

9:00 CATL 20. Response of alloy catalyst surfaces to changes in reaction conditions by LEIS. C. Mims, P. Brodersen, Y. Chin, A. Hensley, H. Nie, H. Cai

9:30 CATL 21. Environmental sensitivity of spectroscopic properties for Cu cations in Cu-SSZ-13: XANES and XES studies from first principles. R. Zhang, H. Li, K. Groden, E. Anderst, F. Gao, J. Szanyi, S.L. Scott, J. McEwen

10:00 Intermission.

10:15 CATL 22. Ten years of diesel and natural gas NO_x emission control catalysis: Empirical and modeling insights into catalyst lifecycles. A. Yezerets, K. Kamasamudram, J. Luo, J. Saurabh, Y. Tang, A. Srinivasan, Y. Zha, H. An, A. Kumar, D. Wang, J. Gong, M. Kim, J. Li, M. Cunningham, N. Currier

10:45 CATL 23. Imaging and chemical probing of the catalytic NO_x and O₂ reduction over Pt and Rh with sub-nanoscale lateral resolution. N. Kruse

11:15 CATL 24. Low temperature carbon monoxide oxidation on transition metal and metal oxide catalysts. Z. Lu, W. Chen, Y. Chin

Section D

Orange County Convention Center
Room W309B

Data Science for Catalysis Research

Cosponsored by CINF, COMP and ENFL
B. R. Goldsmith, H. J. Kulik, H. Xin, *Organizers, Presiding*

8:00 CATL 25. Possibilities and roadblocks in the machine-learning acceleration of atomistic calculations. A. Peterson

8:45 CATL 26. Simulating complex inorganic materials for energy applications with machine-learning potentials. N. Artrith

9:15 CATL 27. Design and analysis of machine-learning exchange-correlation functionals based on convolutional descriptors. A.J. Medford

9:45 CATL 28. Machine learning for accelerating discovery of perovskite electrocatalysts. H. Xin, Z. Li, N. Omidvar, L.E. Achenie

10:15 CATL 29. Utilizing machine learning for high throughput screening of bimetallic alloy catalysts for Fischer-Tropsch synthesis. O. Mamun, T. Bligaard

10:30 CATL 30. AI and machine learning guided design of electrocatalysts. S. Sankaranarayanan

11:00 CATL 31. Unraveling local atomic structures from X-ray absorption spectroscopy using theory and machine learning. D. Lu



TECHNICAL PROGRAM

11:30 CATL 32. Neural network approach for operando characterization of catalysts: From ultra-small clusters to nanoparticles. **A. Frenkel**, J. Timoshenko, N. Marcella, Y. Liu

Section E

Orange County Convention Center
Room W307A

Elucidation of Mechanisms & Kinetics on Surfaces

Mechanisms on Surfaces: C-C Coupling, C-H & C-O Bond Manipulations

Cosponsored by ENFL, ENVR, INOR and PHYS
L. Baker, S. Laursen, *Organizers*
A. Ignatchenko, A. Savara, *Organizers, Presiding*

8:00 CATL 33. Influence of support acid sites on Cu catalyzed non-oxidative dehydrogenation of ethanol to acetaldehyde. **P. Christopher**

8:20 CATL 34. Alkane dehydrogenation and wet/dry reforming over intermetallic compound catalysts: Tuning surface reactivity towards C, H, and O. **S. Laursen**, Y. Song, Y. He

9:00 CATL 35. Theoretical study of complex reaction mechanism, competitive reaction paths and the role of co-adsorbates. **L. Arnadottir**, K. Chukwu

9:20 CATL 36. Propane dehydrogenation on bimetallic alloys: selectivity descriptors and deactivation modes. R. Seemakurthi, Y. Xu, B. Bukowski, Y. Lee, E. Wegener, Z. Wu, J.T. Miller, **J.P. Greeley**

9:40 Intermission.

10:00 CATL 37. Ketonization of aldehydes on zirconium and cerium oxide surfaces. **M. Renz**, L.M. Orozco, A. Corma

10:20 CATL 38. Mechanism of the ketonic decarboxylation of carboxylic acids on zirconium oxide and other oxides. **M. Renz**, B. Oliver-Tomas, A. Corma

10:40 CATL 39. Decarboxylative ketonization mechanism: Rates of individual steps. **A. Ignatchenko**, M.E. Springer, R.M. Ibrahim

11:20 CATL 40. Mechanistic insights for C-C coupling of simple carbonyl compounds on CeO₂(111). C. Zhao, S.H. Overbury, D.R. Mullins, F.C. Calaza, A. Savara, **Y. Xu**

11:40 CATL 41. Transformations of metal oxides under reaction conditions and their consequence on lewis-acid catalyzed conversion of oxygenates. S. Najmi, C. Chang, M. Rasmussen, W. Medlin, A.J. Medford, **C. Sievers**

Section F

Orange County Convention Center
Room W310A

Computational Electrocatalysis



TECHNICAL PROGRAM

Cosponsored by COMP and ENFL
K. Schwarz, *Organizer*
R. Sundararaman, *Organizer, Presiding*

8:00 CATL 42. Universal scaling relations for the rational design of molecular water oxidation catalysts with near-zero overpotential. **M. Craig**, G. Coulter, E. Dolan, J. Soriano-López, M. Garcia-Melchor

8:20 CATL 43. Computational rational design of high-performance water oxidation electrocatalysts. **M. Garcia-Melchor**, M. Bajdich, A. Vojvodic

8:40 CATL 44. Exploring electrocatalytic processes at the Pt/water interface with cluster models and density functional theory. **J.A. Santana**, Y. Ishikawa

9:10 CATL 45. Electrochemical synthesis of hydrogen peroxide via different routes. **S. Siahrostami**

9:30 CATL 46. Toward understanding activity and selectivity trends in electrocatalytic nitrate reduction. **B.R. Goldsmith**, J. Liu, N. Singh, D. Richards

10:00 Intermission.

10:10 CATL 47. Understanding solvation effects on hydrogenation barriers for CO₂ reduction on zigzag edges of nitrogen-doped graphene. **Y. Basdogan**, J.A. Keith

10:40 CATL 48. Impacts of electrochemical environments on the catalytic activities of transition metals in C-C cleavage and C-O coupling towards complete ethanol oxidation. Z. Wu, B. Miao, R. Wu, **L. Wang**

11:00 CATL 49. Reaction mechanisms and design of electrocatalysts: oxygen reduction reaction (ORR), CO₂ reduction reaction (CO₂RR), and oxygen evolution reaction (OER). **W.A. Goddard**

11:40 CATL 50. Electrons in flatland: The electronic structure underlying electrocatalysis of 2D materials. **Y. Liu**

Section G

Orange County Convention Center
Room W310B

Advances in Methods for Comparing Molecular & Supramolecular Simulations to Experiments

Cosponsored by CINF, COMP and PHYS
D. Le, *Organizer*
T. S. Rahman, A. Savara, *Organizers, Presiding*

8:00 CATL 51. Advances in subensemble sampling to identify speciation, organization and dynamic response in complex solutions and interfaces. **A.E. Clark**

8:40 CATL 52. Accelerated molecular dynamics methods. **A.F. Voter**

9:00 CATL 53. Markov state model approach to simulating self-assembly at low concentrations. **M.F. Hagan**, S. Paquay



TECHNICAL PROGRAM

9:20 CATL 54. Parallel approaches to long-time atomistic simulations: Decomposition, replication, and speculation. **D. Perez**

9:40 Intermission.

10:00 CATL 55. Overcoming the time limitation in molecular dynamics simulation of crystal nucleation: A persistent-embryo approach. **K. Ho**, F. Zhang, Y. Sun, M. Mendeleev, C. Wang

10:20 CATL 56. GPU accelerated computation of isotropic chemical shifts offers new dimension of structure refinement in largescale molecular dynamics simulation. A. Bryer, S. Chandrasekaran, E. Wright, M. Ferrato, T. Huber, E. Ortiz, R. Searles, **J.R. Perilla**

10:40 CATL 57. Mechanism of the polymorphism and curvature control of the HIV capsid protein assemblies probed by a novel coarse grain model. **B. Chen**

11:00 CATL 58. Growth of fivefold-twinned Cu and Ag nanowires. **K.A. Fichthorn**, Z. Chen, X. Qi

11:20 CATL 59. Self Learning Kinetic Monte Carlo (SLKMC) method for cluster diffusion on surfaces. **T.S. Rahman**

11:40 CATL 60. SQERTSS & SQERTT: Dynamic throttling of KMC rate constants to achieve experimental timescales in simulations. T. Danielson, J. Sutton, C. Hin, **A. Savara**

Innovative Chemistry & Materials for Electrochemical Energy Storage

Li-Ion & Na-Ion

Sponsored by ENFL, Cosponsored by CATL, INOR and PMSE

Carbon Dioxide Conversion & Utilization

CO₂ Hydrogenation to Fuels & Chemicals

Sponsored by ENFL, Cosponsored by CATL, COMP and GEOC

SUNDAY AFTERNOON

Section A

Orange County Convention Center
Room W306A

Ipatieff Prize : Symposium in Honor of Ivo Hermans



TECHNICAL PROGRAM

D. Rosenfeld, *Organizer*
C. A. Carrero, L. Grabow, *Organizers, Presiding*

1:00 CATL 61. Getting the most from molecular oxygen: Low overpotential O₂ reduction and its implications for aerobic oxidation reactions and fuel cells. **S.S. Stahl**

1:30 CATL 62. Selective oxidation of hydrocarbons over metal oxides: Effects of metal oxide and hydrocarbon properties. **A.T. Bell**

2:00 CATL 63. Catalysis researchers caused climate change: What can we do to reverse it? **C.W. Jones**

2:30 CATL 64. *N*-hydroxyphthalimide catalysis in liquid phase aerobic oxidations: An ongoing story. **C. Punta**, M. Petroselli, M. Caruso, L. Melone, M. Cametti

3:00 Intermission .

3:10 CATL 65. C-H activation by ozone in liquid carbon dioxide at ambient temperatures. X. Chen, D. Rice, A.M. Danby, M.D. Lundin, T.A. Jackson, **B. Subramaniam**

3:40 CATL 66. Drowning out the uncertainty of using catalysis to recycle water. **M.A. Reynolds**, M.S. Wong, C.L. Coonrod, Y. Yin

4:10 CATL 67. Complex kinetics of oxidative coupling and hydro-deoxygenation. **W.H. Green**

Section B

Orange County Convention Center
Room W306B

Mechano- & Tribochemistry & Catalysis

Cosponsored by I&EC
R. G. Blair, *Organizer*
J. Mack, *Organizer, Presiding*

1:00 CATL 68. Mechanocatalytic reduction of carbon dioxide for the realization of formic acid. R.G. Blair, **K.L. Chagoya**, D.J. Nash

1:20 CATL 69. Mechanochemical synthesis of supported nanoparticles on porous materials: the MOF effect. **R. Luque**

1:40 CATL 70. Role of the support and the solvent on the transfer hydrodeoxygenation of HMF to DMF on carbon supported ruthenium catalysts.. **S. Prodinge**r, R.F. Lobo

2:00 CATL 71. Understanding mechanocatalytic reaction pathways: Surface chemistry at the solid-solid interface. **W.T. Tysoe**

2:40 Intermission.



TECHNICAL PROGRAM

3:00 CATL 72. Evaluating the mechanisms of catalysis of defect laden *h*-BN at the micro- and nano-scales. F. Torres-Davila, Y. Ding, **L. Tetard**

3:20 CATL 73. Mechanochemical synthesis of supported catalysts. **F. Schueth**, M. Felderhoff, S. Immohr, H. Schreyer, A. Amrute

3:40 CATL 74. Mechanochemical and aging-based methods towards metal nanoparticles synthesis and biopolymers functionalization. **A.H. Moores**

4:00 CATL 75. Mechanocatalytic depolymerization of lignin. A. Tricker, K. Hebisch, A. Brittain, V. Thomas, M.J. Realff, **C. Sievers**

4:20 Concluding Remarks.

Section C

Orange County Convention Center
Room W309A

Symposium in Honor of Chuck Peden's Research Career: Catalysis for Energy & the Environment

Cosponsored by ENFL, ENVR, I&EC and PHYS
Y. Wang, *Organizer*
F. Gao, J. Szanyi, *Organizers, Presiding*

1:00 CATL 76. Computational studies of catalytic reactions of metal oxide clusters and single site metals. **D.A. Dixon**

1:30 CATL 77. Selective review of reactions and catalysts important in automotive emissions control. **G.B. Fisher**, C. Seo, X. Chen, A. Hill, J.W. Schwank, A. Reihani, J.W. Hoard

2:00 CATL 78. Activation of H-H and C-H bonds on oxide supported single Pd atoms. **Z. Dohnalek**

2:30 CATL 79. Characterization of the surface species on carbon supported Pd and Pt catalysts. **S.F. Parker**, S. Mukhopadhyay, M. Jiménez-Ruiz, P.W. Albers

3:00 Intermission.

3:15 CATL 80. Review of fuel sulfur effects on vehicle emissions and catalyst monitoring systems. **S. Oh**

3:40 CATL 81. Advancement of automotive catalysts: Journey to the zero NO_x and hydrocarbon emissions for internal combustion engines. **C.H. Kim**

4:05 CATL 82. Combining in situ NMR and reaction calorimetry to study the catalytic reduction of phenol in aqueous media. **T. Autrey**, T. He, R. Kumar, A.J. Karkamkar, J.C. Linehan

4:30 CATL 83. Copper mobility in zeolite-based SCR catalysts. **M. Skoglundh**, S. Shwan, L. Chen, P.N. Vennestrøm, T.V. Janssens, L.F. Lundegaard, R. Tiruvalam, H. Falsig, A. Carlsson, J. Jansson

4:55 CATL 84. Catalysis for energy and the environment: A research career (so far). **C.H. Peden**



TECHNICAL PROGRAM

Section D

Orange County Convention Center
Room W309B

Data Science for Catalysis Research

Cosponsored by CINF, COMP and ENFL
B. R. Goldsmith, H. J. Kulik, H. Xin, *Organizers, Presiding*

- 1:00 CATL 85.** Text and data mining for material synthesis. **E. Olivetti**
- 1:45 CATL 86.** Artificial intelligence for chemical sciences. J. Lansford, J. Feng, M. Katsoulakis, **D.G. Vlachos**
- 2:15 CATL 87.** Identifying physical descriptors for predicting metal-support interactions in catalysis. **T. Senftle**
- 2:45 CATL 88.** Catalysis-hub.org: An open electronic structure database for surface reactions and catalytic materials. **K.T. Winther**, M.J. Hoffmann, O. Mamun, J.R. Boes, M. Bajdich, T. Bligaard
- 3:15 CATL 89.** Addressing uncertainty in machine learning model predictions for inorganic complex discovery. **J. Janet**, A. Nandy, C. Duan, H.J. Kulik
- 3:45 CATL 90.** Structure–activity relationships to identify promising metal–organic frameworks for the catalytic oxidation of methane. **A.S. Rosen**, J.M. Notestein, R. Snurr
- 4:00 CATL 91.** Sequential learning for (autonomous) design of catalysts. **B. Meredig**
- 4:30 CATL 92.** Break the limitation of small dataset in materials science. **C. Ling**
- 5:00 CATL 93.** Using artificial intelligence to discover new materials. **C. Wolverton**

Section E

Orange County Convention Center
Room W307A

Elucidation of Mechanisms & Kinetics on Surfaces

Reductions & Hydrogenations

Cosponsored by ENFL, ENVR, INOR and PHYS
A. Ignatchenko, S. Laursen, A. Savara, *Organizers*
L. Baker, *Organizer, Presiding*
S. Laursen, *Presiding*

- 1:00 CATL 94.** Mechanistic study of CO₂ reduction on metal-oxide catalysts. **P. Liu**, J.G. Chen, J. Rodriguez, S. Kattel
- 1:20 CATL 95.** Mechanistic studies for the forward and reverse water-gas shift reaction on Cu-ceria catalysts. **J. Rodriguez**



TECHNICAL PROGRAM

1:40 CATL 96. Nanoscale engineering of efficient oxygen reduction electrocatalysts by tailoring the local chemical environment of Pt surface sites. **S. Linic**

2:20 CATL 97. Formation and thermal stability of subsurface hydrogen and its reactivity for the hydrogenation of CO on Ni(110). **B.E. Koel**

2:40 CATL 98. Control of hydrogenation vs. H₂ evolution selectivity in photocatalytic CO₂ reduction by H₂O only. **S. Laursen, S. Poudyal**

3:00 Intermission.

3:20 CATL 99. *Ab Initio* prediction of proton exchange barriers for alkanes at brønsted sites of zeolite H-MFI. **J. Sauer**

3:40 CATL 100. Computational operando spectroscopy and kinetics for single atom catalysis. K. Alexopoulos, Y. Wang, **D.G. Vlachos**

4:00 CATL 101. Mechanistic role of ionic Cu species in dimethyl ether homologation. **C.A. Farberow, S. Kim, S. Habas, C. Nash, A.T. To, J. Hensley, J. Schaidle, D.A. Ruddy**

4:20 CATL 102. Bayesian chemisorption theory of catalysis. **H. Xin, S. Wang**

4:40 CATL 103. H₂ oxidation over supported Au nanoparticle catalysts: Mechanistic evidence for heterolytic H₂ activation at the metal-support interface. **B.D. Chandler, T. Whittaker, S. Kumar, L. Grabow**

5:00 CATL 104. Mechanistic description of the ring hydrogenation of m-cresol on Pt catalysts. N. Duong, C. Abreu Teles, F. Noronha, **D.E. Resasco**

Section F

Orange County Convention Center
Room W310A

Computational Electrocatalysis

Cosponsored by COMP and ENFL
K. Schwarz, R. Sundararaman, *Organizers*
K. Schwarz, *Presiding*

1:00 CATL 105. Understanding structure-property relationships in catalysts using cluster expansions. **C. Li, T. Mueller**

1:20 CATL 106. Computational chemistry for understanding and simulating single-crystal voltammetry. **M. Koper**

2:00 CATL 107. Azide anion formation during electrochemical oxidation of ammonia on Pt(100) electrode: First-principles study. **D. Skachkov, V. Chitturi, Y. Ishikawa**

2:20 CATL 108. Computational design of two-dimensional pentagonal materials for hydrogen evolution reaction. **H. Zhuang, L. Liu, D. Wang**

2:50 Intermission.



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- 3:00 CATL 109.** Carbon capture properties of two-dimensional calcium hydroxide. V.O. Ozcelik, K. Gong, **C.E. White**
- 3:30 CATL 110.** Analyzing halide promoted corrosion of Pd surfaces with density functional theory. **M. Groenenboom**
- 4:00 CATL 111.** Electrochemical reduction of CO₂ on ligand-protected metal nanoclusters. **D. Alfonso**, D. Kauffman, D. Tafen
- 4:30 CATL 112.** Large-scale DFT simulation on metallic nanoparticle catalysts. **A. Nakata**, T. Miyazaki

Section G

Orange County Convention Center
Room W310B

Advances in Methods for Comparing Molecular & Supramolecular Simulations to Experiments

Cosponsored by CINF, COMP and PHYS
T. S. Rahman, *Organizer*
D. Le, A. Savara, *Organizers, Presiding*

- 1:00 CATL 113.** Generalized temporal acceleration scheme for kinetic Monte Carlo simulations of surface catalytic processes by scaling the rates of fast reactions. **C. Plaisance**, E. Dybeck, M. Andersen, M. Neurock, K.U. Reuter
- 1:20 CATL 114.** Multiscale modeling, coupling DFT to KMC to CFD and comparison to experiment: A success story with CO oxidation over RuO₂. J.E. Sutton, J. Lorenzi, J. Krogel, Q. Xiong, S. Pannala, S. Matera, **A. Savara**
- 1:40 CATL 115.** Another approach to heterogeneous catalysis. **M.A. Gosalvez**, J. Alberdi-Rodriguez
- 2:00 CATL 116.** Machine-learning and energy decomposition analysis of adsorbate binding on low-symmetry catalyst nanoclusters. **A. Ramasubramaniam**
- 2:20 CATL 117.** "multi-timescale" model for calculating energies, free energies, activation energies, and rate constants of heterogeneously catalyzed reactions under liquid phase. **R. Getman**
- 2:40** Intermission.
- 3:00 CATL 118.** Ionic polyimide composite membranes for gas separation: Predicting experimental performance with Kinetic Monte Carlo. **C.H. Turner**, J.E. Bara, A. Abedini
- 3:20 CATL 119.** Theoretical study of oxygen reduction reactions in alkaline solution. S. Liu, **P. Liu**
- 3:40 CATL 120.** Simulation and optimization of temporal analysis of products (TAP) curves from micro-kinetic models. **A.J. Medford**, A. Yonge
- 4:00 CATL 121.** Extending attainable timescales in molecular dynamics simulations using adaptive Kinetic Monte Carlo: structural rearrangements in catalytic core-shell nanoparticles. **L. Koziol**, L. Li, Z. Duan, G. Henkelman
- 4:20 CATL 122.** Combined quantum mechanical and molecular mechanical methods and software for metal-organic frameworks. **X. Wu**, L. Gagliardi, D.G. Truhlar



TECHNICAL PROGRAM

Innovative Chemistry & Materials for Electrochemical Energy Storage

Li-Ion & Na-Ion

Sponsored by ENFL, Cosponsored by CATL, INOR and PMSE

Carbon Dioxide Conversion & Utilization

CO₂ Conversion to Carbonates

Sponsored by ENFL, Cosponsored by CATL, COMP and GEOC

MONDAY MORNING

Section A

Orange County Convention Center
Room W306A

Ipatieff Prize : Symposium in Honor of Ive Hermans

L. Grabow, *Organizer*

C. A. Carrero, D. Rosenfeld, *Organizers, Presiding*

8:00 CATL 123. Analysis of coverage transients (ACT): Application to propylene epoxidation on gold/titanosilicate catalysts. **S.T. Oyama**, J.J. Bravo Suarez, K. Bando

8:30 CATL 124. Catalytic activity of ultra-small, homogeneously alloyed bimetallic nanoparticles prepared by co-electrostatic adsorption. L.T. De Castro, A. Shakouri, R.D. Adams, C.T. Williams, **J.R. Regalbuto**

9:00 CATL 125. Supported bimetallic noble metal catalysts prepared by use of bifunctional organic chelates. **S. Soled**, S. Miseo, C.E. Kliewer, M.P. Lanci, J. Guzman

9:30 CATL 126. Elucidating structure-performance relationships in zeolite catalysis. **J.D. Rimer**

10:00 Intermission .

10:10 CATL 127. Metal organic framework-based catalysts for oxidation of light hydrocarbons to alcohols. J. Vitillo, M. Simons, A. Bhan, C.J. Cramer, C.C. Lu, **L. Gagliardi**

10:40 CATL 128. C-H bond activation by single metal atom catalysts under mild conditions. **M. Flytzani-Stephanopoulos**, M. Li, J. Shan, G. Giannakakis, J. Liu, A. Trimpalis



TECHNICAL PROGRAM

11:10 CATL 129. Characterization of ODH heterogeneous boron catalysts by high-resolution solid-state NMR spectroscopy. B. Thomas, A. Love, M. Cendejas, I. Hermans, **A.J. Rossini**

11:40 CATL 130. Cost advantaged feeds for creating new businesses for ExxonMobil using oxidation technology. **J.M. Dakka**

Section B

Orange County Convention Center
Room W306B

Gabor A. Somorjai Award for Creative Research in Catalysis: Symposium in Honor of Manos Mavrikakis

S. Rangarajan, L. T. Roling, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 CATL 131. Heterogeneous catalyst design at the single atom limit. **M. Flytzani-Stephanopoulos**

8:35 CATL 132. Trends in catalysis by atomically dispersed supported metals. **B.C. Gates**

9:05 CATL 133. Electrochemical ammonia synthesis. **J.K. Nørskov**

9:35 Intermission.

9:55 CATL 134. Catalytic conversion of biomass-derived oxygenated hydrocarbons. **J.A. Dumesic**

10:25 CATL 135. Identifying the rate- and selectivity-determining steps for heterogeneously catalyzed reactions. **A.T. Bell**

10:55 CATL 136. Surface science approach to the molecular level integration of the principles in heterogeneous, homogeneous, and enzymatic catalysis. **G.A. Somorjai**

11:25 CATL 137. Aqueous-phase hydrogenation of phenol and benzaldehyde on carbon-supported Pt, Pd and Rh. N. Singh, U. Sanyal, O.Y. Gutiérrez, D.M. Camaioni, J. Lercher, **C.T. Campbell**

Section C

Orange County Convention Center
Room W309A

Symposium in Honor of Chuck Peden's Research Career: Catalysis for Energy & the Environment

Cosponsored by ENFL, ENVR, I&EC and PHYS

Y. Wang, *Organizer*

F. Gao, J. Szanyi, *Organizers, Presiding*

8:00 CATL 138. Strong metal-support interactions and the generation of highly active catalysts for C1 chemistry. **J. Rodriguez**



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

8:30 CATL 139. Catalysis for automotive emission control: Lessons learned and next challenges. **C. Lambert**

9:00 CATL 140. Towards atomic level understanding of structures and surfaces of transition aluminas. **L. Kovarik**, M. Bowden, A. Andersen, N. Washton, D. Shi, K. Khivantsev, J. Szanyi, J. Kwak, C.H. Peden

9:30 CATL 141. Catalytic approaches to reducing automotive exhaust emissions at low temperatures. **T.J. Toops**, M. Kidder, S. Tan, E. Kyriakidou

10:00 Intermission.

10:15 CATL 142. Catalytic science of nitrogen oxides, through a computational lense. **W.F. Schneider**

10:45 CATL 143. Boron effect on low temperature H₂-SCR catalysts. M. Hu, **X. Wang**

11:15 CATL 144. Operando Infrared and XAS study of NO adsorption on zeolite supported Pd catalysts under complex gas feeds. **H. Chen**

Section D

Orange County Convention Center
Room W309B

Data Science for Catalysis Research

Cosponsored by CINF, COMP and ENFL
B. R. Goldsmith, H. J. Kulik, H. Xin, *Organizers, Presiding*

8:00 CATL 145. Cluster regularization: A machine learned artificial energy landscape. **B. Hammer**

8:45 CATL 146. Towards automated discovery of plausible reaction paths in complex catalytic systems using network generation and optimization. **S. Rangarajan**, B. Li

9:15 CATL 147. Guiding materials discovery using reaction informatics. **A.J. Norquist**

9:45 CATL 148. Double-ended transition state search combined with a reaction exploration algorithm. D.S. Levine, L.D. Jacobson, **A. Bochevarov**

10:15 Intermission.

10:25 CATL 149. Understanding the limits of machines in learning chemical reactivity. **J. Kammeraad**, J. Goetz, E. Walker, A. Tewari, P.M. Zimmerman

10:40 CATL 150. Combining machine learning models and Sabatier's principle to predict the activity of homogeneous catalysts. **C. Corminboeuf**, B. Meyer, B. Sawatlon, A. von Lilienfeld

11:10 CATL 151. Data science in enzymatic catalysis. **H. Mayes**

11:40 CATL 152. Machine learning framework for the analysis of catalyst performance. **A. Smith**, A. Keane, J.A. Dumesic, G.W. Huber, V. Zavala



TECHNICAL PROGRAM

Section E

Orange County Convention Center
Room W307A

Frontiers in Catalysis for Energy & Sustainability

Cosponsored by ENFL[†]

E. Bergin, M. S. Wong, *Organizers*

F. Jentoft, D. E. Resasco, M. A. Reynolds, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 CATL 153. Gaseous carbon waste streams utilization: Status and research needs. **C.L. Tway**, D.T. Allen, M. Barteau, M.D. Burkart, J. Dunn, A.M. Gaffney, R. Gupta, N. Hazari, M. Kanan, P.J. Kenis, H. Klee, G. Sant

8:30 CATL 154. New frontiers in CCUS: Integrated capture and catalytic conversion of CO₂. **D.J. Heldebrant**, J. Kothandaraman, E. Walter, D.W. Hoyt, S. Burton, R. Dagle, V. Lebarbier Dagle, S. Davidson

8:55 CATL 155. Theory-guided design of diesel oxidation catalysts with improved low temperature activity. Y. Song, **L. Grabow**

9:20 CATL 156. Towards clean and usable water using heterogenous metal catalysis. **M.S. Wong**, Y. Yin, S. Guo, K.N. Heck, C.A. Clark, C.L. Coonrod

9:45 Intermission.

10:05 CATL 157. Catalytic conversion of renewable resources using sustainable 'cleave and couple' strategies. **K. Barta**, Z. Sun

10:30 CATL 158. Use of carbon nanotube hydrogen highways to identify active sites over metals supported on reducible oxides. L. Barrett, N. Briggs, A. Gomez, D. Jones, L. Herrera, T. Pham, H. Chau, **S. Crossley**

10:55 CATL 159. Earth abundant Fe-based catalysts for selective hydrodeoxygenation. **Y. Wang**

11:20 CATL 160. Catalysts live & up close. **B.M. Weckhuysen**

Section F

Orange County Convention Center
Room W310A

Computational Electrocatalysis

Cosponsored by COMP and ENFL

K. Schwarz, R. Sundaraman, *Organizers*

K. Schwarz, *Presiding*

8:00 CATL 161. Understanding the apparent fractional charge of protons in the aqueous electrochemical double layer. **L.D. Chen**, M. Bajdich, J.P. Martinez, C. Krauter, J.A. Gauthier, E.A. Carter, A.C. Luntz, K. Chan, J.K. Nørskov



TECHNICAL PROGRAM

8:30 CATL 162. Developing DFT-based models for describing electrochemical reactions: implicit treatments of electrolytes. **J. Goodpaster**

9:00 CATL 163. Exploring polarization and double-layer effects at electrochemical interfaces within the Effective Screening Medium method. **B. Wood**, S. Weitzner, C. Zhan, T. Pham, J. Varley, T. Ogitsu, M. Otani

9:30 CATL 164. Key aspects in modeling the solvent in electrocatalysis. **C. Michel**, S.N. Steinmann

9:50 Intermission.

10:00 CATL 165. Key role of antibonding electron transfer in surface chemisorption and heterogeneous catalysis. **L. Yu**, Q. Yan, A. Ruzsinszky

10:20 CATL 166. Computational methods for the determination of electrocatalytic mechanisms. **R. Nielsen**, Y. Huang, Y. Ping, W.A. Goddard

10:50 CATL 167. Computational electrocatalysis: Methods, challenges, and applications to the CO₂ reduction reaction. **M.P. Head-Gordon**

11:30 CATL 168. Ab initio modeling of electrified metal-water interfaces. J. Le, **J. Cheng**

Section G

Orange County Convention Center
Room W310B

Recent Advances in Plasma-Enhanced Catalysis

Cosponsored by ENFL, ENVR and PHYS
J. C. Hicks, W. F. Schneider, R. Van De Sanden, *Organizers, Presiding*

8:00 CATL 169. Summary of two decades of plasma-catalyst research for environmental emissions control. **G.B. Fisher**, J.W. Hoard

8:30 CATL 170. Superlocal chemical reaction equilibrium in low temperature plasmas. **E. Thimsen**, N.B. Uner

8:50 CATL 171. Plasmas for catalysis: from surface chemistry activation to synthesis of novel nanomaterials. **L. Mangolini**

9:20 CATL 172. Understanding molecular factors influencing plasma-catalytic phenomena using theory and experiment. **P. Mehta**, P. Barboun, F. Herrera, D. Go, J.C. Hicks, W.F. Schneider

9:40 CATL 173. Vibrational activation in energetic environments: Lessons from state-resolved studies of methane activation on Ni surfaces. **A.L. Utz**

10:10 Intermission.

10:20 CATL 174. Plasma-enhanced catalysis for ammonia production. J. Hong, S. Prawer, **A.B. Murphy**



TECHNICAL PROGRAM

10:50 CATL 175. Plasma-based electrolytic synthesis of ammonia from nitrogen and water. J. Toth, R. Hawtof, S. Ghosh, D.J. Lacks, J. Renner, **R. Sankaran**

11:10 CATL 176. Plasma catalysis as vibrational activation of surface interactions for the RWGS reaction. **Q. Ong**

11:30 CATL 177. Relationships between plasma and plasmon mediated catalysis. **P. Christopher**

ACS Award in Surface Chemistry: Symposium in Honor of Hajo Freund

Sponsored by COLL, Cosponsored by CATL⁺ and PHYS

Innovative Chemistry & Materials for Electrochemical Energy Storage

Solid & Polymer Electrolytes

Sponsored by ENFL, Cosponsored by CATL, INOR and PMSE

Carbon Dioxide Conversion & Utilization

CO₂ Capture & Separation

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Celebrating 50 Years of ExxonMobil's Corporate Strategic Research Laboratories: A View Forward from a Retrospective

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Celebrating 50 Years of ExxonMobil's Corporate Strategic Research Laboratories: A View Forward from a Retrospective

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MONDAY AFTERNOON

Section A

Orange County Convention Center
Room W306A



TECHNICAL PROGRAM

Ipatieff Prize : Symposium in Honor of Ivo Hermans

C. A. Carrero, *Organizer*
L. Grabow, D. Rosenfeld, *Organizers, Presiding*

1:00 CATL 178. 1,6-Hexanediol synthesis from cellulose. J. He, S. Burt, M. Ball, I. Hermans, J.A. Dumesic, **G.W. Huber**

1:30 CATL 179. Influence of water molecules in second-order C-C bond forming reactions. **D.E. Resasco**, G. Li, D. Ngo, B. Wang

2:00 CATL 180. Oxidative methane activation over Cu-containing zeolites. **R.F. Lobo**

2:30 CATL 181. Solvent effects in the catalytic conversion of C6 sugars to α -hydroxy acids. C.G. Rivera-Goyco, I. Hortal-Sanchez, Y.J. Pagan Torres, **N. Cardona-Martinez**

3:00 Intermission .

3:10 CATL 182. Role of heterogeneous catalysis in biomass conversion. **B. Sels**

3:40 CATL 183. Selective oxidation, reforming and combustion of methane over NiO/Ni on ceria-zirconia. Y. Lyu, J. Jocz, R. Xu, **C. Sievers**

4:10 CATL 184. Metal carbides for the upgrading of natural gas. **C.A. Carrero**

4:30 CATL 185. Award Address (Ipatieff Prize sponsored by the Ipatieff Trust Fund).. **I. Hermans**

Section B

Orange County Convention Center
Room W306B

Gabor A. Somorjai Award for Creative Research in Catalysis: Symposium in Honor of Manos Mavrikakis

S. Rangarajan, L. T. Roling, *Organizers, Presiding*

1:00 Introductory Remarks.

1:05 CATL 186. Award Address (Gabor A. Somorjai Award for Creative Research in Catalysis sponsored by the Gabor A. and Judith K. Somorjai Endowment Fund). Nature of the active site in and improved catalysts for heterogeneous catalysis: Insights from molecular modeling. **M. Mavrikakis**

1:50 CATL 187. Using liquid crystals to report reactions at surfaces. **N.L. Abbott**

2:20 CATL 188. Shape-controlled metal nanocrystals: The next-generation heterogeneous catalysts? **Y. Xia**

2:50 Intermission.



TECHNICAL PROGRAM

3:10 CATL 189. Predicting reactor performance for oxygen-assisted coupling of alcohols: DFT-based versus ultrahigh vacuum kinetics-based microkinetic modeling. **R.J. Madix**, I. Fampiou, C. Reece

3:40 CATL 190. Electrified interfaces for energy applications. **V. Stamenkovic**

Section C

Orange County Convention Center
Room W309A

Symposium in Honor of Chuck Peden's Research Career: Catalysis for Energy & the Environment

Cosponsored by ENFL, ENVR, I&EC and PHYS

Y. Wang, *Organizer*

F. Gao, J. Szanyi, *Organizers, Presiding*

1:00 CATL 191. Dry reforming of glycerol over ceria, zirconia and alumina-zirconia-titania supported Rh, Co, Ni catalysts: New insights on catalyst activity and stability. **E. Ozensoy**, A.K. Avci

1:30 CATL 192. Catalytic methane pyrolysis for hydrogen production. M. Gordon, E.W. McFarland, **H. Metiu**

2:00 CATL 193. Investigation of the robust hydrothermal stability of Cu/LTA for NH₃-SCR reaction. A. Wang, P. Arora, D. Bernin, A. Kumar, K. Kamasamudram, **L. Olsson**

2:30 Intermission.

2:45 CATL 194. Low temperature NO adsorption over Pd based catalysts for cold start application. **D.H. Kim**

3:15 CATL 195. Multi-component oxide catalysts for low-temperature CO oxidation. **S. Dai**

3:45 CATL 196. Radiation and thermal chemistries of organometallic clusters. **G.S. Herman**

4:15 CATL 197. SO₂ oxidation over monometallic and bimetallic Pt and Pd catalysts. **W. Epling**, M.S. Wilburn, M. Cortez-Reyes

Section D

Orange County Convention Center
Room W309B

Elucidation of Mechanisms & Kinetics on Surfaces

Experimental Surface Science

Cosponsored by ENFL, ENVR, INOR and PHYS

A. Ignatchenko, S. Laursen, A. Savara, *Organizers*

L. Baker, *Organizer, Presiding*

S. Laursen, *Presiding*



TECHNICAL PROGRAM

1:00 CATL 198. Gaining Insights into catalytic performance from fundamental studies in ultrahigh vacuum combined with Knudsen pulse flow reactor analysis. **R.J. Madix**, C. Reece, M. Luneau

1:40 CATL 199. Chiral molecules and the electron's spin: A new pathway to spin selective chemistry. **R. Naaman**

2:20 CATL 200. Structure and reactivity of nanocatalysts prepared by mass-selected cluster deposition. **M.G. White**, K.R. Goodman, Y. Ma, J. Wang

2:40 CATL 201. Shining light on complexity: State- and energy-resolved studies of gas-surface reaction dynamics and mechanism. **A.L. Utz**

3:00 Intermission.

3:20 CATL 202. Spatio-temporal reaction kinetics at interfaces. **S.J. Sibener**, R. Edel, T. Grabnic, B. Wiggins, S. Brown, J. Sayler

4:00 CATL 203. Identifying the influence of reaction conditions on site-dependent reactivity of Pt particles. **E. Gross**

4:20 CATL 204. Encapsulation of metal nano-islands at the surface of graphite. **P.A. Thiel**, A. Lii-Rosales, Y. Han, D. Jing, C. Wang, J. Evans, M. Tringides

4:40 CATL 205. Following charge transfer dynamics in molecular catalyst/semiconductor systems by transient laser spectroscopy. **L. Hammarstrom**, L. D'Amario, J. Föhlinger, H. Tian, L. Tian

5:00 CATL 206. Two-dimensional (alumino)silicate-noble gas clathrates formation mechanism. **J.A. Boscoboinik**, J. Zhong, M. Wang, D. Lu

Section E

Orange County Convention Center
Room W307A

Frontiers in Catalysis for Energy & Sustainability

Cosponsored by ENFL⁺
D. E. Resasco, M. A. Reynolds, *Organizers*
E. Bergin, F. Jentoft, M. S. Wong, *Organizers, Presiding*

1:00 Introductory Remarks.

1:05 CATL 207. Activity and stability: All simultaneously please. **A. Vojvodic**

1:30 CATL 208. Non-innocent solvents, hydrogen transfer, and oxygen dissociation on nanoparticles during the direct synthesis of H₂O₂. J. Adams, P. Priyadarshini, T. Ricciardulli, Y. Lu, A. Chemburkar, A.M. Karim, M. Neurock, **D. Flaherty**

1:55 CATL 209. Fuel cell cathodic chemistry research in the context of synthetic models for copper or heme-copper enzyme active-site O₂-reduction and/or O–O bond reductive cleavage. **K.D. Karlin**

2:20 CATL 210. Molecular design and stabilization of metal oxo clusters for challenging electrocatalytic, sustainable transformations. **T. Tilley**



TECHNICAL PROGRAM

2:45 Intermission.

3:05 **CATL 211.** Tailoring the active surface phase for oxygen electrocatalysis. **M. Escudero-Escribano**

3:30 **CATL 212.** Kinetic fingerprints of catalysis by subsurface hydrogen on Pd-Ag alloys. I. Sen, **A.J. Gellman**

3:55 **CATL 213.** Bridging the gaps between homogeneous and heterogeneous catalysis: Hammett studies and active site kinetics studies to better understand alcohol oxidation over Au catalysts. **B.D. Chandler**

4:20 **CATL 214.** Designing for selectivity in heterogeneous catalysis. **C.M. Friend**

Section F

Orange County Convention Center
Room W310A

Computational Electrocatalysis

Cosponsored by COMP and ENFL
K. Schwarz, *Organizer*
R. Sundararaman, *Organizer, Presiding*

1:00 **CATL 215.** First-principles kinetic Monte Carlo approach for simulating electrochemical processes. **K. Honkala**

1:30 **CATL 216.** Unified electrochemical band diagram framework: Understanding the driving forces of material electrochemistry. **C. Musgrave**, A. Holder, M. Young

2:10 **CATL 217.** Data- and theory-driven design of metastable materials for energy conversion. **A. Holder**

2:40 Intermission.

2:50 **CATL 218.** Excited states in liquid environments with GW and continuum models. **A. Habib**, D. Vigil-Fowler, R. Sundararaman

3:10 **CATL 219.** Studying heterogeneous catalysis via solvated random phase approximation (RPA) calculations in a plane-wave basis. **D. Vigil-Fowler**, R. Sundararaman

3:40 **CATL 220.** Beyond Born-Oppenheimer dynamics at metal surfaces: Surface hopping and electronic friction. **W. Dou**, J.E. Subotnik

4:10 Concluding Remarks.

Section G

Orange County Convention Center
Room W310B

Recent Advances in Plasma-Enhanced Catalysis



TECHNICAL PROGRAM

Cosponsored by ENFL, ENVR and PHYS

J. C. Hicks, W. F. Schneider, R. Van De Sanden, *Organizers, Presiding*

1:00 CATL 221. Plasma aided electrocatalysis for nitrogen fixation. **M. Tsampas**, H. Patel, R. Sharma, A. Pandiyan, V. Kyriakou, S. Welzel, R. Van de Sanden

1:30 CATL 222. Coupling of heterogeneous catalysts with non-thermal plasma for CO₂ methanation: probing the reaction mechanisms using *in-situ* DRIFTS. **H. Chen**, Y. Mu, S. Chansai, C. Stere, X. Fan, C. Hardacre

1:50 CATL 223. Plasma-enhanced catalysis: a promising solution to turn CO₂ into value-added fuels and chemicals. **X. Tu**

2:20 CATL 224. Plasma catalysis for methane dissociation: Investigation of optimal reaction conditions for C₂H_x formation. **Y. Engelmann**, P. Mehta, E.C. Neyts, W.F. Schneider, A. Bogaerts

2:40 CATL 225. Energy-efficient CO₂ conversion with renewable electricity storage by plasma catalysis. **J. Liu**

3:10 Intermission.

3:25 CATL 226. Plasma based nitrogen fixation: better insights from computer modelling. **W. Wang**

3:45 CATL 227. Addressing catalytic challenges using non-thermal plasma (NTP) activation: A case study of NTP activated MOFs catalysis. S. Xu, Y. Mu, H. Chen, C. Hardacre, **X. Fan**

4:05 CATL 228. Cold plasma catalysis for SO₂ reduction with CH₄ over metal sulfide catalysts. **M. AlQahtani**, S. Knecht, X. Wang, S. Bilén, C. Song

4:25 CATL 229. Non-equilibrium transformation of biomass into hydrocarbons in a low temperature plasma fluidized bed reactor. **N.B. Uner**, E. Thimsen

ACS Award in Surface Chemistry: Symposium in Honor of Hajo Freund

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Innovative Chemistry & Materials for Electrochemical Energy Storage

Supercapacitors

Sponsored by ENFL, Cosponsored by CATL, INOR and PMSE

Carbon Dioxide Conversion & Utilization

CO₂ as an Oxidant



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

Sponsored by ENFL, Cosponsored by CATL, COMP and GEOC

Celebrating 50 Years of ExxonMobil's Corporate Strategic Research Laboratories: A View Forward from a Retrospective

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Celebrating 50 Years of ExxonMobil's Corporate Strategic Research Laboratories: A View Forward from a Retrospective

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MONDAY EVENING

Section A

Orange County Convention Center
West Hall C

Sci-Mix

A. Savara, *Organizer*

8:00 - 10:00

371, 395, 398-400, 408. See subsequent listings.

TUESDAY MORNING

Section A

Orange County Convention Center
Room W306A

Elucidation of Mechanisms & Kinetics on Surfaces

Kinetic Modeling

Cosponsored by ENFL, ENVR, INOR and PHYS

S. Laursen, A. Savara, *Organizers*

L. Baker, A. Ignatchenko, *Organizers, Presiding*



TECHNICAL PROGRAM

8:00 CATL 230. Kinetics and mechanism of aspartic acid adsorption and its explosive decomposition on Cu(hkl) surfaces. B. Karagoz, A. Reinicker, B. Mhatre, **A.J. Gellman**

8:20 CATL 231. Selectivity in multiple guises: Microkinetic models of NH₃ catalytic oxidation. H. Ma, **W.F. Schneider**

8:40 CATL 232. Low temperature SO₂ poisoning mechanism of Cu/CHA selective catalytic reduction (SCR) catalysts. **W. Epling**, Y. Jangjou, I.S. Pieta

9:00 CATL 233. Experimental study and kinetic modeling of the transformation of ethanol and acetaldehyde mixture into butadiene. **D. Dussol**, N. Cadran, N. Laloue, J. Schweitzer

9:20 CATL 234. Thiele moduli for complex reaction systems: A case study of methanol-to-olefins catalysis. **A. Bhan**

9:40 Intermission.

9:55 CATL 235. Catalytic and thermodynamic effects of hydrogen bonding on epoxidations within Ti-substituted zeolites. **D. Flaherty**, D.T. Bregante

10:20 CATL 236. Active site ensemble requirements in selective hydrogenation: Nuclearity and composition effects. **R.M. Rioux**, A. Dasgupta, H. He, R. Meyer, M. Janik

10:40 CATL 237. Reaction mechanisms and microkinetic modeling of nitrile hydrogenation to higher amines on Pd(111) and Co(0001) surfaces. G. Lozano-Blanco, **A.J. Adamczyk**

11:00 CATL 238. Kinetic simulations and parameter estimation: Bayesian kinetic parameter estimation to include errors from both experiment and theory. **A. Savara**, S.D. Sawtelle

11:20 CATL 239. Decomposition mechanism of lignin models on Pt(111) combining single crystal experiments and first principle calculations. **C. Michel**, R. Réocreux, P. Sautet, C.A. Ould Hamou, J. Giorgi

11:40 CATL 240. Reaction kinetics analysis of acrolein hydrodeoxygenation over a WO₃ catalyst. T.J. Thibodeau, J. Tavana, C.M. Goodwin, F.G. Amar, **T.J. Schwartz**, B.G. Frederick

Section B

Orange County Convention Center
Room W306B

Gabor A. Somorjai Award for Creative Research in Catalysis: Symposium in Honor of Manos Mavrikakis

S. Rangarajan, L. T. Roling, *Organizers*
J. P. Greeley, Y. Xu, *Presiding*

8:00 Introductory Remarks.

8:05 CATL 241. Computational catalysis: Rigor and relevance. **J. Sauer**

8:35 CATL 242. Computational design of functionalized metal–organic frameworks for catalysis. **L. Gagliardi**



TECHNICAL PROGRAM

9:05 CATL 243. Understanding strain in defective near surface alloys: Going beyond the epitaxial relationship. **L. Grabow**

9:35 Intermission.

9:55 CATL 244. Preparation of Pt-containing bimetallic and trimetallic catalysts using continuous electroless deposition methods. G. Tate, A. Kevlin, B.A. Tavakoli Mehrabadi, **J.R. Monnier**

10:25 CATL 245. Olefin oligomerization on carbon supported cobalt catalyst. **G.W. Huber**, Z. Xu, J. Chada, D. Zhao, L. Xu, Y. Li, X. Liu, J. Xu, J. Rogers, M. Mavrikakis, D. Rosenfeld, I. Hermans

10:55 CATL 246. Hydrogen shuffling catalysis: A generalized mechanistic interpretation for hydrogenation and hydrodeoxygenation on transition metal clusters. **Y. Chin**

11:25 CATL 247. Heterogeneous catalysis by homogeneous complexes: Silica-supported iridium-pincer complexes catalyze alkane dehydrogenation at elevated temperatures. **F.E. Celik**

Section C

Orange County Convention Center
Room W309A

Well-Defined Materials for Heterogeneous Catalysis: Synthesis, Characterization, & Performance Studies

Synthesis & Performance

Cosponsored by ENFL

H. Zhu, *Organizer*

M. Cargnello, D. Su, *Organizers, Presiding*

8:00 CATL 248. Fundamental studies of C1 chemistry on novel metal-carbide catalysts. **J. Rodriguez**

8:35 CATL 249. Catalytic alkene hydrosilylation with oxide-supported Pt single-site catalysts (SSCs). **L. Chen**, I.S. Ali, G.E. Sterbinsky, S.L. Tait

8:55 CATL 250. Shape effect in oxide catalysis: from binary to ternary oxides. **Z. Wu**

9:30 CATL 251. Hydrodechlorination of 1,2-dichloroethane over AgPd catalysts prepared by controlled surface reactions. **M. Ball**, K. Rivera-Dones, E.E. Stangland, M. Mavrikakis, J.A. Dumesic

9:50 CATL 252. Small pore zeolite SSZ-13 supported Pd as highly stable low-temperature methane combustion catalysts. **F. Gao**, Y. Cui, L. Kovarik, Y. Wang, B. Peng

10:25 CATL 253. High yield of hierarchical SAPO-34 with excellent MTO performance by solid acid-treatment. X. Chen, C. Yang, **Z. Liu**

10:45 CATL 254. Atomic layer deposition (ALD) as a way to produce well-defined mixed-oxide and metal-oxide interfaces for catalysis. **F. Zaera**

11:20 CATL 255. Synthesis of supported bimetallic nanoparticles via surface inorganometallic chemistry. **K. Ding**



TECHNICAL PROGRAM

Section D

Orange County Convention Center
Room W309B

Light-Driven Chemistry: Photoelectrochemistry & Photocatalysis

Cosponsored by COLL, ENFL, I&EC, INOR and PHYS
G. Dukovic, *Organizer*
S. Ardo, D. Esposito, I. Sharp, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 CATL 256. Inverted metamorphic multijunction III-Vs for photo-electrochemical hydrogen production systems: Challenges in absorber stabilization and device scale-up. **T.G. Deutsch**, J. Young, E. Klein, M. Steiner

8:35 CATL 257. Multifunctional atomic layer deposited metal oxide alloy catalysts and schottky contacts for protected silicon photoanodes. **P.C. McIntyre**

9:05 CATL 258. Regio- and diastereoselective triplet-initiated intermolecular [2+2] cycloadditions photocatalyzed by visible-light-absorbing quantum dots. **E.A. Weiss**, Y. Jiang, C. Wang, C. Rogers

9:35 Intermission.

9:50 CATL 259. Time resolved in operando optical spectroscopy of (photo)electrochemical water oxidation. **J.R. Durrant**

10:20 CATL 260. Capturing intermediates of solar fuels catalysis by transient mid-IR spectroscopy. **L. Hammarstrom**, R. Lomoth, S. Wang

10:50 CATL 261. Electronic structures of metal centers in OER catalyst models and electron/energy relays in the excited state supramolecular dinuclear transition metal complexes. **L.X. Chen**

11:20 CATL 262. Metal Carbodiimides as materials for (photo)electrochemical water oxidation. **A. Slabon**

Section E

Orange County Convention Center
Room W307A

Frontiers in Catalysis for Energy & Sustainability

Cosponsored by ENFL[†]
F. Jentoft, M. A. Reynolds, *Organizers*
E. Bergin, D. E. Resasco, M. S. Wong, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 CATL 263. Positioning active sites in catalytic materials: from cooperative catalysis to cascade catalysis in multicompartment nanoreactors. S. Jang, **C.W. Jones**, M. Weck



TECHNICAL PROGRAM

8:35 CATL 264. Metal/organo hybrid catalysis for group 9 metal-catalyzed enantioselective C-H functionalization. **T. Yoshino**

9:05 CATL 265. Stereospecific N-H/N-alkyl aziridination of unactivated olefins, C-H amination of arenes and primary/secondary amination of (hetero)arylmets. **L. Kurti**

9:35 CATL 266. Advances in the cross coupling of alkyl electrophiles and nucleophiles for the preparation of chiral organic molecules.. **C.M. Crudden**

10:05 Intermission.

10:25 CATL 267. Biocatalysis at Merck. **J.C. Moore**

10:55 CATL 268. Frontiers in biocatalysis. **A.R. Narayan**

11:25 CATL 269. Newest advances in enzymatic carbene- and nitrene-transfer catalysis. **F.H. Arnold**

Section F

Orange County Convention Center
Room W310A

Elucidating the Roles of Electric Fields in Catalysis

Cosponsored by ENFL and PHYS
C. Barroo, S. L. Scott, *Organizers*
J. McEwen, *Organizer, Presiding*

8:00 CATL 270. Role of external and internal electric fields in catalysis at interfaces: A computational perspective. **A. Gross**

8:30 CATL 271. Density functional theory approach to electrocatalytic reaction barriers. **M.J. Janik**

9:00 Intermission.

9:25 CATL 272. Computational optimization of electric fields for better catalysis design. **T.L. Head-Gordon**

9:55 CATL 273. Capturing the electric field effects on solvent structure and electronic structure at electrochemical interfaces. **K. Schwarz**

10:25 CATL 274. Electric field and voltages fluctuations in condensed phases. **S. Kathmann**

Section G

Orange County Convention Center
Room W310B

Catalytic Chemistry over Metal Oxides



TECHNICAL PROGRAM

Oxide-Supported Metals

D. Jiang, *Organizer*
S. D. Senanayake, Z. Wu, *Organizers, Presiding*
W. Huang, *Presiding*

8:00 Introductory Remarks.

8:05 CATL 275. Adsorption energies of metal atoms and adhesion energies of metal nanoparticles on oxide surfaces: relationships to catalyst performance. **C.T. Campbell**

8:35 CATL 276. Metal nodes in bimetallic metal-organic frameworks as isolated sites for hydrogenation reactions. D. Shakya, O. Ejegbavwo, A. Brandt, R. Thayalan, S. Farzandh, S.D. Senanayake, J.R. Monnier, K.D. Vogiatzis, N.B. Shustova, **D.A. Chen**

9:05 CATL 277. Substantially enhanced reduction of oxyanions through the integration of Group 6– 8 metal oxides into supported hydrogenation catalyst. **C. Ren**, J. Gao, J. Liu

9:25 CATL 278. Controlling leaching of supported oxo-rhenium species during deoxydehydration. **B.E. Sharkey**, F. Jentoft

9:45 Intermission.

9:55 CATL 279. Gold nanoparticle interactions with rutile TiO₂(110). **G. Thornton**

10:25 CATL 280. TiO₂ morphology effect in Au-TiO₂ catalysis. **W. Huang**

10:55 CATL 281. Characteristics of quad-functional catalytic sites on Au/Anatase TiO₂. J. Mao, P. Yan, J. Zhou, Z. Xia, Z. Xu, X. Guo, **Z. Zhang**

11:25 CATL 282. Morphology control for NO_x storage catalysts. **K.L. Stamm Masias**, T.C. Peck

ACS Award in Surface Chemistry: Symposium in Honor of Hajo Freund

Sponsored by COLL, Cosponsored by CATL⁺ and PHYS

Innovative Chemistry & Materials for Electrochemical Energy Storage

Flow Batteries

Sponsored by ENFL, Cosponsored by CATL, INOR and PMSE



TECHNICAL PROGRAM

Carbon Dioxide Conversion & Utilization

Electrocatalysis

Sponsored by ENFL, Cosponsored by CATL, COMP and GEOC

Carbon Dioxide Conversion & Utilization

Electrocatalysis

Sponsored by ENFL, Cosponsored by CATL, COMP and GEOC

TUESDAY AFTERNOON

Section A

Orange County Convention Center
Room W306A

Elucidation of Mechanisms & Kinetics on Surfaces

Catalysis on Metal Interfaces with Metal Oxides

Cosponsored by ENFL, ENVR, INOR and PHYS
A. Ignatchenko, S. Laursen, *Organizers*
L. Baker, A. Savara, *Organizers, Presiding*

1:00 CATL 283. Promotional effects of potassium on reducible oxide catalysts. **D.J. Stacchiola**

1:20 CATL 284. Selective furfural ring rearrangement reactions over TiO₂ supported catalysts in the vapor phase. L. Herrera, A. Gomez, T. Pham, L. Barrett, D. Jones, N. Briggs, B. Wang, **S. Crossley**

1:40 CATL 285. Phenol hydrodeoxygenation in a high-pressure liquid-phase flow reactor over Ru/TiO₂. **D.I. Stuck**, B.G. Frederick, R.N. Austin, L. Grabow, T.J. Schwartz

2:00 CATL 286. From catalyst design to technology validation: Elucidating reaction mechanisms and kinetics for complex biomass conversion processes. C. Mukarakate, K. Iisa, C. Nash, C.A. Farberow, M. Griffin, R.J. French, S. Habas, D.A. Ruddy, M. Yung, M.R. Nimlos, **J. Schaidle**

2:20 Intermission.

2:40 CATL 287. Molecular mechanism of ethanol steam reforming on bifunctional nickel-cerium oxide catalysts. **L. Baker**, Y. Mueannern

3:00 CATL 288. Intermetallic nanoparticles with atomic precision for selective catalytic transformations. **W. Huang**, Y. Pei



TECHNICAL PROGRAM

3:20 CATL 289. First principles microkinetic analysis on water-gas shift reaction over Rh/ZrO₂. **K. Honkala**, M.M. Kauppinen, M. Melander, A.S. Bazhenov

3:40 CATL 290. First-principles kinetic Monte Carlo study of hydrodeoxygenation at metal-support interfaces. X. Li, **L. Grabow**

4:00 CATL 291. Novel designs for tandem catalysis. **F. Zaera**

4:20 CATL 292. New insight into CO₂ reduction on Pd/Al₂O₃. **J. Szanyi**, N. Nelson

4:40 CATL 293. Kinetics and mechanism of alcohol conversions over shape-controlled oxide nanocrystals. **Z. Wu**

Section B

Orange County Convention Center
Room W306B

Gabor A. Somorjai Award for Creative Research in Catalysis: Symposium in Honor of Manos Mavrikakis

S. Rangarajan, L. T. Roling, *Organizers*
F. E. Celik, L. Grabow, *Presiding*

1:00 Introductory Remarks.

1:05 CATL 294. H₂O₂ formation in alcohol-assisted catalytic oxidation of water. J. Ye, J. Dombrowski, R. Han, A. Prokofjevs, M. Kung, **H. Kung**

1:35 CATL 295. First principles analysis of reactivity trends at metal/oxide interfaces. P. Majumdar, T.S. Choksi, Y. Cui, N. Delgass, F. Ribeiro, **J.P. Greeley**

2:05 CATL 296. Random alloys for fundamental electrocatalytic reactions. Y. Fang, F. McKay, S. Zhang, P.T. Sprunger, J.C. Flake, W.A. Shelton, **Y. Xu**

2:35 Intermission.

2:55 CATL 297. In search of an efficient approach to condensed phase catalyst design. **L.T. Roling**

3:25 CATL 298. Deoxygenation on molybdenum carbide catalysts: Fundamentals of the surface reactivity. **C.A. Farberow**, C. Nash, A.T. To, D.A. Ruddy, J. Schaidle

3:55 CATL 299. Elucidating the mechanism of reverse water gas shift reaction on molybdenum sulfides. R. Upadhyay, L. Sharma, J. Baltrusaitis, **S. Rangarajan**

Section C

Orange County Convention Center
Room W309A



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

Well-Defined Materials for Heterogeneous Catalysis: Synthesis, Characterization, & Performance Studies

Synthesis & Performance

Cosponsored by ENFL
M. Cargnello, D. Su, H. Zhu, *Organizers*
M. Cargnello, H. Zhu, *Presiding*

1:00 CATL 300. Catalyst discovery and development: From bulk to nanoscale materials. **R.E. Schaak**

1:35 CATL 301. Modifying titania support for enhanced alkene hydrosilylation using Pt single-site catalyst. **X. Zhou, S.L. Tait**

1:55 CATL 302. Tailoring cooperative metal-support interfaces for catalysis. **S. Dai**

2:30 CATL 303. Introducing nonstructural ligands to MOF nodes to tune the activity and selectivity of node-supported nickel catalysts for ethylene conversion. **J. Liu, J. Ye, Z. Li, X. Zhang, K. Otake, D.G. Truhlar, L. Gagliardi, C.J. Cramer, O.K. Farha, J.T. Hupp**

2:50 CATL 304. New routes to engineer the physicochemical properties of zeolite catalysts. **J.D. Rimer**

3:25 CATL 305. Effects of acid site proximity on acid strength and the rates and mechanism of methanol dehydration in zeolites. **D.D. Hibbitts, A. Hoffman, S. Nystrom, J. Di Iorio, C. Nimlos, R. Gounder**

4:00 Intermission.

4:15 CATL 306. Double-shelled nanoreactor as support for confined catalytic reactions. **G. Arora**

4:35 CATL 307. Well-defined olefin metathesis catalysts by the activation of molecular rhenium complexes on solid supports. F. Zhang, **S.L. Scott**

5:10 CATL 308. Heterogeneous nanocatalytic surfaces. **Y. Huang**

5:35 CATL 309. Encapsulating catalysts and biocatalysts into metal-organic frameworks with defined interfaces. **C. Tsung**

Section D

Orange County Convention Center
Room W309B

Light-Driven Chemistry: Photoelectrochemistry & Photocatalysis

Cosponsored by COLL, ENFL, I&EC, INOR and PHYS
G. Dukovic, *Organizer*
S. Ardo, D. Esposito, I. Sharp, *Organizers, Presiding*

1:00 CATL 310. Photo-electrocatalytic alcohol oxidation by a multi-component metal organic framework. S. Lin, **A.J. Morris**



TECHNICAL PROGRAM

- 1:25 CATL 311.** From light harvesting to photoelectrochemistry: Optoelectronic processes in covalent organic frameworks. **T. Bein**
- 1:50 CATL 312.** Porous boron nitride for combined CO₂ capture and photoreduction. **R. Shankar**, A. Hankin, C. Petit
- 2:10 CATL 313.** Strongly reducing organic dihydrophenazine and phenoxazine photoredox catalysts for visible light-driven synthesis of polymers and small molecules. **C. Lim**, G. Miyake
- 2:30 CATL 314.** Colloidal quantum dots as enantioselective photocatalysts for carbon-carbon bond formation. **Y. Jiang**
- 2:50** Intermission.
- 3:05 CATL 315.** “Rust” challenge: Solar water splitting with hematite photoanodes. **D. Grave**
- 3:30 CATL 316.** Complex metal oxide photoanodes for solar water splitting. M. Lamers, M. Kölbach, M. Favaro, D. Starr, D. Friedrich, R. Van de Krol, **F. Abdi**
- 3:55 CATL 317.** Investigation of CuWO₄/electrocatalyst interface for photoelectrochemical water oxidation. **P. Shadabipour**, H. Hajibabaei Najafabadi, T. Hamann
- 4:15 CATL 318.** Quaternary SCIGS chalcopyrite semiconductors with improved photocatalytic H₂ evolution performance. **D. Ni**, H. Kuo, R. Cava, A.B. Bocarsly
- 4:35 CATL 319.** Simultaneous non-metal doping and cocatalyst decoration for efficient photoelectrochemical water splitting on hematite photoanodes. **D. Wu**

Section E

Orange County Convention Center
Room W307A

Frontiers in Catalysis for Energy & Sustainability

Cosponsored by ENFL⁺
E. Bergin, M. S. Wong, *Organizers*
F. Jentoft, D. E. Resasco, M. A. Reynolds, *Organizers, Presiding*

- 1:00** Introductory Remarks.
- 1:05 CATL 320.** Serendipity in catalysis research: Boron-based materials for alkane oxidative dehydrogenation. **I. Hermans**
- 1:35 CATL 321.** Electrochemical opportunities for catalytic conversion of light alkanes. Y. Xu, G. Zhang, T. Krause, **A. Hock**
- 2:05 CATL 322.** Controlling the local coordination and reactivity of supported Pt-group atoms. **P. Christopher**
- 2:35 CATL 323.** Single site heterogeneous catalysts for the selective oxidation of alcohols and hydrocarbons. **R.J. Davis**, J. Xie, G. Brezicki



TECHNICAL PROGRAM

3:05 Intermission.

3:25 **CATL 324.** Development of advanced catalysts with atomically dispersed active sites. P. Xie, **C. Wang**

3:55 **CATL 325.** Proximity matters: Catalytic consequences and control of active site proximity in zeolites. **W.F. Schneider**, S. Li

4:25 **CATL 326.** Understanding and controlling catalysis in crowded environments. **J.A. Lercher**

Section F

Orange County Convention Center
Room W310A

Elucidating the Roles of Electric Fields in Catalysis

Cosponsored by ENFL and PHYS
C. Barroo, J. McEwen, S. L. Scott, *Organizers*
C. Barroo, *Presiding*

1:00 **CATL 327.** Experimental evidences of the effects of electric fields in catalysis. C. Barroo, L. Jacobs, S. Owczarek, Z. Wang, B. von Boehn, M. Homann, R. Bryl, L. Markowski, M. Willinger, R. Imbihl, **T. Visart de Bocarmé**

1:30 **CATL 328.** Nanoscale characterization of zeolites using atom probe tomography. **S.R. Bare**, **J.D. Poplawsky**, J.E. Schmidt, B.M. Weckhuysen

2:00 **CATL 329.** Electric fields, catalysis, and electrochemistry: A stark shift spectroscopy perspective. J. Patrow, S. Sarkar, M.J. Voegtle, A. Pennathur, **J. Dawlaty**

2:30 Intermission.

2:55 **CATL 330.** Exploring electric field assisted steam reforming of methane. J.T. Gray, F. Che, J. McEwen, **S. Ha**

3:25 **CATL 331.** Highly efficient Pt and PtCo nanoparticle catalysts prepared by electrochemical deposition for PEM fuel cells. **S. Buratto**

3:55 **CATL 332.** Mimicing electrocatalytic reactions with atom-probe devices. **N. Kruse**

Section G

Orange County Convention Center
Room W310B

Catalytic Chemistry over Metal Oxides

Titania Catalysis

S. D. Senanayake, *Organizer*



TECHNICAL PROGRAM

D. Jiang, Z. Wu, *Organizers, Presiding*
J. Zhou, *Presiding*

1:00 Introductory Remarks.

1:05 **CATL 333.** Structure, polarization and sum frequency generation spectrum of the anatase TiO₂-water interface. M. Calegari Andrade, H. Ko, R. Car, **A. Selloni**

1:35 **CATL 334.** Understanding the photocatalytic properties of titanium dioxides from first-principles electronic structure calculations. F. Li, **X. Gong**

2:05 **CATL 335.** Role of adventitious carbon on photocatalytic nitrogen fixation by titania. **B. Comer**, M. Hatzell, A.J. Medford

2:25 **CATL 336.** Use of surface hydroxyl frequencies to identify the exposed facets of pyrogenic TiO₂ nanoparticles. **A. Mahdavi-Shakib**, J. Arce-Ramos, R.N. Austin, T.J. Schwartz, L. Grabow, **B.G. Frederick**

2:45 Intermission.

2:55 **CATL 337.** Morphology dependence of stability and properties of stoichiometric TiO₂ nanoparticles. A. Morales García, A. Macià, S. Thomas, **F. Illas**

3:25 **CATL 338.** Single-facet dominant anatase Titania model catalysts to elucidate the active sites for O elimination and C-C bond formation. **Y. Wang**

3:55 **CATL 339.** Time resolved spectroscopy of charge carriers in TiO₂ single crystals and powder. Effect of adsorbates and reaction media. K. Katsiev, **H. Idriss**

4:25 **CATL 340.** X-ray Radiocatalysis of semiconductors. **M.C. Higgins**, J. Rojas

Innovative Chemistry & Materials for Electrochemical Energy Storage

Beyond Li-Ion

Sponsored by ENFL, Cosponsored by CATL, INOR and PMSE

Carbon Dioxide Conversion & Utilization

Photo, Electro & Plasma Catalysis

Sponsored by ENFL, Cosponsored by CATL, COMP and GEOC

TUESDAY EVENING

Section A



TECHNICAL PROGRAM

Orange County Convention Center
West Hall C

General Catalysis

A. Savara, *Organizer*

7:00 - 9:00

CATL 341. Pd-catalysed Suzuki cross-coupling of aryl halides and aryl boronic acids, by using new phenoxy-pyrazole-based *N^O^N*-type bis-pyrazole ligands. **Z. Hussain**, C.S. Schwalm, R.S. Rambo, R. Stieler, A.L. Monteiro

CATL 342. Photoreduction of carbon dioxide by biomimetic polyimide-supported cuprous oxide/graphitic carbon nitride photocatalytic films. **I. Tseng**, Y. Chen, P. Chang

CATL 343. Pt-Mo catalysts for acetic acid hydrodeoxygenation. **Y. Zheng**, S.G. Podkolzin, Z. Tang

CATL 344. Photocatalytic production of H₂O₂ through selective two-electron reduction of O₂. **W. Choi**, G. Moon, P. Zhang, S. Kim

CATL 345. Tunable doping of chromium Cr³⁺ in TiO₂ nanocrystals via ion diffusion. **R. Hossain**, J.D. Hoefelmeyer

CATL 346. Iron(0) nanoparticle-catalyzed ligand-free C-C/C-N bond forming tandem reaction. T. Akiyama, T. Honma, K. Tsuruta, Y. Tamenori, Y. Ueda, H. Tsurugi, K. Murai, O. Shohei, K. Mashima, H. Fujioka, Y. Sato, **M. Arisawa**

CATL 347. Silver modified hollow mesoporous carbon/silica nanospheres for selective adsorptive desulfurization. **C. Liu**, A. Duan, Q. Meng, D. Hu, Y. Gong

CATL 348. Effect of various amounts of boron on the catalytic performance of nanocrystalline ZSM-5 zeolites in methanol to propylene reaction. **Y. Zhai**, Y. Song, Y. Shang, L. Zhang, T. Ma, W. Wang, Y. Gong

CATL 349. Synthesis of the novel ZSM-5-KIT-5 composite material and its performance of hydrodenitrogenation. Q. Meng, C. Liu, D. Hu, **A. Duan**

CATL 350. Synthesis and catalytic performance of a dual-sites Fe-Zn catalyst based on ordered mesoporous Al₂O₃ for isobutane dehydrogenation. M. Cheng, H. Song, C. Xia, **L. Chou**

CATL 351. Excellent effect of solid acid WO₃/TiO₂-supported lithium-manganese oxides for oxidative coupling of methane. F. Cheng, H. Song, C. Xia, **L. Chou**

CATL 352. Hydrodehalogenation of polyhalogenated aromatics catalyzed by NiPd nanoparticles supported on nitrogen-doped graphene. **X. Guo**, C. Yu, S. Sun, C. Seto

CATL 353. Direct C-H activation by nanostructured MnWO₄ for selective oxidation of toluene to benzaldehyde. **D. Mal**, D. Pradhan

CATL 354. Carbohydrate-triazole-steroid bifunctional compounds: Enhancers of corrosion resistance of API 5L X52 steel and versatile ligands for the development of lanthanide coordination compounds. **B.I. Vergara-Arenas**, D. Pérez-Martínez, L. Lomas-Romero, G.E. Negrón-Silva, A. Espinoza-Vázquez, D. Angeles-Beltrán



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- CATL 355.** Entropy-stabilized metal oxides for efficient CO oxidation with high-temperature stability. **H. Chen**, S. Dai
- CATL 356.** Specific metal-support interactions of layered nanoparticle catalysts in catalytic methanol oxidation. **S. Yoon**, K. An
- CATL 357.** Cu-Ni/Al mixed oxide carboxylative coupling: synthesis of benzyl-2-alkynoates under ambient pressure of CO₂. B. Garcia Maximiliano, **D. Pérez-Martínez**, L. Lomas-Romero, G. Negrón Silva, D. Angeles-Beltrán
- CATL 358.** Visible light driven photocatalytic H₂-production activity of CuS/TiO₂ heterostructured nanocomposites based on type-II band alignment. **M. Chandra**, D. Pradhan
- CATL 359.** Effective structural descriptor to quantify the reactivity of lattice oxygen in CeO₂ subnanoclusters. **C. Zhou**, H.F. Wang, P. Hu
- CATL 360.** Palladium speciation in beta and chabazite zeolites for passive NO_x adsorption. T.M. Lardinois, **J.S. Bates**, K.A. Unocic, J. Choi, V. Prikhodko, J.T. Miller, R. Gounder
- CATL 361.** Activity enhancement in photocatalytic reduction of CO₂ over nano ZnO anchored on graphene. **X. Yin**
- CATL 362.** Surface Pd-rich PdAg nanowires as highly efficient catalysts for formic acid dehydrogenation and subsequent adiponitrile hydrogenation. **M. Shen**, H. Liu
- CATL 363.** Indium based catalyst for CO₂ conversion to cyclic carbonates. **H. Baalbaki**, P. Mehrkhodavandi
- CATL 364.** Pyridine derived post-synthetic modification of metal-organic frameworks catalyst for the efficient base-promoted Knoevenagel condensation reaction. **X. Li**
- CATL 365.** Copper modified Zr-based metal-organic framework (MOF) as an efficient catalyst for aerobic epoxidation of olefins. **Y. Luan**
- CATL 366.** Application of *N,N*-diaryl dihydrophenazine and *N*-aryl phenoxazine organic photoredox catalysts in organocatalyzed atom transfer radical polymerization. **D. Corbin**, B. McCarthy, G. Miyake
- CATL 367.** Synthesis of dual functional metal-organic framework for the aerobic oxidation/Knoevenagel condensation sequential reaction. **Y. Qi**
- CATL 368.** Insight Into the superior catalytic activity of MnO₂ for low-content NO oxidation at room temperature. H. Yuan, **J. Chen**, Y. Guo, H.F. Wang, P. Hu
- CATL 369.** Active site and confining environment requirements for glucose-sorbose isomerization in microporous Lewis acids. M. Cordon, **J. Vega-Vila**, A. LaRue, Z. Huang, R. Gounder
- CATL 370.** Ligand-free gold nanoclusters confined in mesoporous silica nanoparticles for styrene epoxidation. **B. Alshankiti**, **N.M. Khashab**, **W. Almaksoud**, **H. Abubaker**, **A. Chaix**, **D. Anjum**
- CATL 371.** Mesoporous silica supported perovskite oxide for low temperature thermochemical CO₂ conversion. **J. Brower**, B. Hare, A. Ramos, V. Bhethanabotla, J. Kuhn
- CATL 372.** Stable vanadium nanocatalysts for the partial oxidation of methane to formaldehyde. **E. Yang**, K. An



TECHNICAL PROGRAM

- CATL 373.** CO₂ reduction on defect rich 2D-TaS₂ layers on Cu(111). **C. Jordan**, B. Blue, M. Pathan, B. Young, M. Ishigami, M. Vaida
- CATL 374.** Mechanistic investigation of dissociation of β-O-4 linkage in the gas phase on Zn and Sn contained MWW-2D zeolite framework. **V. Jain**, N. Rai
- CATL 375.** Understanding exothermic catalytic decomposition of ADN based green propellants under anaerobic conditions. **M. Kurt**, S. Senol, K. Ercan, P. Beyazkilic, H. Esiyok, E. Ozensoy
- CATL 376.** Withdrawn
- CATL 377.** Chemically modified proteins as highly selective artificial metalloenzymes. **S.A. Wilhelm**, M. Leurs, S. Konieczny, B. Dorn, M. Manisegaran, J.C. Tiller
- CATL 378.** Adsorption-induced reconstruction on Cd-Au during CO₂ reducing reaction: A density functional theory study. **S. Bao**, X. Gong
- CATL 379.** Molybdenum nitride thin-film development and screening. **M. Sajid**, A. Khaniya, W. Kaden, A. Kara
- CATL 380.** Benzene, toluene and tetralin adsorption on palladium catalysts benzene, toluene and tetralin adsorption on palladium catalysts. **Z. Tang**, Y. Zheng, J.P. Robbins, S.G. Podkolzin
- CATL 381.** First principle calculations on electrochemical conversion of methane to alcohols on iron oxide-zirconia and Nb-doped nickel oxide-zirconia composites. **S. Kwak**, Y. Choi, H. Kim, G. Choi, M. Park, J. Moon, W. Lee
- CATL 382.** Catalytic hydrogenation of quinoline on composites of graphene-like carbon and 3D-metals or their oxides. **S. Ryabukhin**, D. Volochnyuk, S. Kolotilov, V. Buryanov, V. Asaula, O. Pariiska
- CATL 383.** Understanding the mechanism of photo-redox catalysis. K. Fogarty, A.J. Wommack, **C. Goudarzi**
- CATL 384.** Synergetic roles of photogenerated carriers in the oxidation of methane on TiO₂ (110): A first-principles study. **M. Zhou**, H.F. Wang, P. Hu
- CATL 385.** Oxygen, hydroperoxy and hydrogen peroxide structures on gold surfaces. **J.P. Robbins**, K. Liu, F. Tian, S.G. Podkolzin
- CATL 386.** Pulse laser synthesis of Ag-Rh and Ag-Pt heterostructures for 4-nitrophenol reduction: Potential antenna-reactor type photocatalysts. **K. Kane**, M. Bertino
- CATL 387.** New insights on the *redox* properties of two- and three-dimensional supported vanadium oxide catalysts: A Raman-spectrokinetics study. J.A. Moncada, **W.R. Adams**, C.A. Carrero
- CATL 388.** Rational engineer of Ag-based catalyst for ethylene epoxidation. **L. Zhu**, J. Zhu
- CATL 389.** Facile one-pot synthesis of single-atom platinum embedded porous gC₃N₄ nanosheets as efficient electrocatalysts for oxygen reduction reaction. **K. Eid**, M.H. Sliem, A. Abdullah
- CATL 390.** Rational design of transition metal nanocatalyst by structure descriptor. **H. Xu**, D. Cheng
- CATL 391.** Withdrawn



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- CATL 392.** Enhanced hydrogenation activity for palladium catalysts supported on carbon. **D.M. Shakya**, S. Farzandh, R. Banerjee, J.R. Regalbutto, D.A. Chen
- CATL 393.** Growth and activity studies of titania-supported Pt-Sn model catalysts for selective hydrogenation reactions. **T.D. Maddumapatabandi**, A. Brandt, S. Farzanadh, D.M. Shakya, W. Chai, G. Henkelman, D.A. Chen
- CATL 394.** Oxidative treatment of simulated produced water through the catalytic generation of hydroxyl radicals. **Y. Yin**, K.N. Heck, C.L. Coonrod, C. Powell, S. Guo, M.A. Reynolds, M.S. Wong
- CATL 395.** Broad-scope investigation of gold, silver, platinum, and palladium nanoparticles for the catalytic reduction of nitrophenols and azo dyes. **L.R. Shultz**, X. Feng, T. Jurca
- CATL 396.** Synthesis of baicalin esters mediated by lipase biocatalysts in organic solvents and their antibacterial activities. **X. Xin**, **X. Li**, S. Zhang, G. Zhao
- CATL 397.** Immobilization of strong field ligands on UiO-66 metal organic frameworks (UiO66-MOFs) surface and their catalysis applications. **P. Elumalai**, S. T. Madrahimov
- CATL 398.** Toward biphasic photocatalysis using water-soluble nano cavities as phase transfer catalysts: Kinetic studies of the host:guest complexation. **W.M. Blodgett**, **A. DeSimone**, N. Kamatham, A.J. Ayitou
- CATL 399.** Altering surface chemistry of SrTiO₃ for enhanced oxygen evolution reaction activity. **V.C. Bhethanabotla**, R. Wexler, A.M. Rappe
- CATL 400.** Catalytic conversion of carbon dioxide via hydrogenation to light olefins over Fe₂O₃ supported Pd-Co catalysts. **A. Leichnam**, C. Zhang
- CATL 401.** Heterogeneous IR single-sites catalysts (SSCs) for hydrogenation reactions. **L. Chen**, I.S. Ali, X. Zhou, S.L. Tait
- CATL 402.** Tuning the carburization of metal oxides for the activation of light hydrocarbons. **J.T. Smith**, R.K. Thakur, C. Carrero
- CATL 403.** Mechanism of acetylene formation via CO hydrogenation on defect rich 2D-MoS₂. **B. Young**, M. Pathan, C. Jordan, T. Nguyen, N. Marrow, D.M. Popolan-Vaida, M. Vaida
- CATL 404.** Synthesis of resveratrol analogues for cancer research via sonogashira coupling and stereoselective reduction by green methods. **I. Baxter**, M. Tase, D. Paull
- CATL 405.** Low-coordinated surface Ta atoms on 2D-TaS₂ for enhanced CO hydrogenation at low temperatures. **M. Pathan**, B. Young, C. Jordan, B. Blue, M. Ishigami, M. Vaida
- CATL 406.** Effect of WS₂ photocatalyst morphology on the activity and selectivity in photocatalytic oxidation of benzyl alcohol. **J. Ludwig**, T.S. Zubkov
- CATL 407.** Synthesis, analysis, and utility of green, solid-supported palladium—NHC complexes. **N. Cyr**, R.T. Johnson, D. Paull
- CATL 408.** Catalytic conversion of carbon dioxide via hydrogenation to light olefins over Fe₂O₃ supported Cu-CO catalysts. **D. Triger**, C. Zhang



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

CATL 409. Biocatalytic synthesis of phenol glycoside esters by whole-cell biocatalyst in nonaqueous medium. **X. Li**, H. Xu, C. Xie, G. Zhao

CATL 410. Rational design of (111) surfaces of Pt-Ni solid solutions for ORR using a strain-dependent cluster expansion. **L. Cao**, L. Niu, T. Mueller

CATL 411. Optimizing the particle size and geometry of Cu₂O nanoparticles for water splitting using DFT trained neural network potential. **B. Selvaratnam**, P. Miro, R.T. Koodali

CATL 412. Assessment of more than 200 density functional approximations for binding energies and spin states of porphyrins. **P. Morgante**, R. Peverati

CATL 413. Hammett neural networks: Prediction of frontier orbital energies of tungsten-benzylidyne photoredox complexes. **A.M. Chang**, J. Freeze, V.S. Batista

CATL 414. Intermittent plasma-assisted selective catalytic reduction of NO_x with hydrocarbon for the improvement of low-temperature catalytic activity. **Y. Mok**, D. Nguyen, V. Nguyen

WEDNESDAY MORNING

Section A

Orange County Convention Center
Room W306A

Elucidating the Roles of Electric Fields in Catalysis

Cosponsored by ENFL and PHYS
C. Barroo, J. McEwen, *Organizers*
S. L. Scott, *Organizer, Presiding*

8:00 CATL 415. Atomically-defined model systems for oxide-based electrodes: From surface science to the electrified interface. **J. Libuda**

8:30 CATL 416. Potential-dependent discharge product distribution in Li-oxygen cathodes. **E. Nikolla**

9:00 Intermission.

9:25 CATL 417. Double-layer effects in electrocatalysis. **M. Koper**

9:55 CATL 418. Influence of electric field at the electrode/electrolyte interface as determined by studies of field emitter tips. **E.M. Stuve**

10:25 CATL 419. Controlling the selectivity of electrochemical carbon monoxide reduction via cation-induced restructuring of interfacial water. **M. Waagele**



TECHNICAL PROGRAM

10:55 CATL 420. Hydrogenation of carbonyl compounds in aqueous phase: On the role of cathodic potential and pH. G. Chen, **O. Gutierrez-Tinoco**, U. Sanyal, L.C. Meyer, E. Ember, A. Jentys, J. Lercher

11:15 Concluding Remarks.

Section B

Orange County Convention Center
Room W306B

Activation of Light (C1-C4) Hydrocarbons: Theory & Experiments

Cosponsored by ENFL, ENVR, INOR and PHYS
F. Tao, *Organizer*
C. A. Carrero, I. Hermans, *Organizers, Presiding*

8:00 CATL 421. Methane dehydroaromatization on Mo/HZSM-5 with transient hydrogen removal. A. Kumar, N. Razdan, **A. Bhan**

8:40 CATL 422. Uncovering the details of methane combustion on palladium catalysts using well-defined nanocrystal precursors. **M. Cargnello**, W. Huang, E. Goodman, J. Willis, A. Yang, F. Abild-Pedersen, A. Johnston-Peck, S. Bare

9:10 CATL 423. Barrier response analysis framework to probe CH activation mechanisms. **S. Mallikarjun Sharada**, Z. Lan

9:30 CATL 424. Effect of framework Al location in metal cation-exchanged zeolites on methane conversion. **T. Yokoi**, Y. Kunitake, R. Osuga, K. Sago, T. Nishitoba, J. Kondo

9:50 Intermission.

10:00 CATL 425. Oxidative coupling of light alkanes using isobutane as oxygen carrier: Alkane structure reactivity relationship. **K. Wang**, J.E. Mitchell

10:20 CATL 426. Enhancement of catalytic properties of Mo/ZSM-5 catalysts for methane dehydroaromatization by ex situ formation of metal carbides. **S. Jatib Khatib**, M. Rahman, A. Sridhar, A. Infantes Molina

10:40 CATL 427. Impacts of activation area during high-coverage alkane hydrogenolysis and CO hydrogenation. **D.D. Hibbitts**, A. Almithn, D. Flaherty, J. Liu, E. Iglesia

11:00 CATL 428. Robust fuel cell operated on nearly dry methane at 500 C enabled by synergistic thermal catalysis and electrocatalysis. Y. Chen, B. deGlee, Y. Tang, **F. Tao**, M. Liu

11:20 CATL 429. Thermo-photo hybrid catalysis for methane conversion. **Y.H. Hu**

11:40 CATL 430. Light alkanes activation using ALD modified catalysts. Z. Gan, **Y. Lei**

Section C

Orange County Convention Center
Room W309A



TECHNICAL PROGRAM

Well-Defined Materials for Heterogeneous Catalysis: Synthesis, Characterization, & Performance Studies

Electrochemistry

Cosponsored by ENFL
M. Cargnello, H. Zhu, *Organizers*
D. Su, *Organizer, Presiding*
H. Zhu, *Presiding*

8:00 CATL 431. Shape-controlled bimetallic nanocatalysts for fuel cell applications. **Y. Xia**

8:35 CATL 432. Low-coordinated sites over metal catalysts boosting carbon dioxide electroreduction. **W. Zhu**, L. ZHANG, J. Gong, P. Yang, Z. Zhao

8:55 CATL 433. Three-dimensional copper electrodes for CO₂ and CO reduction. Y. Wang, D. Raciti, **C. Wang**

9:30 Intermission.

9:45 CATL 434. Controlling the growth of M-Ru nanoparticles for active and stable oxygen evolution reaction electrocatalysis. **L. Gloag**, R.D. Tilley

10:05 CATL 435. Hard-magnetic L₁₀-CoPt/Pt nanoparticles for fuel cell catalysis. **S. Sun**

10:40 CATL 436. Design of heterostructures for heterogeneous catalysis towards oxygen reduction and evolution reactions. **H. Yang**

11:15 CATL 437. Synthetic control of interfacial cooperation for enhanced electrocatalysis. **S. Zhang**, Z. Zhang, C. Liu

Section D

Orange County Convention Center
Room W309B

Light-Driven Chemistry: Photoelectrochemistry & Photocatalysis

Cosponsored by COLL, ENFL, I&EC, INOR and PHYS
G. Dukovic, *Organizer*
S. Ardo, D. Esposito, I. Sharp, *Organizers, Presiding*

8:00 CATL 438. Structural influences and non-covalent interactions in photocatalytic CO₂ reduction by the M(bpy-R)(CO)₃X (M = Mn or Re) class of complexes. **C.P. Kubiak**

8:25 CATL 439. Photocatalytic CO₂ reduction by biomimetic NADH analogs. **K. Glusac**

8:50 CATL 440. Roles of triethanolamine in photochemical CO₂ reduction with [Ru(dmb)₂(CO)₂]²⁺ and Ru(II)-Ru(II) supramolecular systems. R. Sampaio, D.C. Grills, D.E. Polyansky, Y. Tamaki, O. Ishitani, **E. Fujita**

9:15 CATL 441. Role of the metal in Au-TiO₂ catalysts during the H₂ photoproduction from water. **F. Zaera**



TECHNICAL PROGRAM

9:35 CATL 442. Photodriven deprotonation of proton donor solvents by N-heterocyclic aromatics. **J.R. Hunt**, C. Tseng, J. Dawlaty

9:55 Intermission.

10:10 CATL 443. Ultrafast electron trapping and defect-mediated recombination in nickel oxide: Resolving the effects of oxygen vacancies and grain boundary defects. **L. Baker**, S. Biswas, J. Husek, S. Londo

10:35 CATL 444. Plasmonic Au/p-GaN photocathodes for artificial photosynthesis: Ultrafast hot-carrier dynamics and photoelectrochemical CO₂ reduction. **J. DuChene**, G. Tagliabue, M. Abdellah, A. Habib, D.J. Gosztola, W. Cheng, R. Sundararaman, J. Sa, H. Atwater

10:55 CATL 445. Exciton dynamics and photoreduction of water in 1D and 2D semiconductor/metal nanoheterostructures. **T. Lian**

11:20 CATL 446. Direct observation of plasmon-induced interfacial charge separation in metal/semiconductor hybrid nanostructures by measuring surface potentials. **S. Lee**, S. Lee, T. Oh, S.A. Petrosko, C.A. Mirkin, **J. Jang**

11:40 CATL 447. Exploring the excited state manifold of organic photocatalysts using pump-push-probe spectroscopy. **K.L. Corp**, C.W. Schlenker, E.J. Rabe

Section E

Orange County Convention Center
Room W307A

Chemical Catalysis for Bioenergy Consortium: Addressing Deactivation during Biomass Conversion

Cosponsored by ENFL, ENVR and INOR
S. Habas, D. A. Ruddy, J. Schaidle, *Organizers*
D. Ruddy, *Presiding*

8:00 CATL 448. Chemical catalysis for bioenergy consortium: Enabling production of biofuels and bioproducts through catalysis. **J. Schaidle**

8:20 CATL 449. Effect of Pt addition on m-cresol hydrodeoxygenation reaction pathways over Mo₂C catalyst. **A.T. To**, C.A. Farberow, D.A. Ruddy, S. Habas, F.G. Baddour, C. Nash, J. Schaidle

8:40 CATL 450. CFD simulation of hydrodynamics, RTD, heat transfer and chemical reaction in a pilot-scale biomass pyrolysis vapor phase upgrading (VPU) reactor. **X. Gao**, L. Tingwen, W. Rogers

9:00 CATL 451. Deactivation and regeneration of Mo₂C used for hydrodeoxygenation of biomass fast pyrolysis vapors. **M. Yung**, C. Mukarakate, K. Iisa, S. Habas, J. Schaidle

9:20 Intermission.

9:50 CATL 452. Insights into the electrochemical conversion of biomass derivatives to fuels and chemicals. A. Román, Z. Barton, **A. Holewinski**



TECHNICAL PROGRAM

10:10 CATL 453. Catalytic conversion of carbohydrates to 5-hydroxymethylfurfural (HMF) and its potential for the production of non-isocyanate polyurethanes. **L. Zhang**, A. Co

10:30 CATL 454. Electrochemical conversion of carbon dioxide as an approach to make waste-derived feedstocks. **S. Ma**, A. Zeng, Z. Huo, M. George, E. Cave, N. Flanders, K. Kuhl

10:50 CATL 455. CO₂ utilization: Electrochemical and thermochemical pathways. **J. Ferrell**, S. Habas, F.G. Baddour, K.M. Van Allsburg, E. White, A.T. To, C. Downes

11:10 CATL 456. Carbon nanospikes as a physical catalyst for the electrolysis of carbon dioxide. **A. Rondinone**

Section F

Orange County Convention Center
Room W310A

Model Catalysis & Materials Complexity Frontiers

Cosponsored by PHYS

J. A. Boscoboinik, F. C. Calaza, W. Kaden, *Organizers, Presiding*

8:00 CATL 457. Bifunctional aldol condensation on metal oxides: The unusual case of oxygen vacancy assisted aldol coupling of acetaldehyde to crotonaldehyde on CeO_{2-x}(111). C. Zhao, C. Watt, P. Kent, S.H. Overbury, D.R. Mullins, F.C. Calaza, Y. Xu, **A. Savara**

8:20 CATL 458. Development of epitaxially supported molybdenum-nitride thin-films suitable for HDN materials-gap investigations. A. Khaniya, M. Sajid, A. Kara, **W. Kaden**

8:40 CATL 459. Role of O vacancies and presence of hydridic H in the alkyne semi-hydrogenation reaction on CeO₂(111). K. Werner, X. Weng, **F. Calaza**, M. Sterrer, T. Kropp, J.A. Paier, J. Sauer, M. Wilde, K. Fukutani, S. Shaikhutdinov, H. Freund

9:00 CATL 460. Metal-oxide kinetic coupling during CO oxidation on partially-reduced PdO(101). **J.F. Weaver**, V. Mehar, A.R. Asthagiri, M. Kim, J. Choi, C. Wu

9:20 CATL 461. Mass-selected clusters for supported nanocatalysts: Surface morphology. **K. Goodman**, J. Wang, Y. Ma, M.G. White

9:40 Intermission.

10:00 CATL 462. Steady-state catalytic decomposition of aspartic acid on Cu(111). Y. Yun, P. Kondratyuk, **A.J. Gellman**

10:20 CATL 463. Exploring enantioselective reactions on chirally modified surfaces in ultrahigh vacuum. **W.T. Tysoe**

10:40 CATL 464. Electrical potential changes at liquid/solid interfaces measured by ambient pressure XPS. **H. Bluhm**, A. Shavorskiy

11:00 CATL 465. Supported catalytically active liquid metal solutions: From operando studies to model catalysis. **J. Libuda**



TECHNICAL PROGRAM

11:20 CATL 466. Grain-boundary-supported active sites in heterogeneous electrocatalysis. **X. Feng**

11:40 CATL 467. Colloidal synthesis of powder catalysts with well-defined nanoparticle ensembles. **E.D. Goodman**, A. Holm, E.Z. Carlson, M. Cargnello

Section G

Orange County Convention Center
Room W310B

Catalytic Chemistry over Metal Oxides

Oxide Surfaces

D. Jiang, *Organizer*
S. D. Senanayake, Z. Wu, *Organizers, Presiding*
W. Huang, *Presiding*

8:00 CATL 468. Oxide surfaces and its interaction with water. **H. Freund**

8:30 CATL 469. Complex-mediated methane conversion over metal oxides from first principles. **V. Fung**, F. Tao, Z. Wu, D. Jiang

8:50 CATL 470. Synergy effect of two sets of single-atom sites (Ni_1 and Ru_1) on catalyst surface for reforming CH_4 . **F. Tao**, Y. Tang, Z. Wang

9:20 CATL 471. Computational studies of aldol condensation over MgO catalyst surfaces. **M. Zhou**, L.A. Curtiss, R.S. Assary

9:40 Intermission.

9:50 CATL 472. Mechanistic investigation of hydrogenation and dehydrogenation promoted by a silica supported organovanadium(III) catalyst. **D. Kaphan**, M. Delferro, R.R. Langeslay, C. Liu

10:20 CATL 473. Surface chemistry of $\text{IrO}_2(110)$. **J.F. Weaver**, A.R. Asthagiri, Z. Liang, T. Li, R. Martin, A. Franklin, Y. Bian, M. Kim

10:50 CATL 474. Dry reforming of methane on single site Ni-MgO catalysts. Z. Zuo, S. Liu, Z. Wang, C. Liu, J. Huang, **P. Liu**

11:20 CATL 475. Active phase in catalytic combustion of methane. **A.C. Banerjee**, K.W. Golub, M. Hakim

11:40 CATL 476. Dry reforming of methane over a Ni-Mo-MgO nanocatalyst. **C.T. Yavuz**, Y. Song, E. Ozdemir, A. Adishev, S. Subramanian, A. Harale, M. Albuali, B. Fadhel, A. Jamal, D. Moon, S. Ramesh

Innovative Chemistry & Materials for Electrochemical Energy Storage



TECHNICAL PROGRAM

Beyond Li-Ion

Sponsored by ENFL, Cosponsored by CATL, INOR and PMSE

Carbon Dioxide Conversion & Utilization

CO₂ Capture & Conversion

Sponsored by ENFL, Cosponsored by CATL, COMP and GEOC

WEDNESDAY AFTERNOON

Section A

Orange County Convention Center
Room W306A

Activation of Light (C1-C4) Hydrocarbons: Theory & Experiments

Cosponsored by ENFL, ENVR, INOR and PHYS

C. A. Carrero, *Organizer*

I. Hermans, F. Tao, *Organizers, Presiding*

1:00 CATL 477. Support-dependent nuclearity in supported zinc and gallium catalysts for alkane dehydrogenation. **S.L. Scott**, Z. Jones, S. Fleischman, A. Gallo

1:40 CATL 478. Stability analysis of electroless deposition derived Ni-Pt catalysts for the dry reforming of methane. B. Egelske, J. Keels, J.R. Monnier, **J.R. Regalbuto**

2:10 CATL 479. Alkane activation on late transition-metal oxides. **J.F. Weaver**, A.R. Asthagiri, Z. Liang, T. Li, R. Martin, A. Franklin, Y. Bian, M. Kim, F. Zhang

2:30 CATL 480. Carbonylation of dimethyl ether over MOR and Cu/H-MOR catalysts: comparative investigation of deactivation behavior. **Z. Cheng**, S. Huang, Y. Li, X. Ma

2:50 Intermission.

3:00 CATL 481. Continuous anaerobic conversion of methane into methanol over Cu-zeolites. J. Kang, S. Lee, Y. Jeong, **E. Park**

3:20 CATL 482. Driving the ethane dehydroaromatization pathway in Zn/ZSM-5 via speciation of Zn sites. **A. Mehdad**, R.F. Lobo

3:40 CATL 483. Computation study of methane borylation in transition metal functionalized metal-organic frameworks. **B. Yang**, X. Wu, M. Delferro, O.K. Farha, L. Gagliardi, D.G. Truhlar



TECHNICAL PROGRAM

4:00 CATL 484. Computational study of the stability and catalytic activity of a copper-oxo cluster supported on the NU-1000 metal–organic framework for methane oxidation to methanol. **J. Ye**, D.G. Truhlar, C.J. Cramer

4:20 CATL 485. Investigating the interaction of surface and gas-phase chemistry on the boron nitride-catalyzed oxidative dehydrogenation of propane. **J. Venegas**, W.P. McDermott, I. Hermans

4:40 CATL 486. DFT study on the effect of the distribution of aluminum atoms in Zn-exchanged MFI on methane activation. **S. Albarracin**, Y.J. Pagan-Torres, M.C. Curet-Arana

Section B

Orange County Convention Center
Room W306B

Light-Driven Chemistry: Photoelectrochemistry & Photocatalysis

Cosponsored by COLL, ENFL, I&EC, INOR and PHYS
G. Dukovic, *Organizer*
S. Ardo, D. Esposito, I. Sharp, *Organizers, Presiding*

1:00 CATL 487. Studies of PCET in natural and artificial photosynthesis. **V.S. Batista**

1:25 CATL 488. Sustainable hydrogen peroxide production from water and oxygen by graphitic carbon nitride (g-C₃N₄)-based photocatalyst. **Q. Zheng**, D. Shuai, H. Chen

1:45 CATL 489. Integrating simulations and experiments to probe complex photoelectrochemical interfaces under realistic operating conditions. **B. Wood**, T. Ogitsu, T. Pham, X. Zhang, S. Ptasinska

2:10 CATL 490. Design considerations of sunlight-driven organic electrosynthetic processes. **M. Modestino**, D. Blanco

2:35 CATL 491. Multiscale modeling of carrier transport in photocatalytic materials: Application to bismuth vanadate BiVO₄. **V. Pasumarthi**, M. Dupuis, T. Liu, C. Li

2:55 Intermission.

3:10 CATL 492. Electrolyte engineering for water splitting at mild pH. **K. Takanabe**

3:35 CATL 493. Understanding nanoscale and interfacial charge transport in water splitting photoanodes. **F. Toma**

4:00 CATL 494. Photoelectrochemical characterization of infrared-absorbing osmium-polypyridyl dyes bound to TiO₂. **J.M. Cardon**, K. Tkaczibson, G.D. Hogrebe, C. Feltenberger, N. Farhang, G.R. Krueper, H. Chen, S. Ardo

4:20 CATL 495. Implications of electron scavenging character of sulfated titania for photochemistry. A. Mahdavi-Shakib, A. Rahmani-Chokanlu, T.J. Schwartz, R.N. Austin, **B.G. Frederick**

4:40 CATL 496. Photocatalysis in nanomaterial-redox enzyme hybrid complexes. **K.A. Brown**, J. Ruzicka, D. Harris, H. Kallas, J. Peters, L.C. Seefeldt, G. Dukovic, P.W. King

5:00 CATL 497. Nanorod-enzyme conjugates for photoinduced turnover of [FeFe] hydrogenase. **M. Sanchez**, J. Birrell, E. Reijerse, W. Lubitz, R.B. Dyer



TECHNICAL PROGRAM

Section C

Orange County Convention Center
Room W309A

Well-Defined Materials for Heterogeneous Catalysis: Synthesis, Characterization, & Performance Studies

Electrochemistry

Cosponsored by ENFL
M. Cargnello, H. Zhu, *Organizers*
D. Su, *Organizer, Presiding*
M. Cargnello, *Presiding*

1:00 CATL 498. Colloidal synthesis of metal nanoparticles for electrochemical transformations of carbon dioxide. **D. Kim**, P. Yang

1:35 CATL 499. Electrochemical behavior of lithium-promoted mesoporous tantalum oxide. **A. Shirazi Amin**, P. Toloueinia, Y. Wu, A. Meguerdichian, P. Kerns, S.L. Suib

1:55 CATL 500. Highly ordered PtM alloy catalysts derived from MOFs for oxygen reduction. **G. Wu**

2:30 Intermission.

2:40 CATL 501. Low-dimensional materials in heterogeneous electrocatalysis: from understanding to nanoengineering. **M. Liu**, Q. Wu

3:00 CATL 502. Device engineering for solar fuel harvesting photoelectrodes. **M. Liu**

3:35 CATL 503. Probing the *in situ* electrochemical reduction of hierarchical oxide-derived inverse opals during the conversion of carbon dioxide into fuels. **T. Nguyen Phan**, D. Kauffman, Y. Zhou, Y. Yu, E. Stavitski, W. Xu, B. Howard, M.Y. Stuckman, C. Wang, C.M. Marin, I. Waluyo, P. Ohodnicki

3:55 CATL 504. Metal ion cycling of Cu foil for selective C–C coupling in electrochemical CO₂ reduction. **H. Wang**

4:30 CATL 505. Microstructural effects on photocatalytic performance in Bi₂MoO₆/Ag₃PO₄ Z-Scheme systems. **K. Ayalew**, X.I. Morgan-Lange, J. Moon

4:50 CATL 506. Influence of three-dimensional macro-porous copper electrodes on the electrochemical reduction of CO₂. **M. Duran**, J. Sanabria-Chinchilla

Section D

Orange County Convention Center
Room W309B

Model Catalysis & Materials Complexity Frontiers

Cosponsored by PHYS
J. A. Boscoboinik, F. C. Calaza, W. Kaden, *Organizers, Presiding*



TECHNICAL PROGRAM

1:30 CATL 507. Synthesis and characterization of chemically active 2D Nanoporous materials.. **D.J. Stacchiola**

1:50 CATL 508. Looking into the atomic structure of glass films. **M. Heyde**

2:10 CATL 509. Exploring confinement effects in two-dimensional porous materials: A surface science approach. **J.A. Boscoboinik**

2:30 CATL 510. Spectromicroscopy of ultrathin bilayer silicate films on Pd(100) and Pd(111). **S.A. Tenney**, V. Lee, C. Eads, M. Wang, J. Kelber, D.J. Stacchiola

2:50 CATL 511. Reactivity of model transition metal-supported zeolites. J. Jhang, G.S. Hutchings, C. Zhou, J.A. Boscoboinik, U. Schwarz, **E. Altman**

3:10 CATL 512. Ionization-facilitated noble gas trapping in two-dimensional (alumino)silicate bilayer films. **M. Wang**, J. Zhong, J.A. Boscoboinik, D. Lu

3:30 Intermission.

3:50 CATL 513. Kinetics-based computational catalyst design strategy for the oxygen evolution reaction on transition metal oxide surfaces. **C. Plaisance**, S. Beinlich, K.U. Reuter

4:10 CATL 514. Dynamic catalytic interfaces: statistical ensembles of multiple metastable states dictate the properties. **A. Alexandrova**

4:30 CATL 515. Quantum nutcracker for near-room-temperature H₂ dissociation. **Y. Zhang**, L. Tao, W. Guo, S.T. Pantelides, S. Du

Section E

Orange County Convention Center
Room W307A

Chemical Catalysis for Bioenergy Consortium: Addressing Deactivation during Biomass Conversion

Cosponsored by ENFL, ENVR and INOR
D. A. Ruddy, J. Schaidle, *Organizers*
S. Habas, *Organizer, Presiding*

1:00 CATL 516. Mitigating deactivation of low temperature biogas reforming catalysts. **J. Kuhn**, S. Tosin, B. Joseph, M. Yung

1:20 CATL 517. Ethanol conversion to gasoline and higher value chemicals (BTEX). **J. Hannon**

1:40 CATL 518. Changes in product selectivity with time: Producing high octane fuels from biomethanol at the pilot scale. **J. Hensley**, S. Marie-Rose, E. Christensen, D.A. Ruddy, A.T. To, C. Nash, J. Schaidle

2:00 CATL 519. Developing bimetallic BEA zeolite catalysts to control the paraffin-olefin ratio during DME homologation. **C. Nash**, D.A. Ruddy, D. DuPuis, A.T. To, C.A. Farberow, K.A. Unocic, C. Yang, J.T. Miller, S. Habas

2:20 Intermission.



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

2:50 CATL 520. Metal encapsulation in zeolites: An approach for stable catalysts. **J. Guzman**

3:10 CATL 521. Role of mesopore generation method in structure, activity and stability of MFI zeolites in glycerol acetylation. **Q. Almas**, C. Sievers, C.W. Jones

3:30 CATL 522. Effects of confining environment polarity on reactivity and stability of Sn-Beta zeolites during gas-phase and liquid-phase catalysis. **J.S. Bates**, M. Cordon, J.N. Hall, J.W. Harris, R. Gounder

3:50 CATL 523. Metal-organic frameworks for biomass up-conversion catalysis with high selectivity: Investigation of C—C bonds formation by aldol condensation in a pre-defined pore space. **T. Wang**, V. Stavila, M. Allendorf

4:10 CATL 524. Optimizing metal oxide catalyst combinations for enhanced stability and selectivity towards production of industrially relevant bio-based olefins, ketones, and aldehydes. **J.O. Smith**

Section G

Orange County Convention Center
Room W310B

Catalytic Chemistry over Metal Oxides

Ceria Catalysis

Z. Wu, *Organizer*

D. Jiang, S. D. Senanayake, *Organizers, Presiding*

J. Zhou, *Presiding*

1:00 Introductory Remarks.

1:05 CATL 525. Inverse oxide/metal catalysts and the hydrogenation of CO₂. **J. Rodriguez**

1:35 CATL 526. Growth and sintering of Ni-based bimetallic nanoparticles over reducible CeO₂(111) thin films. **J. Zhou**, L. Du

2:05 CATL 527. Redox materials chemistry at the nanoscale. **Y. Lykhach**, T. Skála, N. Tsud, J. Mysliveček, K.C. Prince, V. Matolin, J. Libuda

2:25 CATL 528. Computational modeling of stability and properties of cerium dioxide supported platinum clusters and isolated platinum species. **G.N. Vayssilov**, H. Aleksandrov, I. Koleva

2:45 Intermission.

2:55 CATL 529. Ceria catalysts for stitching small molecules via multiple bond formation reactions. **F. Wang**

3:25 CATL 530. CeO₂-based model catalysts: Reducibility and interaction with hydrogen. **P. Luches**, J. Pelli Cresi, S. Benedetti, G. Gasperi, S. D'Addato, S. Valeri

3:55 CATL 531. Identifying the active structures of metal nanoparticles supported on CeO₂ for CO oxidation. **J. Liu**, M. Yang, E. Hensen, B.R. Goldsmith



TECHNICAL PROGRAM

4:15 CATL 532. Selective oxidation of hydrocarbons by La doped cerium oxide catalysts. **S. Dissanayake**, S.L. Suib

4:35 CATL 533. Controlling the concentration of oxygen vacancies in CeO₂-ZrO₂ nanoparticles via spatial tailoring of the active site. B. Safavinia, Y. Wang, S. Sahu, J. Larriviere, K.M. Dooley, **J. Dorman**

Innovative Chemistry & Materials for Electrochemical Energy Storage

Advanced Materials & Synthesis

Sponsored by ENFL, Cosponsored by CATL, INOR and PMSE

THURSDAY MORNING

Section A

Orange County Convention Center
Room W232C

General Catalysis

A. Savara, *Organizer*
F. C. Calaza, *Organizer, Presiding*
A. Dutta Chowdhury, *Presiding*

8:20 CATL 534. Highly dispersed metal catalyst synthesized through a metal@carbon core-shell precursor through simple impregnation method. **S. Das**, A. Jangam, N. Dewangan, S. Kawi

8:40 CATL 535. Rational and microwave-assisted synthesis of noble metals-promoted carbon-supported transition metal catalysts for CO hydrogenation reaction. **F. Almalki**, F. Gupton

9:00 CATL 536. Catalytic decomposition of NaBH₄ using dendrimer encapsulated nanoparticles (DENS). **A. Jacobsen**

9:20 CATL 537. Tunable aryl alkyl ionic liquids (TAAILs) and transition metal catalysis. **S. Lerch**, T. Strassner

9:40 Intermission.

10:00 CATL 538. Amphiphilic graphene oxide nanosheet catalysts via layer-by-layer assembly with high catalytic activity and stability. **Y. Ko**, C. Kwon, J. Choi, J. Cho

10:20 CATL 539. Synthesis and catalytic properties of Graphene based mesoporous silica (SBA-15) doped titania nanocomposites(Graphene/SBA15/TiO₂). **A. Ali**, B. Li, M. Asim khan

10:40 CATL 540. Engineering functional coordination space in MOFs. **H. Yu**, J. Jiang, M. Pan, Z. Wei

11:00 CATL 541. Nanoengineering of yolk-shell MOF@MOF nanomaterials for catalytic reactions. **T. Pan**



TECHNICAL PROGRAM

11:20 CATL 542. Biphasic nickel phosphide nanosheets electrocatalyst for sensitive electrochemical H₂O₂ detection. **S. Tong**

Section B

Orange County Convention Center
Room W240D

Well-Defined Materials for Heterogeneous Catalysis: Synthesis, Characterization, & Performance Studies

Selectivity

Cosponsored by ENFL
M. Cargnello, D. Su, H. Zhu, *Organizers*
M. Cargnello, H. Zhu, *Presiding*

8:00 CATL 543. Multi-functional Pd-Re catalysts for the reduction of carboxylic acids. **R.J. Davis**, J. Kammert

8:35 CATL 544. Withdrawn

8:55 CATL 545. Toward more sustainable MPd (M = Au, Ag) catalysis for dehydrogenation/hydrogenation reactions through nanomaterials design. **M. Muzzio**, H. Lin, C. Yu, S. Sun

9:15 CATL 546. Effects of hydrophilic binding site density in Lewis acid zeolites on glucose isomerization catalysis. **J. Vega-Vila**, M. Cordon, R. Gounder

9:35 Intermission.

9:45 CATL 547. Pt-Re nanoporous networks: A well-defined model system for elucidating composition-reactivity correlations in bimetallic catalysts. **E. Gross**

10:20 CATL 548. Highly active and stable carbon nanosheets supported iron oxide for Fischer-Tropsch to olefins synthesis. **C. Wang**

10:40 CATL 549. Elucidating electronic metal-support interactions for Pd-graphene systems. **K. Dreyer**, D.D. Hibbitts, R. Rao, J. Tessonnier

11:00 CATL 550. Investigation how to control surface reactivity towards carbon, oxygen, and hydrogen of intermetallic compounds in wet reforming of hydrocarbons and oxygenates. **Y. Song**, Y. He, S. Laursen

11:20 CATL 551. Effect of surface composition change of non-noble metal intermetallic compounds on the activation of C-H and C=C bonds in the dehydrogenation of light hydrocarbons. **Y. He**, Y. Song, S. Laursen

11:40 CATL 552. Synthesis of ionic liquid supported silica-coated magnetic nanocatalyst for the straightforward one-pot synthesis of bioactive *N*-aryl oxazolidin-2-ones. **R. Gupta**

Section C

Orange County Convention Center
Room W311D



TECHNICAL PROGRAM

In Situ & Operando Spectroscopy/Microscopy Studies of Catalysis

F. Tao, Z. Wu, *Organizers, Presiding*
L. Nguyen, Y. Tang, *Presiding*

8:00 CATL 553. Catalytic hydrogenation of carbon dioxide: Structure sensitivity and mechanistic insights to steer activity and selectivity. **B.M. Weckhuysen**

8:30 CATL 554. Active species and active sites in water gas shift reaction over Pt/CeO₂ catalysts. Y. Li, M. Kottwitz, R.G. Nuzzo, **A. Frenkel**

9:00 CATL 555. Catalytic oxidation of 2-propanol on SnO₂(110) studied with ambient-pressure X-ray photoelectron spectroscopy. T.T. Diulus, **G.S. Herman**

9:20 CATL 556. Probing synthesis and reaction mechanisms of core-shell metal nanoparticles via *in situ* environmental and liquid STEM. **M. Chi**

9:50 Intermission.

10:00 CATL 557. *in-situ* combined XAS and SAXS study of nanocatalysts under realistic reaction conditions: understanding of the size and reactivity relationship in catalysis. **S. Lee**, S. Lee, R.E. Winans

10:30 CATL 558. Developing a Raman-spectrokinetic approach to gain insights on the structure-reactivity relationship of supported metal oxide catalysts. J.A. Moncada, W.R. Adams, R.K. Thakur, **C.A. Carrero**

10:50 CATL 559. X-ray photoelectron spectroscopy studies of nanoparticles dispersed in static liquid. **F. Tao**, L. Nguyen

11:20 CATL 560. Scanning tunneling microscopy and spectroscopy of Ar-sputtered TaS₂/Cu(111) at 78K: Investigating catalytic mechanisms. **B. Blue**, D. Le, M. Ishigami, T. Rahman, M. Vaida

11:40 CATL 561. Active site of atomically dispersed metal-catalysts for CO₂ reduction reaction. **J. Ou**

Section D

Orange County Convention Center
Room W311E

Chemical Catalysis for Bioenergy Consortium: Addressing Deactivation during Biomass Conversion

Cosponsored by ENFL, ENVR and INOR
S. Habas, D. A. Ruddy, *Organizers*
J. Schaidle, *Organizer, Presiding*

8:00 CATL 562. Catalyst deactivation mitigation in biomass conversion and their correlation to feedstock properties and catalyst functionalities. **H. Wang**

8:20 CATL 563. Zeolite catalyst deactivations during the conversion of bio-derived 2,3-butanediol and ethanol. **Z. Li**, J. Zhang, S. Adhikari, C. Yang, N. LiBretto, J.T. Miller, T. Krause, K.A. Unocic



TECHNICAL PROGRAM

8:40 CATL 564. Single step conversion of ethanol to butadiene and butenes over Ag/ZrO₂/SiO₂ catalysts. **V. Dagle**, J. Saavedra Lopez, S. Akhade, V. Glezakou, R. Rousseau, S. Habas, Y. Tang, F. Tao, A. Winkelman, R. Dagle

9:00 CATL 565. Inverse bimetallic catalysts for selective reduction of propionic acid. **V. Vorotnikov**, T. Eaton, A. Settle, K. Orton, E. Wegener, C. Yang, J.T. Miller, G. Beckham, D. Vardon

9:20 Intermission.

9:50 CATL 566. Deactivation mechanism of zeolite (HZSM-5) catalyst from biomass derived small oxygenates conversion. **K.K. Ramasamy**, A. Devaraj

10:10 CATL 567. Catalyst considerations for upgrading biomass pyrolysis vapors and liquids to fungible hydrocarbon intermediates. **K.A. Magrini**, J. Olstad, B. Peterson, Y. Parent, S. Deutch, K. Lisa, M. Yung

10:30 CATL 568. Hydrodeoxygenation of biomass-derived intermediates to paraffins for blending into jet or diesel fuels. **D.K. Johnson**

10:50 CATL 569. Reactivity of model oxygenates on heterogeneous catalysts: Insights from first principles Simulations. **R. Surendran Assary**, L.A. Curtiss, M. Zhou

Section E

Orange County Convention Center
Room W311C

Elucidation of Mechanisms & Kinetics on Surfaces

Cosponsored by ENFL, ENVR, INOR and PHYS
L. Baker, A. Ignatchenko, S. Laursen, *Organizers*
A. Savara, *Organizer, Presiding*

8:00 CATL 570. Elucidation of reaction mechanisms of bifunctional metal oxide-zeolite catalyzed hydrogenation of carbon dioxide to hydrocarbons. **A. Dutta Chowdhury**, A. Ramirez, E. AbouHamad, A. Dokania, J. Gascon

8:20 CATL 571. Methanol dehydration over H-SSZ-13 with controlled site proximity: Effects of site proximity and coverage. **A. Hoffman**, J. Di Iorio, S. Nystrom, C. Nimlos, R. Gounder, D.D. Hibbitts

8:40 CATL 572. Large impact of approximate exchange-correlation functionals on predicting the mechanisms of water-gas shift reaction and methanol synthesis. M.S. Tameh, A.K. Dearden, **C. Huang**

9:00 CATL 573. Propyne hydrogenation over a Pd/Cu(111) single atom alloy catalyst studied with infrared spectroscopy. **M.K. Abdel-Rahman**, M. Trenary

9:20 Intermission.

9:40 CATL 574. Atomic-scale observation of diffusion on a crowded catalyst surface. **A. Henß**, S. Sakong, P. Messer, J. Wiechers, R. Schuster, D. Lamb, A. Gross, J. Winterlin

10:00 CATL 575. Solvation effects on deoxygenation reactions over bimetallic phosphide catalysts. **V. Jain**, N. Rai



TECHNICAL PROGRAM

10:20 CATL 576. On the rational design of zeolite clusters for converging reaction barriers: Quantum study of aldol kinetics confined in HZSM-5. **A.N. Miguez**, Q. Sun, S. Vaitheeswaran, W. Sherman, S.M. Auerbach

10:40 CATL 577. Electrocatalytic hydrogenation of lignin dimers & derivatives: Towards selectivity of C-O cleavage over Raney® nickel surface. **Y. Zhou**, P. Hao, J.E. Jackson

Section F

Orange County Convention Center
Room W311F

General Catalysis

A. Savara, *Organizer*

F. C. Calaza, *Organizer, Presiding*

8:00 CATL 578. Oxidative dehydrogenation of propane over Pt-Sn/Si-beta catalysts: Key role of Pt-Sn interaction. **L. Sun**

8:20 CATL 579. High-performance CoCu catalyst encapsulated in KIT-6 for higher alcohol synthesis from syngas. **Z. Li**, Y. Wang, X. Ma

8:40 CATL 580. Effect of bi-metallic heterogeneous catalysts for the hydrogenation of carbon dioxide to light olefins. **C. Zhang**, A. Rosario, D. Triger, A. Leichnam, S.D. Senanayake

9:00 CATL 581. Discovery of a reactive oxygen structure on catalytic gold nanoparticles. J.P. Robbins, K. Liu, T. Chen, S. He, F. Tian, **S.G. Podkolzin**

9:20 Intermission.

9:30 CATL 582. Withdrawn

9:50 CATL 583. Electrocatalysts as aerobic oxidation catalysts and the use of organic redox mediators as “soluble electrodes”. **S. Biswas**, T.W. Root, S.S. Stahl

10:10 CATL 584. Design principles for dihydrophenazine-mediated photoredox applications. **J. Cole**

10:30 CATL 585. Highly active and stable bimetallic Ni-Mo₂C catalyst for a partial oxidation of jet fuel. **Q. Bkour**, M. Norton, S. Ha

10:50 CATL 586. Electrochemical structure of water in contact with low temperature plasma. **T. Oldham**, E. Thimsen

11:10 CATL 587. Withdrawn

Innovative Chemistry & Materials for Electrochemical Energy Storage

General



TECHNICAL PROGRAM

Sponsored by ENFL, Cosponsored by CATL, INOR and PMSE

THURSDAY AFTERNOON

Section A

Orange County Convention Center
Room W232C

General Catalysis

F. C. Calaza, A. Savara, *Organizers*
A. Dutta Chowdhury, *Presiding*

1:00 CATL 588. Probes into acid-base sites on geopolymeric catalyst: A DFT study. **S. Sinha**, S. Karri, S. Sharma, P. Deshpande

1:20 CATL 589. DFT studies on palladium catalyzed Suzuki-Miyaura reaction. **S. Karri**, P. Deshpande

1:40 CATL 590. Development of bio-inspired synthetic metallohydrolases. T.J. Paul, G. Sharma, Q. Hu, V. Jayasinghe-Arachchige, **R. Prabhakar**

2:00 CATL 591. Mn-promoted cobalt catalysts for light olefin production. E.Ø. Pedersen, **I. Svenum**, E.A. Blekkan

2:20 CATL 592. CO₂ microwave plasma: Efficient production of CO at moderate pressures. **F. Peeters**, B. Wolf, T. Righart, V. Reddy, Y. Liu, P. Groen, R. Van de Sanden, W. Bongers

2:40 Intermission.

2:50 CATL 593. Are urban environmental contaminants beneficial or detrimental to chemical warfare agent destruction on zirconium hydroxide nanoparticles? **R.B. Balow**, M.L. McEntee, G.C. Daniels, W.O. Gordon, J.H. Wynne, G.W. Peterson, P.E. Pehrsson

3:10 CATL 594. Machine learning enhanced global optimization by clustering local environments. **S. Meldgaard**, B. Hammer

3:30 CATL 595. ACCDB: A collection of chemistry databases for broad computational purposes, and its reduction to statistically significant subsets. P. Morgante, **R. Peverati**

3:50 CATL 596. Mechanistic insights into interactions between bacterial class I P450 enzymes and redox partners. **W. Zhang**

4:10 CATL 597. Efficient and stable Ru(III)/choline chloride catalyst system with low Ru content for non-mercury acetylene hydrochlorination. **H. Li**, B. Wu, F. Wang, X. Zhang

Section B



TECHNICAL PROGRAM

Orange County Convention Center
Room W240D

General Catalysis

A. Savara, *Organizer*
F. C. Calaza, *Organizer, Presiding*

1:30 CATL 598. Rhodium-catalyzed hydroformylation of vinyl acetate: Effect of phosphine ligands on regioselectivity. **X. Xu**, H. Feng, D. Liu, S. Zhao, H. Liu, Y. Shao

1:50 CATL 599. Reaction pathways of cyclohexene oxidation in the presence of transition-metal-substituted phosphotungstates and hydrogen peroxide. **Y. Song**, F. Xin

2:10 CATL 600. Methane pyrolysis catalyzed by liquid and gas phase tellurium. **J. Zeng**, T. Pennebaker, M. Tarazkar, M. Gordon, H. Metiu, E.W. McFarland

2:30 CATL 601. Electroactivated alkylation of amines with alcohols via borrowing hydrogen methodology. **B. Appiagyei**, **S. Bhatia**, **G. Keeney**, **J.E. Jackson**

2:50 CATL 602. Long chain hydrocarbons synthesis from quaiacol ring opening reactions. **F.A. Agblevor**, H. Jahromi

3:10 CATL 603. Vibrational signatures of sarin adsorption on anatase surfaces by density functional theory. **N.Q. Le**, I. Schweigert, D. Gunlycke

3:30 Intermission.

3:40 CATL 604. Reusable reaction media and catalysts for the Friedel-Crafts alkylation of indole with alcohols. **F.G. García Cirujano**, M. Stalpaert, D. De Vos

4:00 CATL 605. Small concentrations of non-framework Bronsted sites impact HZSM-5 reactivity. **M. Abdolrahmani**, K. Chen, J.L. White

4:20 CATL 606. Superacidic mesoporous catalysts of alkylation of aromatic compounds. A.A. Kuvayskaya, **A. Vasiliev**

4:40 CATL 607. Synthesis of mesoporous Al-SBA-15 with enhanced acidity and hydrothermal stability for hydrocracking process. **H.H. Habboubi**

Section C

Orange County Convention Center
Room W311D

Well-Defined Materials for Heterogeneous Catalysis: Synthesis, Characterization, & Performance Studies

Characterization

Cosponsored by ENFL
M. Cargnello, H. Zhu, *Organizers*



TECHNICAL PROGRAM

D. Su, *Organizer, Presiding*
H. Zhu, *Presiding*

1:00 CATL 608. Rational design and synthesis of bifunctional metal nanocrystals for probing catalytic reactions by surface-enhanced raman scattering. **D. Qin**

1:35 CATL 609. In situ study on abnormal pore size changes of Zr based metal-organic frameworks using low-dose high resolution TEM. **P. Tieu**, W. Gao, L. Muqing, Z. Xu, X. Pan

1:55 CATL 610. Surface plasmon resonance spectroscopy as a tool for distinguishing homogeneous versus heterogeneous catalytic pathways for metal nano-catalyzed C-C coupling reactions. **F. Mohammadparast**, A. Dadgar, R. Tirumala, M. Andiappan

2:15 CATL 611. Understanding boron-containing oxidative dehydrogenation catalysts through well-defined supported materials. **M. Cendejas**, I. Hermans, A.J. Rossini

2:35 Intermission.

2:45 CATL 612. Advances in the use of advanced solid state NMR for the study of alumina supports and alumina-supported organometallic catalysts. L. Delevoye, N. Merle, K. Szeto, F. Zhang, S.L. Scott, M. Taoufik, **R. Gauvin**

3:05 CATL 613. Spectroscopy and structural characterization of single site Mo metathesis catalyst. A. Hoffman, L. Li, N. Peek, S.L. Scott, **A.E. Stiegman**

3:25 CATL 614. Deconvoluting the role of defects and hydronium ion concentration on the stability of zeolites in aqueous phase reactions. **S. Proding**, M.A. Derewinski, J.A. Lercher

3:45 CATL 615. Quantitative studying the formation kinetics and energetics of intermetallic nanoparticles. M. Chen, Y. Han, C. Tsung, J. Evans, **W. Huang**

4:20 CATL 616. Growth, structure and catalytic properties of ZnO grown on Cu(111). **M. Mahapatra**, J. Rodriguez

4:40 CATL 617. Surface construction of nitrogen-functionalized graphene for enhanced sulfacetamide degradation via peroxymonosulfate activation. **X. Chen**, T.T. Lim

Section D

Orange County Convention Center
Room W311E

In Situ & Operando Spectroscopy/Microscopy Studies of Catalysis

F. Tao, Z. Wu, *Organizers, Presiding*
L. Nguyen, Y. Tang, *Presiding*

1:00 CATL 618. Insights into the mechanism for oxidation of volatile organic compounds on ceria based catalysts. M. Brites Helu, S. Collins, **F.C. Calaza**

1:20 CATL 619. Probing catalytic interfaces with in situ neutron pair distribution function studies. **K. Page**



TECHNICAL PROGRAM

1:50 CATL 620. Elucidating the mechanism of ethanol coupling to *n*-butanol over hydroxyapatite with diffuse reflectance infrared fourier transform spectroscopy and mass spectrometry (DRIFTS-MS). **S. Wang**, I. Hermans

2:30 CATL 621. *in-situ* NMR of the catalytic depolymerization of lignin. **M.B. Foston**, Y. Gao, L. Qi, D.W. Hoyt

2:50 Intermission.

3:00 CATL 622. VISION and VirtuES: Modeling and interpreting inelastic neutron scattering applications to catalysis and chemistry. **A. Ramirez-Cuesta**, Y. Cheng

3:30 CATL 623. Surface restructuring of transition metal phosphide nanoparticles under electrochemical water-splitting conditions. **Z. Wu**, L. Huang, H. Liu, H. Wang

3:50 CATL 624. *Operando* MAS-NMR spectroscopy in catalytic lignin hydrogenolysis. **L. Qi**, A. Chamas, D.W. Hoyt, E. Walter, N. Washton, S.L. Scott

4:20 CATL 625. *Operando* studies of carbon removal and contaminants in solid oxide fuel cells. **W.A. Maza**, S.D. Tsoi, D.A. Steinhurst, B.C. Eigenbrodt, R.A. Walker, J. Owrutsky

4:40 CATL 626. *Operando* synchrotron infrared microspectroscopy: Insight into the direct formation of olefins in the MTG process over H-ZSM-5. **I. Minova**, P.A. Wright, A. Greenaway, S. Matam, R. Catlow, M. Frogley, G. Cinque, R. Howe

Section E

Orange County Convention Center
Room W311C

Activation of Light (C1-C4) Hydrocarbons: Theory & Experiments

Cosponsored by ENFL, ENVR, INOR and PHYS
I. Hermans, *Organizer*
C. A. Carrero, F. Tao, *Organizers, Presiding*

1:00 CATL 627. Mechanistic insights on Ag/CaCO₃ catalyzed aerobic propylene epoxidation under complex reaction conditions. **S.E. Specht**, I. Hermans

1:20 CATL 628. Density-dependent deactivation mechanism in supported catalysts by high-temperature decomposition of particles into single atoms. **E.D. Goodman**, A. Johnston-Peck, E. Dietze, C.J. Wrasman, A.S. Hoffman, F. Abild-Pedersen, S. Bare, P.N. Plessow, M. Cargnello

1:40 CATL 629. Dry reforming using modified metal carbides. **R.K. Thakur**, C.A. Carrero

2:00 CATL 630. Hexagonal boron nitride as a catalyst for the oxidative cracking of *n*-butane. **W.P. McDermott**, J. Venegas, I. Hermans

2:20 CATL 631. Methane to value-added chemicals using a solid superacid. S. Kanitkar, J. Carter, K. Ding, G. Hutchings, **J.J. Spivey**

2:40 Intermission.



TECHNICAL PROGRAM

2:50 CATL 632. Computational study of the selective hydrogenation of alkynes to alkenes on 2D materials. **E. Mates-Torres**, M. Garcia-Melchor

3:10 CATL 633. Oxidation of methane to methanol using $(\text{DMSO})_2\text{PtCl}_2$ catalyst in $\text{SO}_3\text{--H}_2\text{SO}_4$ system. **H. Dang**, H. Lee, S. Hong, M. Cheong, H. Lee

3:30 CATL 634. Isolated effect of metal content on the performance of Pt/CeZrO_2 dry reforming catalysts. **Y.O. Sokefun**, B. Joseph, J. Kuhn

3:50 CATL 635. Lifetime improvement in methanol-to-olefins catalysis over chabazite materials by high-pressure H_2 co-feeds. **S.S. Arora**, D.L. Nieskens, A. Malek, A. Bhan

4:10 CATL 636. Direct conversion of methane to aromatics on stable Mo@HZSM-5 catalyst. **Y. Liu**, Y. Zhang

4:30 CATL 637. DFT studies of C-H and C-C bond activations in n-butane on nickel based catalysts. **C. Wu**, L. Wang, Z. Xiao, G. Li, **L. Wang**

Section F

Orange County Convention Center
Room W311F

Elucidation of Mechanisms & Kinetics on Surfaces

Cosponsored by ENFL, ENVR, INOR and PHYS
L. Baker, A. Ignatchenko, S. Laursen, *Organizers*
A. Savara, *Organizer, Presiding*

1:00 CATL 638. Adaptive kinetic Monte Carlo simulations of surface segregation in PdAu nanoparticles. **L. Li**, L. Koziol, G. Henkelman

1:20 CATL 639. Computational screening of NU-1000-supported transition metal catalysts for the hydrolysis of sarin. **M. Mendonca**, R. Snurr

1:40 CATL 640. Interconversion of aromatic co-catalysts during MTO in H-MFI zeolites: Reacting methanol and dimethyl ether with $\text{C}_6\text{--C}_{12}$ methylbenzenes. **M. DeLuca**, P. Kravchenko, D.D. Hibbitts

2:00 CATL 641. Probing molecular-scale catalytic interactions between oxygen and cobalt phthalocyanine supported on metal surfaces. **D. Nguyen**, G. Kang, M. Hersam, G.C. Schatz, R.P. Van Duyne

2:20 CATL 642. Measurements of oxygen electroadsorption kinetics on $\text{RuO}_2(110)$ and $\text{IrO}_2(110)$. **D. Kuo**, H. Paik, J. Nelson, K. Shen, D. Schlom, J. Suntivich

2:40 Intermission.

3:00 CATL 643. $\text{NO} + \text{CO}$ reaction on Rh surface: DFT investigation combined with microkinetic analysis. **A. Ishikawa**, Y. Tateyama

3:20 CATL 644. Mechanistic insights into the CO_2 hydration reaction over biomimetic graphene and CNT surfaces. **S. Vangala**, P. Deshpande



TECHNICAL PROGRAM

3:40 CATL 645. Reaction and deactivation mechanism insights into catalytic conversion of ethanol to butadiene over bifunctional Zn-Y/Beta zeolite. **T. Yan**

4:00 CATL 646. Interfacial effects in CO₂ hydrogenation of CeO₂ supported metal single atoms, nanoclusters and nanoparticles. **Y. Guo**, Y. Zhang

Section G

Orange County Convention Center
Room W311A

Catalytic Chemistry over Metal Oxides

Oxide Catalysis: Others

S. D. Senanayake, *Organizer*
D. Jiang, Z. Wu, *Organizers, Presiding*
F. Wang, *Presiding*

1:00 Introductory Remarks.

1:05 CATL 647. Surface science approach to the study of cobalt based oxides for electrocatalytic applications. **S. Agnoli**, G. Granozzi, L. Calvillo Lamana

1:35 CATL 648. Towards efficient N₂ electroreduction to ammonia through DFT investigation of mixed iron/nickel oxides. **Y. Li**, M.J. Janik

1:55 CATL 649. Intimate role of a basis set on the outcomes of external energy mediated chemical reactions. **S. Yamijala**, Z. Ali, B.M. Wong

2:15 CATL 650. Light Absorption management by systematic ytterbium doping in monoclinic BiVO₄ for enhancement in photoelectrochemical water oxidation. **U. Prasad**, J. Prakash, B. Azeredo, A.M. Kannan

2:35 CATL 651. Layered double hydroxide nanosheets decorated with metal or metal oxides for oxygen evolution and reduction reactions. S. Chala, M. Tsai, W. Su, H. Dai, **B. Hwang**

2:55 Intermission.

3:05 CATL 652. MOF-derived CuO clusters in large pore zeolites for C-C bond formation: A new catalyst strategy toward substituted indoles and propargylamines. **N. Martin Garcia**, M. Dusselier, D. De Vos, F.G. García Cirujano

3:25 CATL 653. Mesoporous transition metal-aluminum oxide prepared via mechanochemical nonhydrolytic sol-gel route. **Z. Zhang**, S. Dai

3:45 CATL 654. Metal oxide nanoparticles as catalysts for chalcone and intermolecular cyclization reactions. **A. Alayyaf**, A.W. Apblett

4:05 CATL 655. Does bulk matter?: Controlling bulk oxygen vacancies enhances catalytic reactivity of perovskite surfaces. **K. Ercan**, Z. Say, M. Kurt, M. Karatok, Z.A. Ok, A.V. Koç, E. Ozensoy



TECHNICAL PROGRAM

CELL

Division of Cellulose & Renewable Materials

W. Thielemans and G. Larkin, *Program Chairs*

SUNDAY MORNING

Section A

Orange County Convention Center
Room W304A

Engineered Lignocellulosic Materials & Multiphase Systems: Anselme Payen Award Symposium in Honor of Orlando Rojas

Sustainable Nanofibers

Cosponsored by ANYL and COLL

Financially supported by EPNOE Martin and Lora Kelley Family Foundation ACS Cellulose and Renewable Materials Division Department of Forest Biomaterials, NC State Elsevier Ronalds W. Gonzalez Stephen S. Kelley Daniel E. Saloni College of Natural Resources, NC State Eastman Chemical Company NonWoven Institute, NC State Sunkyu Park Springer Nature BV VTT Hasan Jameel Nathalie M. Lavoine Lucian Lucia Lokendra Pal Richard A. Venditti Yuan Yao K. J. Edgar, S. S. Kelley, J. Zhu, J. O. Zoppe, *Organizers*
L. Berglund, *Presiding*

8:00 Introductory remarks.

8:05 CELL 1. Fiber spinning of nanocellulose composite fibers and supramolecular polysaccharides. **O.T. Ikkala**

8:30 CELL 2. Challenges in the development of novel regenerated cellulose fibers. **H. Sixta**, M. Hummel

8:55 CELL 3. Analysis of the porous architecture and properties of anisotropic cellulose nanofibril (CNF) foams as a tool to evaluate the CNF quality. K. Kriechbaum, P. Munier, V. Apostolopoulou-Kalkavoura, **N. Lavoine**

9:20 CELL 4. Preparation and characterization of carboxymethylated cellulose nanofibrils for use as engineered material. **H. Youn**, W. Im, S. Park, H. Lee

9:45 Intermission.

10:00 CELL 5. Holocellulose fibers: combining mechanical performance and optical transmittance. **L. Berglund**, X. Yang, F. Berthold

10:25 CELL 6. Development of functional cellulose filament materials from wound healing materials to optical fibers. **H. Orelma**



TECHNICAL PROGRAM

10:50 CELL 7. Cellulose nanofibrils pretreatment: the solution for production of functional CNF by twin screw extrusion. **J. Bras**, F. Rol, N. Belgacem

11:15 CELL 8. Light management with cellulose nanofibers. M. Toivonen, O. Onelli, O. Rojas, O.T. Ikkala, **S. Vignolini**

11:40 CELL 9. Interfacial effect of nanofibrillated cellulose (CNF) on wood-based matrix/resin interactions. **M.S. Peresin**, M.C. Iglesias, M. Hornus, G. Cheng, B. Via

12:05 Concluding remarks.

Section B

Orange County Convention Center
Room W304B

New Horizons: Early-Career Researchers in Renewable Materials: Symposium in honor of the Kingfa & PhD Student Prize Winners

Cosponsored by ANYL and PROF
Financially supported by EPNOE
E. D. Cranston, *Organizer, Presiding*
P. A. Larsson, *Presiding*

8:00 Introductory Remarks.

8:05 CELL 10. Optically transparent composites reinforced with cellulose nanofibers: Enhancing the fracture resistance and impact strength of acrylic with bacterial cellulose. A. Santmarti, J. Teh, **K. Lee**

8:30 CELL 11. Unmodified cellulose nanocrystals as stabilizers of polystyrene latex: parameters tuning the particle size. **C. Jimenez Saelices**, M. Save, I. Capron

8:55 CELL 12. Incorporation of cellulose nanocrystals into polyamide nanocomposites with controlled architecture via interfacial polymerization. **M.S. Reid**, J. Erlandsson, L. Wagberg

9:20 CELL 13. Functionalization of cellulose nanocrystals for development of polymeric bionanocomposites and applications in sustainable chemical processes. **P. Dhar**, A. Kumar, V. Katiyar

9:45 Intermission.

10:00 CELL 14. Nanocellulose as a rheology modifier for use in industrial applications. **E. Heggset**, R. Aaen, F. Brodin, K. Syverud

10:25 CELL 15. Molecular understanding of cellulose interactions. **T. Pettersson**

10:50 CELL 16. Lateral arrangement of cellulose microfibrils in wood secondary cell wall. **Y. Ogawa**, T. Kuribayashi, Y. Nishiyama

11:15 CELL 17. Advances in liquid-state NMR analysis of polysaccharide-containing biomaterials. **A. King**, D.R. del Cerro, V. Mäkelä, S. Heikkinen, T. Koso, S.A. Kedzior, E.D. Cranston, I. Kilpeläinen



TECHNICAL PROGRAM

11:40 Concluding remarks.

Section C

Orange County Convention Center
Room W304C

Bio-Based Materials for Energy Conversion & Storage Applications

Electrolyte & Separators for Battery Applications

Cosponsored by ANYL and BIOL
Financially supported by EPNOE
J. F. Stanzione, *Organizer*
S. K. Dishari, F. Jiang, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 **CELL 18.** Battery separators based on mesoporous cellulose for the next generation of lithium-ion batteries. R. Gonçaves, **E. Lizundia**, M.M. Silva, C. Costa, S. Lanceros-Mendez

8:30 **CELL 19.** Cellulose-inspired solid electrolytes membranes. **K. Fu**

8:55 **CELL 20.** Conductivity and ion transport in lignin-derived solid polymer electrolytes. E. Baroncini, **J.F. Stanzione**

9:20 **CELL 21.** Innovative of bio-based quaternary ammonium electrolyte derived from fatty acid. **F. Jumaah**, N. Mobarak, N. Ahmad Ludin, N. Hassan, S. Mohd Noor, K. Haji Badri, A. Ahmad, M. Suait

9:45 Intermission.

Section C

Orange County Convention Center
Room W304C

Bio-Based Materials for Energy Conversion & Storage Applications

Electrodes for Battery Applications

Cosponsored by ANYL and BIOL
Financially supported by EPNOE
F. Jiang, *Organizer*
S. K. Dishari, J. F. Stanzione, *Organizers, Presiding*

10:00 **CELL 22.** Wood derived materials as high performance anode for Na-ion batteries. **W. Luo**

10:25 **CELL 23.** Lignin derived carbon-silicon nanocomposite materials for electrochemical energy storage applications. **W. Li**, Y. Cheng, J. Shi



TECHNICAL PROGRAM

10:50 CELL 24. Natural polymer based energy storage materials and devices. **J. Xie**

11:15 CELL 25. Wood nanotechnologies. **L. Hu**

11:40 Concluding remarks.

Section D

Orange County Convention Center
Room W304D

Advances in Renewable Materials

Cosponsored by ANYL and CARB
Financially supported by EPNOE
S. M. Murphy, *Organizer*
N. Abidi, G. W. Selling, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 CELL 26. All-cellulose composites via short-fiber dispersion approach. **O. Korhonen**, N. Forsman, M.K. Osterberg, T. Budtova

8:30 CELL 27. Swelling behavior of cellulose rich materials in water. **T. Larsson**, R. Karlsson, L. Wagberg

8:55 CELL 28. Cellulose dissolution in imidazolium-based ionic liquids: Effect of size and shape of cations. **N. Dissanayake**, V. Thalangamaarachchige, S. Troxell, E.L. Quitevis, N. Abidi

9:20 CELL 29. Novel and green approach in engineering transparent and homogenous cellulose nanocrystal/lignin UV protection films. **M.B. Parit**, P. Saha, V.A. Davis, Z. Jiang

9:45 Intermission.

10:00 CELL 30. New eco-friendly high-performance cellulosic fibers for the textile and packaging industries. M. Alam, **L. Christopher**

10:25 CELL 31. Cellulose-based value-added co-products from agricultural materials. **M.P. Yadav**

10:50 CELL 32. Crosslinked cellulose fiber reinforced poly(lactic acid) composites. **K. Li**, H. Tekinalp, S. Ozcan

11:15 CELL 33. Synthesis and characterization of a novel biodegradable cellulose acetate-chitosan biosorbent for water purification and treatment purposes. **E.R. Farag**, T. Madkour, M. El Sayyed

11:40 Concluding remarks.

Section E

Orange County Convention Center
Room W304E



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

Interplay of Cellulose & Other Biopolymers in Biological & Designed Materials Systems

Interactions of Plant Polymers in Model Systems

Cosponsored by ANYL, BIOL and CARB
Financially supported by EPNOE; CP Kelco
H. M. O'Neill, F. J. Vilaplana, *Organizers*
D. Cosgrove, M. Roman, *Organizers, Presiding*

8:00 Introductory remarks.

8:05 CELL 34. Adsorption of xyloglucan onto thin films of cellulose nanocrystals and amorphous cellulose. J. Kittle, C. Qian, E. Edgar, **M. Roman**, A. Esker

8:30 CELL 35. Influence of solubility on the adsorption of different Xyloglucan fractions to cellulose model surfaces. S. Kishani, F.J. Vilaplana, P. Hansson, **L. Wagberg**

8:55 CELL 36. Hemicellulose-cellulose composites reveal differences in cellulose organization after dilute acid pretreatment. **H.M. O'Neill**, R. Shah, S. Huang, S. Pingali, D. Sawada, Y. Pu, A. Ragauskas, S.H. Kim, B.R. Evans, B.H. Davison

9:20 CELL 37. Computer modeling of the structure and dynamics of hemicelluloses. J. Berglund, P. Chen, F. Vilaplana, **J. Wohler**

9:45 Intermission.

10:00 CELL 38. Small-angle scattering studies on biomimetic composites of bacterial cellulose and wood hemicelluloses. **P. Penttilä**, T. Imai, R. Schweins, J. Sugiyama

10:25 CELL 39. Spruce hemicelluloses (galactoglucomannan and arabinoglucuronoxylan): Interplay with cellulose and lignin in softwoods. A. Martínez-Abad, A. Jiménez-Quero, J. Wohler, **F. Vilaplana**

10:50 CELL 40. Hydrogels of bacterial cellulose and wood hemicelluloses as a model of plant secondary cell walls. **J. Berglund**, D. Mikkelsen, B.M. Flanagan, S. Dhital, G. Henriksson, M. Lindström, G.E. Yakubov, M.J. Gidley, F.J. Vilaplana

11:15 CELL 41. Interactions between the building blocks of plant cell walls. **M.S. Skaf**

11:40 Concluding remarks.

Wolfrom Award

Sponsored by CARB, Cosponsored by CELL, MEDI, ORGN and PROF

Horton Award



TECHNICAL PROGRAM

Sponsored by CARB, Cosponsored by CELL, MEDI, ORGN and PROF

Bioenergy & Bioproducts

Biofuel

Sponsored by ENFL, Cosponsored by CELL

SUNDAY AFTERNOON

Section A

Orange County Convention Center
Room W304A

Engineered Lignocellulosic Materials & Multiphase Systems: Anselme Payen Award Symposium in Honor of Orlando Rojas

Cellulose Nanocrystals Enabling Sustainable Materials

Cosponsored by ANYL and COLL

Financially supported by EPNOE Martin and Lora Kelley Family Foundation ACS Cellulose and Renewable Materials Division Department of Forest Biomaterials, NC State Elsevier Ronalds W. Gonzalez Stephen S. Kelley Daniel E. Saloni College of Natural Resources, NC State Eastman Chemical Company NonWoven Institute, NC State Sunkyu Park Springer Nature BV VTT Hasan Jameel Nathalie M. Lavoine Lucian Lucia Lokendra Pal Richard A. Venditti Yuan Yao K. J. Edgar, S. S. Kelley, J. Zhu, J. O. Zoppe, *Organizers*
U. Edlund, *Presiding*

1:15 Introductory remarks.

1:20 CELL 42. Engineering the surface chemistry of nanocelluloses for material applications. **U. Edlund**, J. Navarro, E. Ålander

1:45 CELL 43. Polysaccharide-based microspheres for advanced applications in healthcare. **P.E. Fardim**

2:10 CELL 44. 1D to 3D hierarchical structural materials from biomass. **Y. Hsieh**

2:35 CELL 45. Engineering cellulose nanocrystals from pre-hydrolyzed substrates. **E. Kontturi**, R. Salminen, T. Pääkkönen

3:00 Intermission.

3:15 CELL 46. Design for reinforced nanocomposites having embedded bamboo-ACC nanocellulose honeycomb by fabrication process due to nano-fusion. **T. Kondo**, S. Yokota, E. Uchida, G. Ishikawa, S. Tagawa, M. Kamogawa

3:40 CELL 47. Combining nanocellulose and nanolignin for high-performance materials. **M.K. Osterberg**, M. Sipponen, M. Farooq



TECHNICAL PROGRAM

4:05 CELL 48. Micropatterned nanocellulose films and magnetically responsive cellulose nanocrystals as platforms for microfluidic devices and selective protein separation. J. Guo, **E. Filpponen**, L. Johansson, M.B. Linder, R. Ras, P. Levkin, O. Rojas

4:30 CELL 49. Preparation and characterization of TEMPO-oxidized cellulose nanonetworks, nanofibers, and nanocrystals. **A. Isogai**

4:55 Concluding remarks.

Section B

Orange County Convention Center
Room W304B

New Horizons: Early-Career Researchers in Renewable Materials: Symposium in honor of the Kingfa & PhD Student Prize Winners

Cosponsored by ANYL and PROF
Financially supported by EPNOE
E. D. Cranston, *Organizer*
T. Abitbol, G. Nyström, *Presiding*

1:15 Introductory Remarks.

1:20 CELL 50. Colloidal gels and glasses from nanocelluloses. M. Nordenstrom, G. Nyström, **A.B. Fall**, L. Wagberg

1:45 CELL 51. Role of cellulose nanocrystals in the film formation of latex-based pressure sensitive adhesives. **E. Niinivaara**, A. Ouzas, C. Fraschini, R.M. Berry, M.A. Dubé, E.D. Cranston

2:10 CELL 52. Nanocellulose: From single particle structure to multiscale assembly of functional materials. S. Campioni, T. Geiger, G. Siqueira, **G. Nystroem**

2:35 CELL 53. Investigating the nanostructure of cellulosic materials with small-angle scattering. **P. Penttilä**, N. Carl, R. Schweins, M. Altgen, M.K. Osterberg, L. Rautkari

3:00 Intermission.

3:15 CELL 54. Optical analysis of cellulose nanocrystal films enables access to their self-assembly history. **B. Frka-Petesic**, G. Kamita, G. Guidetti, G. Jacucci, S. Vignolini

3:40 CELL 55. Nanocellulose-based hybrid materials for optical applications. A. Wörnheim, M. Toprak, A. Ahniyaz, A. Swerin, **T. Abitbol**

4:05 CELL 56. Opto-mechanical properties of microtemplated chiral-nematic cellulose nanocrystals films. **B.L. Tardy**, B. Mattos, L. Garcia Greca, T. Kämäräinen, K. Klockars, O. Rojas

4:30 CELL 57. Bio-inspired Photonics: from nature to applications. **S. Vignolini**

5:15 Concluding remarks.



TECHNICAL PROGRAM

Section C

Orange County Convention Center
Room W304C

Bio-Based Materials for Energy Conversion & Storage Applications

Lignin-Based Materials for Supercapacitor & other Applications

Cosponsored by ANYL and BIOL
Financially supported by EPNOE
S. K. Dishari, *Organizer*
F. Jiang, J. F. Stanzione, *Organizers, Presiding*

1:15 Introductory Remarks.

1:20 **CELL 58.** Development of lignin-based electrode for high performance electric double layer capacitor with ionic liquid as an electrolyte. **N. Pakkang**, K. Koda, Y. Uraki

1:45 **CELL 59.** Improving lignin-derived supercapacitor electrode performance by crosslinking lignin and controlling lignin carbon's morphology. **H. Ho**, N. Nguyen, A.K. Naskar

2:10 **CELL 60.** Lignin-based rigid polyurethane foam containing phase change material for thermal energy management element in buildings. X. Zhang, **Y. Kim**

2:35 **CELL 61.** Implementing nitrogen functionalized BioChar for CO₂ capture and storage. H. Bamdad, K. Hawboldt, **S. MacQuarrie**

3:00 Intermission.

Section C

Orange County Convention Center
Room W304C

Bio-Based Materials for Energy Conversion & Storage Applications

Electroconductive Hydrogels

Cosponsored by ANYL and BIOL
Financially supported by EPNOE
J. F. Stanzione, *Organizer*
S. K. Dishari, F. Jiang, *Organizers, Presiding*

3:15 **CELL 62.** Controllable fabrication and modification of bacterial cellulose based electroactive hydrogel. **G. Yang**

3:40 **CELL 63.** Self-healing hydrogels by thermal-induced protein-lipid co-assembly for air-tolerant photon upconversion. **J. Ding**, T. Mani, J. He, C.V. Kumar



TECHNICAL PROGRAM

4:05 CELL 64. Direct microalgae harvesting to prevent harmful algae blooms and produce renewable biofuel. **J.K. Shurtleff**, P. Rich, T. Johnson, A. Bettridge, B. Allred

4:30 CELL 65. Multifunctional piezoelectric elastomer nanocomposites for smart biomedical or wearable electronics. **H. Sanming**, G. Yang

4:55 Concluding Remarks.

Section D

Orange County Convention Center
Room W304D

Advances in Renewable Materials

Cosponsored by ANYL and CARB
Financially supported by EPNOE
G. W. Selling, *Organizer*
N. Abidi, S. M. Murphy, *Organizers, Presiding*

1:15 Introductory Remarks.

1:20 CELL 66. Fabrication of magnetic lignosulfonate-based microspheres for efficient removal of Rhodamine B in wastewater treatment. **J. Geng**, J. Chang

1:45 CELL 67. Cellulose graft copolymers as functional materials. **R. Liu**, H. Kang

2:10 CELL 68. Preparation of cellulosic samples with varied content of residual lignin and hemicelluloses: Impact on nanofibrillation process and nanopaper properties. **D. Carvalho**, C. Moser, M. Lindström, O. Sevastyanova

2:35 CELL 69. Application of molecular dynamics calculations to high-syringyl lignin oligomers. **T.J. Elder**, J.V. Vermaas, G. Beckham

3:00 Intermission.

3:15 CELL 70. Monomers and polymers from plant oils. Z. Demchuk, K. Kingsley, V. Kirianchuk, A. Kohut, O. Shevchuk, S. Voronov, **A. Voronov**

3:40 CELL 71. Cottonseed protein and its use as wood adhesives. **H.N. Cheng**, Z. He, M.K. Dowd, T. Klasson

4:05 CELL 72. Understanding fragmentation and condensation reactions during Organosolv extractions of lignin. **M.B. Foston**

4:30 CELL 73. Comparison of molar mass between technical lignins and 8-O-4' type of polymeric lignin models. **Y. Uraki**, L. Wang, K. Koda, K. Shigetomi

4:55 Concluding remarks.

Section E



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

Orange County Convention Center
Room W304E

Interplay of Cellulose & Other Biopolymers in Biological & Designed Materials Systems

Structure & Mechanics of Plant Cell Walls

Cosponsored by ANYL, BIOL and CARB
Financially supported by EPNOE; CP Kelco
D. Cosgrove, F. J. Vilaplana, *Organizers*
H. M. O'Neill, M. Roman, *Organizers, Presiding*

1:15 Introductory Remarks.

1:20 **CELL 74.** Interaction of cellulose nanocrystals with lipid bilayers. Y. Navon, F. Dahlem, B.R. Jean, J. Putaux, L. Coche-Guérente, A. Bernheim-Grosswasser, **L. Heux**

1:45 **CELL 75.** Modeling the habit and surface chemistry of fundamental plant cellulose microfibrils. **J.D. Kubicki**, H. Yang

2:10 **CELL 76.** Surface interactions of crystalline cellulose with surrounding matrix polymers studied with sum frequency generation (SFG) vibrational spectroscopy. **M. Makarem**, C.M. Lee, D. Sawada, H.M. O'Neill, S.H. Kim

2:35 **CELL 77.** Resonant soft X-ray scattering for chemically-specific structural characterization of plant primary cell walls. **E. Gomez**, D. Ye, S. Rongpipi, S. Kiemle, X. Wang, C. Wang, D. Cosgrove, E. Gomez

3:00 Intermission.

3:15 **CELL 78.** Sum Frequency Generation (SFG) microscopy study of cellulose structures in plant cell walls: Mesoscale structure: Cell function relationship. **S.H. Kim**, M. Makarem, S. Huang, S. Kiemle, J. Burris, A. Chaves, C.H. Haigler, A. Roberts, D. Cosgrove

3:40 **CELL 79.** Xylan domains allow pectin adhesion to cellulose in Arabidopsis seed mucilage. **M. Ralet**, S. Saez-Aguayo, A. Orellana, H.M. North

4:05 **CELL 80.** Investigation of the structure and dynamics of plant cell wall polysaccharides at acidic pH by solid-state NMR. **M. Hong**

4:30 **CELL 81.** Nature of wall extensibility in primary cell walls: insights from imaging, biomechanics and the action of selective enzymes. **D. Cosgrove**, X. Wang, T. Zhang

4:55 Concluding remarks.

Hudson Award

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TECHNICAL PROGRAM

Isabell Award

Sponsored by CARB, Cosponsored by CELL, MEDI, ORGN and PROF

Gin New Investigator Award

Sponsored by CARB, Cosponsored by CELL, MEDI, ORGN and PROF

Bioenergy & Bioproducts

Sponsored by ENFL, Cosponsored by CELL

SUNDAY EVENING

Section A

Orange County Convention Center
West Hall C

General Posters

Cosponsored by ANYL and CARB
Financially supported by EPNOE
M. L. Auad, W. Thielemans, *Organizers*

7:00 - 9:00

CELL 82. Mussel-inspired cellulose nanocomposite tough hydrogels with synergistic self-healing, adhesive, and strain-sensitive properties. **C. Shao**

CELL 83. PolyAESO: Bacterial cellulose nanocomposites: Comparing the reinforcing ability of never-disrupted BC networks vs vacuum filtrated BC networks. **A. Santmarti**, K. Lee

CELL 84. Combination of chemical and enzymatic treatment on cellulose fibre properties. **G. Banvillet**, G. Depres, N. Belgacem, J. Bras

CELL 85. Antimicrobial functionalization of cotton textiles with ZnO NPs and gallic acid embedded in an in-situ sonoenzymatically generated bioadhesive. **J. Hoyo**, T. Tzanov

CELL 86. Impact of the physicochemical environment on clustering-triggered emission in cellulosic nanomaterials: Its effects and uses. **M.A. Johns**, A.E. Lewandowska, S.J. Eichhorn

CELL 87. Nanocellulose/polymer compatibility: State-of-the art review and knowledge gaps. **D. Turpin**

CELL 88. Nanocellulose dewatering and drying: state-of-the art review and knowledge gaps. **D. Turpin**



TECHNICAL PROGRAM

- CELL 89.** Study the effect of nitro-oxidized cellulose nanofibers on growth of fibroblast and dental pulp cells. **P. Sharma**, S. Sharma, K. Che-Fang, M. Rafailovich, B.S. Hsiao
- CELL 90.** Novel approach in developing cellulose nanofiber and polypyrrole based conducting composites with improved conductivity and mechanical strength. **M.B. Parit**, H. Du, X. Zhang, Z. Jiang
- CELL 91.** How the recalcitrance of plant cell wall deconstruction during chemical pretreatment process? **F. Xu**, X. Zhang, T. You
- CELL 92.** Strengthening soy protein-based films by integrating thiol-branched graphene oxide and polydopamine-induced nano-fibrillated cellulose using multiple Michael addition/Schiff base reactions. **X. Liu**, K. Wang, J. Li
- CELL 93.** Facile synthesis of promising phosphorus fertilizer from sewage sludge through calcium oxide enhanced pyrolysis. **S. Tang**, C. Zheng, Z. Zhang
- CELL 94.** Withdrawn
- CELL 95.** Review of solvent chemistry toward sustainable biorefinery in biomass-water-energy nexus. C. Dong, **S. Leu**, M. Islam
- CELL 96.** Withdrawn
- CELL 97.** Construction of robust cellulose hydrogels and films consisted of nanofibers via bottom-up strategy. **L. Zhang**, D. Ye, X. Lei, C. Chang
- CELL 98.** Inkjet printing of conductive nanocellulose inks for flexible electronics. E. Loukiantchenko, A. Denneulin, J. Bras, **E.D. Cranston**
- CELL 99.** Determination of molecular weight of cellulose by diffusion-ordered NMR spectroscopy. **K. Hattori**, A. Arai
- CELL 100.** Drying and NaClO concentration effect on TEMPO-mediated oxidation of bacterial nanocellulose. **E. Martinez**, D. Suarez, M. Osorio, R. Zuluaga Gallego, C. Castro, B. Gómez
- CELL 101.** Optimization of cellulose membranes using artificial neural networks. **B.C. Sulbaran**, V. Romero Arellano, C. Guzmán González, **V. Zuñiga Grajeda**, **K. Gurubel Tun**
- CELL 102.** Electrospinning cellulose from ionic liquid systems: A secondary school research project. J. Perkins, M. Boyer, **M.A. Johns**
- CELL 103.** Adsorption and the associated thermodynamics of different cellulose binding modules of cellulases on model cellulose surfaces. Y. Zhang, P. Wang, X. Zhang, X. Wang, **J. Song**
- CELL 104.** Grafting polycaprolactone onto alkali lignin for improved compatibility and processability. J. Tian, Y. Yang, **J. Song**
- CELL 105.** Bio-based flame retardants on paper substrates. **F. Schäfer**, M. Biesalski
- CELL 106.** Biomimetic mineralization of three-dimensional bacterial nanocellulose for bone tissue regeneration. A. Cañas, **M. Osorio**, D. Arboleda, C. Castro



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- CELL 107.** Nanocellulose foams containing bioglass: A three-dimensional scaffold for bone tissue engineering. **F.V. Ferreira**, L.P. Souza, T.M. Martins, J.H. Lopes, T.M. Valverde, M. Mariano, I.F. Pinheiro, J. Camilli, A.M. Goes, O. Rojas, R.F. Gouveia, L.M. Lona
- CELL 108.** Mussel-inspired clay/carboxymethyl cellulose nanocomposites with high hygromechanical and self-extinguish performance. T. Guo, J. Song, H. Xiao, **Y. Jin**
- CELL 109.** Additive manufacturing of wood. **D. Kam**, M. Layani, O. Shoseyov, S. Magdassi
- CELL 110.** Cutin from agroresidual wastes of *Vitis vinifera* as new raw biomaterials. **D. Arrieta-Baez**, M. Gómez-Patiño, J. Mendez-Mendez, D. Reyes-Duarte
- CELL 111.** 3D bioprinting inks for ultraviolet-assisted direct ink writing technology. **N. Alizadeh**, S. Li, J. Burchfield, B. Cleary, M.L. Auad
- CELL 112.** Recovered compounds from agroresidual wastes of *Musa paradisiaca* for food industrial applications. **D. Arrieta-Baez**, M. Gómez-Patiño, I. Arzate-Vazquez, J. Campos-Teran
- CELL 113.** Effect of the reinforcement architecture on the optical and mechanical properties of bacterial cellulose composites. **A. Santmarti**, K. Lee
- CELL 114.** Chitinous functional materials: Chitosan-poly vinyl alcohol fibers reinforced with TiO₂ nanoparticles. **R.A. Vargas**, E.E. Ruiz, J.H. Mina
- CELL 115.** Designing and production of UV-curable double-network hydrogels for tissue engineering applications by amalgamation of PEGDA macromere with polysaccharides. **P. Joshi**, **M.L. Auad**
- CELL 116.** Distinct antioxidant activity of xylooligosaccharides obtained by several xylanases. **C. Valls**, F. Pastor, T. Vidal, M. Roncero, P. Díaz, J. Martínez, S. Valenzuela
- CELL 117.** Using zinc salts from spent alkaline batteries to produce activated carbon from rice husk. **J. Leiton**
- CELL 118.** Glucose-derived nanotemplated carbon adsorbents for water remediation of organic and inorganic pollutants. **L. Barrera**, A.C. Escobosa, J. Noveron
- CELL 119.** Distribution of carboxyl groups in TEMPO-oxidized celluloses. **Y. Ono**, T. Saito, A. Isogai
- CELL 120.** Influence of regeneration liquid polarity on different material properties of dried cellulose II films. **M. From**, B. Andreasson, I. Svanedal, T. Larsson, H. Edlund, M. Norgren
- CELL 121.** Fabrication of durable superhydrophobic surface using lignocellulose nanofibrils. L. Gu, W. Wu, J. Song, H. Xiao, **Y. Jin**
- CELL 122.** Hydroxyethyl lignin: a robust building block for greener modification of lignin with carboxylic acid and vinyl functionality. **L. Liu**, Q. Hua, S. Renneckar
- CELL 123.** Predicting the behavior of cellulose nanocrystal suspensions and expanding their use at high temperatures. **O.M. Vanderfleet**, J. Bras, A. Yakovlev, J. Godoy, M.K. Panga, V. Lafitte, E.D. Cranston



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- CELL 124.** Spinning of nanocellulose/chitosan hybrid fiber. **H. Tamura**, D. Dechojarassri, T. Kitamura, M. Hashimoto, T. Furuike
- CELL 125.** Bioresource-based Poly(3hydroxybutyrate-co-4-hydroxybutyrate)/ Poly(lactic acid) blend fibers with high strength and toughness via melt-spinning. **Z. Pan**, Z. Zhao, Z. Chen, J. Hong
- CELL 126.** Leather-inspired modification of nanocellulose-based hybrids to enhance wet strength. **K. Kriechbaum**, L. Bergstrom
- CELL 127.** Correlations between the morphology, topology, mechanical and thermal stability of biopolymer scaffolds fabricated from ionic liquids with muscle cell functionalities. **S.A. Love**, K. Rybacky, A. Morales, D. Salas-de la Cruz
- CELL 128.** The relationship between morphology, conductivity and elasticity of silk and cellulose biocomposites fabricated from ionic liquids. **B. Blessing**, C. Trout, K. Rybacky, A. Morales, S. O'Malley, **D. Salas-de la Cruz**
- CELL 129.** Ammonium remediation using nitro-oxidized cellulose nanofibers as a slow release fertilizer. **K.I. Johnson**, S.K. Sharma, P.R. Sharma, H. Chang, B.S. Hsiao
- CELL 130.** Cellulose nanofibrils/silver nanowires suspensions for the development of barrier properties and antibacterial surfaces. H. Spieser, A. Denneulin, D. Gethin, D. Deganello, **J. Bras**
- CELL 131.** Intermolecular interactions of keratin/cellulose biocomposites fabricated using ionic liquids. **K. Rybacky**, S.A. Love, A. Morales, D. Salas-de la Cruz
- CELL 132.** Characterization of silk-cellulose biocomposite for medical application in space exploration. **A. Morales**, K. Rybacky, S.A. Love, D. Salas-de la Cruz
- CELL 133.** Development of supercapacitors using renewable carbon fiber. J.A. Hinkle, A. Bansode, C. Upp, H. Nam, I. Filpponen, S. Adhikari, J. Radich, T.J. Elder, **M.L. Auad**
- CELL 134.** Development of pH responsive cellulose nanofibers for the selective adsorption of emerging organic contaminants in water. **J.L. Ramirez**, T.A. Hines, J.A. Lasalde, J. Herrera, E. Nicolau
- CELL 135.** Antibacterial composite films with high mechanical properties based on hemicellulose/chitosan/graphene oxide. **R. Jun**, Y. Guan, H. Gao
- CELL 136.** High mechanical properties of hemicelluloses films by graphene oxide for humidity sensing. **Y. Guan**, H. Gao, R. Jun, S. Liu
- CELL 137.** Withdrawn
- CELL 138.** Nanocellulose/gelatin composite cryogels for controlled drug release. J. Wu, **W. Wu**
- CELL 139.** Isolation and characterization of nanocrystalline cellulose from corncob. **E.M. Santos Ventura**, A. Gutiérrez Becerra, M. Esquivel Alfaro, M.A. Escalante, G. Toriz, **B.C. Sulbaran**
- CELL 140.** *In vitro* release of microemulsion from nanochitin hydrogel. Z. Wang, R. Wang, J. Yu, **L. Liu**, Y. Fan
- CELL 141.** Preparation of amphoteric chitin nanocrystals and its hydrogels. J. Jiang, L. Liu, J. Yu, **Y. Fan**



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- CELL 142.** Preparation of high-strength sustainable lignocellulose gels cross linked with a silane coupling agent. **Y. Fan**
- CELL 143.** Effects of cellulose on the loading of Zinc oxide on cellulose. X. Li, Z. Wang, J. Song, **J. Ma**
- CELL 144.** Photo-crosslinking strategy constructs tough and green hydrogel-based adhesives through controlling the balance of cohesion and adhesion. **H. Bai**, Z. Li, W. Dong
- CELL 145.** How pH and degree of deacetylation affect the antibacterial property of chitin nanofiber. **J. Xu**, Y. Fan
- CELL 146.** Synthesis and characterization of bio-based poly(Schiff-base) composed of bifurfural. **S. Hayashi**, T. Wasano, Y. Tachibana, K. Kasuya
- CELL 147.** Elucidation of lignin-HEMA hydrogel network using SANS, SAXS and TEM. **K. Rajan**, S. Pingali, D.J. Carrier, S.C. Chmely
- CELL 148.** Selective cleavage of lignin β -O-4 aryl ether bond by β -etherase of the white-rot fungus *Dichomitus squalens*. M. Marinović, P. Nousiainen, A. Dilokpimol, J. Kontro, R. Moore, J. Sipila, R. de Vries, M. Mäkelä, **K. Hilden**
- CELL 149.** Processive action of glycoside hydrolase family 5 endoglucanase from *volvariella volvacea* and its application in the preparation of nanofibers. **S. Wu, S. Wu, J. Song**
- CELL 150.** Enzyme-assisted preparation of nanocellulose from wood holocellulose fibers. **S.M. Koskela**, S. Wang, X. Yang, K. Li, V. Srivastava, L. McKee, L. Berglund, V. Bulone, Q. Zhou
- CELL 151.** Lignomics toolkit analysis of subcritical water treated alkali lignin. **A.L. LaVallie**, J. Bilek, K. Voeller, K. Furey, S. Lu, A. Andrianova, E. Kozliak, A. Kubatova
- CELL 152.** Application of lignomics analytical toolset for comprehensive characterization of SEC fractions of lignin. **S.E. Reagen**, A. Andrianova, S. Lu, E. Kozliak, A. Kubatova
- CELL 153.** Development of a biodegradable wound dressing from aquaculture waste. **M. Esquivel Alfaro**, G. Ramos, S. Madrigal, L. Villegas
- CELL 154.** Effect of laccase mediator system oxidation on various lignin interunit linkages and end-groups. J. Kontro, R. Maltari, J. Mikkilä, K. Hilden, **P. Nousiainen**, J. Sipila
- CELL 155.** Wood-based emerging technologies for sustainable applications. **A.S. Gong**
- CELL 156.** Effect of process parameters on the composition of hemicellulose hydrolyzates from dilute sulfuric acid treatment of hybrid poplar. **W. Liu**, A.F. Astner, J.J. Bozell, M. Roman
- CELL 157.** Alkali lignin solubilization and characterization using lignomics analytical toolset. **B. Yao**, E.R. Tiede, A.L. LaVallie, L. Lilleboe, S. Gupta, E.I. Kozliak, A. Kubatova
- CELL 158.** Physico-chemical characterization of lignins from different sources for the synthesis of lignin based epoxy resins. **A.S. Bansode**
- CELL 159.** Potential of cellulose nanoparticles in biomedical applications. **P. Tumkur**, N. Bayón, K. Prabhakaran, G. Ramesh



TECHNICAL PROGRAM

CELL 160. Towards standardization of laboratory preparation procedure for uniform cellulose nanopapers. **M.B. Parit**, Z. Jiang, B. Aksoy

CELL 161. Withdrawn

CELL 162. Potential of chitin as bio-polymer electrolyte. M. Latifi, H. Kaddami, R. Dieden, A. Ahmad, N. Hassan, **Y. Habibi**

CELL 163. New biopolymers from renewable building blocks derived from woody hemicelluloses. **Y. Habibi**, L. Puchot, R. Dieden, D. Da Silva

CELL 164. Polysaccharide-based microneedles for transdermal delivery of insulin. **C.R. Freire**, D. Fonseca, C. Vilela, P. Costa, I. Almeida, P. Pereira, A. Silvestre

CELL 165. Withdrawn

CELL 166. Bio-based thermosets prepared using Michael addition of furan and isosorbide building blocks. **X. Chu**, J. La Scala, G.R. Palmese

CELL 167. Development of three-dimensional bacterial nanocellulose biomaterials for tissue engineering and regenerative medicine. **M. Osorio**, T. Naranjo, T. van Kooten, I. Ortiz, **C. Castro**

CELL 168. Obtaining pure spectra of hemicellulose and cellulose from poplar cell wall Raman imaging data. **X. Zhang**, F. Xu

CELL 169. In situ acetylation of ground whole plant cell walls: a new method for solution-state NMR in DMSO-d₆. **X. Zhang**

CELL 170. Efficient and highly selective biomass conversion by hydriodic acid mediated hydrogenation. **W. Yang**, T. Li

CELL 171. Withdrawn

CELL 172. Tree bark valorization toward biofuel. **I. Kumaniaev**, J.S. Samec

CELL 173. Withdrawn

CELL 174. Diversifying Klabin's portfolio with Kraft Lignin - recent developments. **M.C. Muguet**, F.R. Milagres

CELL 175. Xyloglucan and cellulose nanocrystals biomimetic aerogels produced by freeze-casting. **Z. Jaafar**, B. Quelenec, C. Moreau, D. Lourdin, J. Maigret, T. Coradin, F. Fernandes, B. Cathala

CELL 176. Aqueous two-phase systems (ATPS) as a tool to overcome product inhibition in lignocellulosic conversions. **B. Consorti Bussamra**, V. Viswanathan, S. Freitas, S. Mussatto, A. Carvalho da Costa, L. van der Wielen, M. Ottens

CELL 177. Functional cellulose nanocrystals and nanofibers obtained by acid hydrolysis of Colombian Figue fibers (*Furcraea* spp). **E.A. Gutiérrez Pineda**, C. Blanco-Tirado, M.Y. Combariza

CELL 178. Cooling properties of textiles with blue pigment. **N. Forsman**, E. Šest, B. Golja, M.K. Osterberg, B. Simončič, I. Jerman



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

CELL 179. Withdrawn

CELL 180. Prebiotic xylooligosaccharide production from biomass autohydrolyzate liquors. **D.B. Corbett**, G. Luo, C. Hong, L. Ou, H. Jameel, R.A. Venditti, S. Park

CELL 181. Bacterial cellulose production using cacao mucilage exudate as culture media. D.R. Durán Riveros, J.T. Cabezas Calderón, O.L. Saavedra Sanabria, I. Hernández Celi, **C. Blanco-Tirado**, M.Y. Combariza

CELL 182. Towards valorization of biorefinery waste to polyhydroxyalkanoate: Structural characterization and mechanisms. **N. Hao**, Z. Liu, S. Shinde, J. Yuan, A. Ragauskas

CELL 183. Use of wood residues for the production of highly porous materials for environmental application and energy storage. **F. Braghiroli**, H. Bouafif, A. Koubaa

CELL 184. Structural characterization of carbonized lignin feedstocks via transmission electron microscopy. **V. Garcia-Negron**, G.J. Duscher, D. Keffer, O. Rios, D.P. Harper

CELL 185. AGRIMAX project: valorization of ferulic acid from wheat bran to obtain bio-based materials for packaging applications. **C. Gioia**, L. Sisti, P. Marchese, A. Celli, M. Ferri, G. Zanaroli, A. Tassoni

CELL 186. Nanocellulose from agroindustrial waste and its potential application in water and energy. **B.C. Sulbaran**, H. Palacios Hinestroza, J.A. Hernandez, M.A. Escalante, G. Toriz, O. Rojas

CELL 187. Revealing the role of phenolic residues co-extracted with hemicelluloses as emulsion stabilizers. **M. Lahtinen**, F. Valoppi, V. Juntti, P. Kilpeläinen, K.S. Mikkonen

CELL 188. Synthesis of nano-cellulose and silica from agricultural waste: A comprehensive utilization of biomass. **N. Shahi**, B. Min, V.K. Rangari, A. Dandy

CELL 189. Highly surface-active citrus fiber as a natural emulsifier for low-energy emulsification. **S. Li**, K. Villwock, B. Lundberg

CELL 190. Biopolymeric nanoparticles as potential stabilizing agents for C-Phycocyanin from cyanobacterium *Desertifilum* sp.. S. Meléndez-Antonio, I. Hernández-Martínez, I. Arroyo Maya, M. Morales-Ibarria, **J. Campos-Teran**

CELL 191. Effects of hardwood lignin model polymers on enzymatic hydrolysis of cellulose. **C. Yue**, H. Guan, M. Tu

CELL 192. Fibrous cellulose/hyaluronic acid composites as transdermal patches for minimizing bacterial infections. **K.M. Lopez**, S. Ravula, R. Pérez, J. Losso, M. Janes, I.M. Warner

CELL 193. Withdrawn

CELL 194. Gelation in natural hydrocolloid composites incorporating hydrophobized nanocellulose. **R. Nigmatullin**, V. Gabrielli, J.C. Muñoz-García, J. Schmitt, M. da Silva, Y. Khimiyak, J. Angulo, J. Scott, K. Edler, S.J. Eichhorn

CELL 195. Nanofiller effect on structure-properties relationship of bio-sourced nanocomposites. **V. Nessi**, C. Chevigny, N. Descamps, V. Gaucher, D. Lourdin

CELL 196. Hairy graphenes: Wrapping nanocellulose nets around graphene oxide sheets. **R. Xiong**, H. Kim, L. Zhang, V. Korolovych, S. Zhang, Y.G. Yingling, V.V. Tsukruk



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

CELL 197. Withdrawn

CELL 198. Twin function of methyl- β -cyclodextrin in emulsion polymerization of monomers from plant oils. **A.S. Voronov**, A. Kohut, Z. Demchuk, S. Voronov

CELL 199. Influence of plant oil-based monomers structure on properties of latex copolymers thereof. **A.S. Voronov**, Z. Demchuk, L. Wing-Sze, H. Eshete, S. Caillol

CELL 200. Epoxy resins based on diamine-functionalized Kraft lignin: The role of the chemical structure of the aminolinker. **S. Trosien**, M.W. Ott, C. Dietz, M. Nau, S. Mehlhase, M. Bitsch, G. Sieger, T. Meckel, R. Stark, M.A. Biesalski

CELL 201. Two-dimensional antifouling fluidic channels on cellulose nanopaper. **K.A. Solin**, H. Orelma, M. Borghei, M. Vuoriluoto, R. Koivunen, O. Rojas

CELL 202. Highly conductive carbon microfibers following low temperature carbonization of wet-spun lignin/nanocellulose hydrogels. **L. Wang**, M. Ago, M. Borghei, A. Ishaq, A. Papageorgiou, O. Rojas

CELL 203. Desarrollo y evaluación de un material compuesto hecho de polietileno reciclado Teraftalato y Eucayptus Nitens Sawdust para ser utilizado en la construcción. **M. Solis**, D. De La Fuente Villanueva

CELL 204. Stratification of lignin particles in waterborne systems via evaporation-induced self-assembly. **O. Cusola**, S. Kivisto, S. Vierros, P. Batys, M. Ago, B.L. Tardy, L. Garcia Greca, M. Roncero, M. Sammalkorpi, O. Rojas

CELL 205. Water-responsive shape-memory, anisotropic, robust, and superhydrophobic aerogel materials with top-down wood nanotechnology for multibehavioral, and reusable oil/water separation. **K. Wang**, X. Liu, S. Zhang

CELL 206. Chitosan enhanced micro-fibrillar cellulose aerogels and application in heavy metal ions separation. **J. Yan**

CELL 207. High-efficiency, energy-saving and “green” route for fabrication of chitin-based materials. **J. Cai**

CELL 208. Nanocellulose-based humidity sensor printed on paper for smart packaging and flexible electronics. **M. Borghei**, K.A. Solin, J. Tallal, O. Rojas

CELL 209. Foam-fiber interaction in tailoring lightweight materials. **A. Ketola**, T. Hjelt, T. Lappalainen, H. Pajari, T. Tammelin, J. Ketoja, W. Xiang, O. Rojas

CELL 210. Xylan-lignin hydrogels. **G. Toriz**, A. Escalante, P. Gatenholm

CELL 211. Evaluation of a cellulose nanocrystals/chitosan composite for its antimicrobial properties and applications in hygiene products. P. Tyagi, R. Mathew, C. Opperman, H. Jameel, R. Gonzalez, L.A. Lucia, M. Hubbe, **L. Pal**

CELL 212. Towards interfacial applications of soybean hull pectins. **V. French**, C.E. Frazier

CELL 213. Preparation and characterization of biomass based copolymer via novel rosin derived ATRP initiator. **J. Yu**, Y. Fan, F. Chu

CELL 214. Nanocellulose-polyelectrolyte superabsorbent composites. L. Hossain, **L. Mendoza**, A. Blanco, C. Negro, J. Tanner, G. Garnier



TECHNICAL PROGRAM

CELL 215. Withdrawn

General Posters

Sponsored by CARB, Cosponsored by CELL

MONDAY MORNING

Section A

Orange County Convention Center
Room W304A

Engineered Lignocellulosic Materials & Multiphase Systems: Anselme Payen Award Symposium in Honor of Orlando Rojas

Creating Sustainable Polymers & Composites

Cosponsored by ANYL and COLL

Financially supported by EPNOE Martin and Lora Kelley Family Foundation ACS Cellulose and Renewable Materials Division Department of Forest Biomaterials, NC State Elsevier Ronalds W. Gonzalez Stephen S. Kelley Daniel E. Saloni College of Natural Resources, NC State Eastman Chemical Company NonWoven Institute, NC State Sunkyu Park Springer Nature BV VTT Hasan Jameel Nathalie M. Lavoine Lucian Lucia Lokendra Pal Richard A. Venditti Yuan Yao S. S. Kelley, J. Zhu, J. O. Zoppe, *Organizers*
K. J. Edgar, *Organizer, Presiding*

8:00 Introductory remarks.

8:05 CELL 216. Silk and cellulose - combining the best of both worlds. **M.B. Linder**

8:30 CELL 217. Selectivity in polysaccharide derivative design. **K.J. Edgar**, J. Chen, B.L. Nichols, C. Gao

8:55 CELL 218. Hexanal releasing packaging materials for extended shelf life of fresh foods. **M. Tenkanen**, M. Lehtonen, H. Zhao, I. Nikkilä, K.S. Mikkonen

9:20 CELL 219. Characterization of hemicellulose in dissolving pulp and its acetylation. J. Lee, C. Kim, T. Treasure, J. Skotty, S.S. Kelley, **S. Park**

9:45 Intermission.

10:00 CELL 220. Diol reactivity in polysaccharides. **E. Bedini**

10:25 CELL 221. Pitfalls in the chemistry of cellulosic chromophores. H. Hettegger, H. Amer, N.S. Zwirchmayr, T. Hosoya, A. Potthast, **T. Rosenau**

10:50 CELL 222. Tailoring the structure of phenylboronic acids grafted on hyaluronic acid to achieve self-crosslinking and stimuli responsive behavior. **R. Auzely-Velty**, T. Figueiredo, Y. Ogawa, V. Cosenza, J. Jing, C. Harris



TECHNICAL PROGRAM

11:15 CELL 223. Tuning cellulose to build renewable biomaterials. **T. Vidal**, A. Torres, C. Valls, O. Cusola, J. Casals-Terré, J. Farré-Lladós, F. Pastor, J. Martínez, M. Roncero

11:40 CELL 224. Modifying latex properties through controlled incorporation of cellulose nanocrystals. S.A. Kedzior, Z. Dastjerdi, A. Ouzas, M. Kiriakou, E. Niinivaara, C. Fraschini, R.M. Berry, M.A. Dubé, **E.D. Cranston**

12:05 Concluding remarks.

Section B

Orange County Convention Center
Room W304B

New Horizons: Early-Career Researchers in Renewable Materials: Symposium in honor of the Kingfa & PhD Student Prize Winners

Cosponsored by ANYL and PROF
Financially supported by EPNOE
E. D. Cranston, *Organizer*
R. Damasio, N. Lavoine, *Presiding*

8:00 Introductory Remarks.

8:05 CELL 225. Chemical modification of cellulose fibres and nanofibrils for an expanded material property space and novel applications. **P.A. Larsson**

8:30 CELL 226. Relationship of hemicelluloses content on grinding process for obtaining cellulose micro/nanofibrils from *Eucalyptus* and *Pinus fibers*. **R. Damásio**, M. Dias, G. Tonoli, M. Mendonça

8:55 CELL 227. Chromophores in pulp and paper: approaches towards their detection and degradation mechanisms. **N.S. Zwirchmayr**, U. Henniges, T.J. Elder, T. Rosenau

9:20 CELL 228. Dissolution of cellulose in NaOH(aq): an unexpected chemisorption of CO₂(g). **M. Hasani**, M. Gunnarsson, B. Swensson, D. Bernin

9:45 Intermission.

10:00 CELL 229. Novel materials from silk proteins and nanocellulose blends- Valorizing sericulture production sidestreams. **M.S. Peresin**, S. Sanchez Diaz, A. Restrepo Osorio, C. Alvarez Lopez, M.C. Arango, T.J. Elder

10:25 CELL 230. Colloidal lignin particles as key to functional renewable materials and applications. **M. Sipponen**, T. Zou, G. Riviere, M. Farooq, M.K. Osterberg

10:50 CELL 231. New chemo-enzymatic pathways for sustainable terpene-based polymeric materials. **L. Fogelstrom**, A. Stamm, M. Tengdelius, P. Syrén, E.E. Malmstrom

11:15 CELL 232. Fungal chitosan-glucan in water remediation applications. **A. Mautner**, J. Janesch, A. Bismarck

11:40 Concluding remarks.



TECHNICAL PROGRAM

Section C

Orange County Convention Center
Room W304C

Understanding Cellulose Crystallinity & Non-Crystalline Aggregated States of Cellulose

Cosponsored by ANYL
Financially supported by EPNOE Bruker Cotton Incorporated
U. P. Agarwal, T. Larsson, *Organizers*
A. D. French, S. H. Kim, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 CELL 233. Crystallinity of nanocellulose: Dispersion-induced disordering of the grain boundary in biologically structured cellulose. **K. Daicho**, T. Saito, S. Fujisawa, A. Isogai

8:30 CELL 234. Crystallinity: Why is cellulose different from other polymers and what are we measuring? **W.T. Winter**

8:55 CELL 235. Anisotropic size-broadening and X-ray diffraction of cellulose: A route towards particle shape and accurate crystallinity determinations. **B. Duchemin**

9:20 CELL 236. Determining cellulose I crystallinity by CP/MAS ¹³C-NMR. **T. Larsson**

9:45 Intermission.

10:00 CELL 237. The pseudo-crystallinity of native celluloses. **R.H. Atalla**

10:25 CELL 238. Multiscale crystallinity and disorder of cellulose: from single fibril properties to liquid crystalline assemblies. **L. Bergstrom**, T. Willhammar, Y. Liu

10:50 CELL 239. Order and Crystallinity in Cellulose Nanocrystals. **W.Y. Hamad**

11:15 CELL 240. Changes in cotton cellulose caused by ball milling - a thirteen technique exploration. **A.D. French**

11:40 Concluding remarks.

Section D

Orange County Convention Center
Room W304D

Advances in Renewable Materials

Cosponsored by ANYL and CARB
Financially supported by EPNOE
N. Abidi, *Organizer*
S. M. Murphy, G. W. Selling, *Organizers, Presiding*



TECHNICAL PROGRAM

8:00 Introductory Remarks.

8:05 **CELL 241.** Superhydrophobic hybrid paper sheets with Janus-type wettability. **C. Kosak Soz**, S. Trosien, M. Biesalski

8:30 **CELL 242.** Preparation and structural characterization of new natural silk non-woven fabrics. **I. Um**, J. Lee, Y. Bae, S. Kim

8:55 **CELL 243.** Use of amylose inclusion complexes to provide high value paper. **G.W. Selling**, W. Hay, G. Fanta, F. Felker, J. Rich

9:20 **CELL 244.** New insight on the preparation of lignin nanoparticles. **B. Li**, W. Qi

9:45 Intermission.

10:00 **CELL 245.** Characterisation of basic properties of ultrahigh-aspect ratio nanocrystals, and nanopapers, made from cellulose of *Cladophora glomerata*-algae. **K. Mihhels**, E. Kontturi, I. Solala

10:25 **CELL 246.** On the role of hot water extraction as a pretreatment method in search for soft pulping methods for modern biorefineries. **J. Sipila**, U. Hyvääkö, R. Maltari, T.A. Kakko, J. Kontro, J. Mikkilä, P.O. Kilpelainen, E. Enqvist, P. Tikka, K. Hilden, P. Nousiainen

10:50 **CELL 247.** Coupling bio-based epoxy resins and recycled carbon fibers: New advances in more sustainable CFRPs. **E. D'Angelo**, L. Mazzocchetti, T. Benelli, L. Giorgini, J.F. Stanzione

11:15 **CELL 248.** Synthesis and characterization of water-soluble anionic carboxylic acid-terminated lignin dendrimer for metal chelating. S. Meng, T. Li, N. Chen, H. Wang, Y. Li, **Z. Tong**

11:40 Concluding Remarks.

Section E

Orange County Convention Center
Room W304E

Interplay of Cellulose & Other Biopolymers in Biological & Designed Materials Systems

Xylan & Lignin Interactions with Cellulose

Cosponsored by ANYL, BIOL and CARB
Financially supported by EPNOE; CP Kelco
H. M. O'Neill, M. Roman, *Organizers*
D. Cosgrove, F. J. Vilaplana, *Organizers, Presiding*

8:00 Introductory remarks.

8:05 **CELL 249.** Structural insights into low and high recalcitrant natural poplar with neutron and X-ray scattering. **R. Shah**, S. Pingali, S. Bhagia, A.J. Ragauskas, B.H. Davison, H.M. O'Neill



TECHNICAL PROGRAM

8:30 CELL 250. Flexibility of xylan and lignin and its effect on interaction with cellulose. **L. Petridis**, U.R. Shrestha, S. Pingali, H.M. O'Neill, M.D. Smith, J. Smith

8:55 CELL 251. Cellulose structure and lignin-carbohydrate interactions in intact secondary plant cell walls from solid-state NMR. X. Kang, A. Kirui, M. Dickwella Widanage, F. Mentink-Vigier, D. Cosgrove, **T. Wang**

9:20 CELL 252. Engineered plant cell walls for improved biomass: exploring the effects on cell wall nanoarchitecture using solid state NMR. **J. Mortimer**

9:45 Intermission.

10:00 CELL 253. Structural colour from a helicoidal cellulose microfibrils-xylan architecture in the cell wall of *Margaritaria nobilis*. **L.M. Steiner**, M. Busse-Wicher, Y. Ogawa, P. Dupree, **S. Vignolini**

10:25 CELL 254. Impact of xylan acetylation on interaction with cellulose. K. Mazeau, Z. Jaafar, C. Moreau, A. Villares, N. Leray, A. Brosse, J. Vigouroux, S. Legall, M. Lahaye, **B. Cathala**

10:50 CELL 255. Interaction between feruloylated arabinoxylan and nanocellulose: Effect on bulk rheological and material properties. **A. Perzon**, J. Muschiol, A.S. Meyer, L. Munk, M. Liu, C. Holland, B. Jørgensen, P. Uivskov

11:15 CELL 256. Occurrence of two- and three-fold chain conformations in homoxylan. **Y. Ogawa**, D. Sawada, Y. Nishiyama

11:40 Concluding remarks.

2019 ACS Sustainable Chemistry & Engineering Lectureship Awards: Symposium in Honor of Paul Dauenhauer

Sponsored by I&EC, Cosponsored by CELL[‡]

Chemical Biology of Glycoproteins

O-Linked Glycosylation

Sponsored by CARB, Cosponsored by CELL

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Sponsored by PROF, Cosponsored by AGFD, ANYL, BIOL, BIOT, CARB, CELL, CHED, CMA, COLL, COMP, ENVR, GEOC, I&EC, MEDI, MPPG, NUCL, ORGN, PHYS, PMSE, POLY, PRES, WCC and YCC

Bioenergy & Bioproducts



TECHNICAL PROGRAM

Bioenergy

Sponsored by ENFL, Cosponsored by CELL

MONDAY AFTERNOON

Section A

Orange County Convention Center
Room W304A

Engineered Lignocellulosic Materials & Multiphase Systems: Anselme Payen Award Symposium in Honor of Orlando Rojas

Creating 21st Century Sustainable Materials from Lignin

Cosponsored by ANYL and COLL

Financially supported by EPNOE Martin and Lora Kelley Family Foundation ACS Cellulose and Renewable Materials Division Department of Forest Biomaterials, NC State Elsevier Ronalds W. Gonzalez Stephen S. Kelley Daniel E. Saloni College of Natural Resources, NC State Eastman Chemical Company NonWoven Institute, NC State Sunkyu Park Springer Nature BV VTT Hasan Jameel Nathalie M. Lavoine Lucian Lucia Lokendra Pal Richard A. Venditti Yuan Yao K. J. Edgar, S. S. Kelley, J. Zhu, J. O. Zoppe, *Organizers*
M. G. Laborie, *Presiding*

1:15 Introductory remarks.

1:20 CELL 257. Distilling the performance of technical softwood lignin with simple solvent fractionation. **S.H. Rennecker**, M. Karaaslan, M. Cho, L. Liu, L. Ji

1:45 CELL 258. Lignin/ Hydroxypropyl cellulose Multiphase Materials: does lignin structure matter? R. Gleuwitz, G. Sirasankarapillai, Y. Chen, C. Friedrich, **M.G. Laborie**

2:10 CELL 259. Utilization of Lignocellulosic Biomass for the development of polymeric materials. **M.L. Auad**, M. Barde

2:35 CELL 260. To understand the enzymatic hydrolysis efficiency promotion by exogenous addition of soluble lignin through the interactions between cellulase and lignin unveiled by QCM and SPR. P. Wang, X. Zhang, X. Wang, J. Tian, **J. Song**, Y. Jin

3:00 CELL 261. Chemical modification of lignin toward functional materials. **Y. Habibi**

3:25 CELL 262. Harmonic analysis of surface instability patterns on colloidal lignin. **T. Kämäräinen**, M. Ago, J. Seitsonen, J. Raula, E. Kauppinen, J. Ruokolainen, O. Rojas

3:50 Concluding remarks.

Section B

Orange County Convention Center
Room W304B



TECHNICAL PROGRAM

New Horizons: Early-Career Researchers in Renewable Materials: Symposium in honor of the Kingfa & PhD Student Prize Winners

Cosponsored by ANYL and PROF
Financially supported by EPNOE
E. D. Cranston, *Organizer*
F. Jiang, E. Niinivaara, *Presiding*

1:15 Introductory Remarks.

1:20 **CELL 263.** Engineering cellulose nanomaterials as alternative supports for heterogeneous cooperative organocatalysis. **N. Ellebracht**, C.W. Jones

1:45 **CELL 264.** Nanocellulose/graphene oxide emulsion-templated aerogels for vanadium redox flow battery electrodes. **S.A. Kedzior**, H. Jahandideh, F. Sharif, M. Trifkovic, S. Bryant

2:10 **CELL 265.** Nature-derived material and structure for sustainable energy storage and generation. **H. Zhu**

2:35 **CELL 266.** Water interactions of man-made cellulose I filaments – threat or opportunity? **M.J. Lundahl**, R. Ajdary, M. Vuoriluoto, H. Orelma, V. Klar, A.G. Cunha, O.J. Rojas

3:00 **CELL 267.** Cellulose nanofibrils as building blocks for advanced structures and applications. **F. Jiang**

3:25 **CELL 268.** Lightweight foams of amine-rich organosilica and cellulose nanofibrils: Processing, properties and potential applications. K. Gordeyeva, H. Voisin, N. Hedin, L. Bergstrom, **N. Lavoine**

3:50 Concluding remarks.

Section C

Orange County Convention Center
Room W304C

Ionic-Liquids Processing of Polysaccharides

Cosponsored by ANYL and CARB
Financially supported by EPNOE
S. J. Eichhorn, J. Scott, *Organizers*
M. Hummel, A. King, *Organizers, Presiding*

1:15 Introductory Remarks.

1:20 **CELL 269.** Cellulose solubility in aqueous quaternary ammonium hydroxide and urea using molecular dynamics simulations. **B. Rabideau**, M. Walters

1:45 **CELL 270.** Biorefining of lignocellulosic biomass in inorganic ionic liquid (molten salt hydrate). **X. Pan**

2:10 **CELL 271.** Understanding the ionic liquid and coagulant role in the formation of cellulose-silk biocomposites for battery and medical applications. **D. Salas-de la Cruz**, S.A. Love, B. Blessing



TECHNICAL PROGRAM

2:35 CELL 272. Manufacturing all-cellulose composites: “selective dissolution” vs “selective swelling”. **F. Chen**, M. Hummel, H. Sixta, T. Budtova

3:00 CELL 273. Dissolution of unbleached wood pulp from low temperature ($\leq 90\text{ }^{\circ}\text{C}$) acid hydrotropic fractionation in an ionic liquid. **J. Zhu**, H. Wang, C. Liu

3:25 CELL 274. Manufacture of high performance all-cellulose nanocomposite fibers using ionic liquid and a co-solvent. **C. Zhu**, J. Van Duijneveldt, R. Richardson, K. Potter, S.J. Eichhorn

3:50 Concluding remarks.

Section D

Orange County Convention Center
Room W304D

Fluorescence Techniques Applied to Lignocellulose Characterization

Cosponsored by ANYL and BIOL
Financially supported by EPNOE

B. Chabbert, L. Donaldson, S. Escamez, A. Gorzsas, F. Guillon, S. Hawkins, G. Paes, *Organizers*
G. Paës, *Presiding*

1:15 Introductory Remarks.

1:20 CELL 275. Fluorescence as a versatile method to characterize lignocellulose. **G. Paes**

1:45 CELL 276. Fiber-level visualization of plant primary cell walls by fluorescently-tagged cellulose binding protein. **X. Wang**, S.N. Kiemle, E. Wagner, L. Wilson, D. Cosgrove

2:10 CELL 277. One, two three, a triple chemical reporter strategy for studying lignification in plant cell walls. C. Simon, C. Lion, F. Baldacci-Cresp, B. Huss, A. Blervacq, C. Spriet, **S. Hawkins**, C. Biot

2:35 CELL 278. Macrofluorescence multispectral image analysis: a promising approach to identify the tissular origin of particles from milled lignocellulosic biomass. **C. Barron**, F. Guillon, M. Devaux

3:00 CELL 279. Two-photon confocal and fluorescence lifetime imaging microscopy as a powerful tool for lignocelluloses characterization. **F.E. Guimaraes**

3:25 CELL 280. Tracking enzymatic modification of cellulose surfaces by fluorescent visualization of oxidized products. **O. Raji**, T.V. Vuong, E.R. Master

3:50 CELL 281. New approaches to the fluorescent labeling of cellulose for visualization at the nanoscale. M. Babi, A. Palermo, A. Fatona, E.D. Cranston, **J. Moran-Mirabal**

4:15 Concluding remarks.

Section E



TECHNICAL PROGRAM

Orange County Convention Center
Room W304E

Hemp Processing: From Weed to Values

Cosponsored by AGRO and ANYL
Financially supported by EPNOE
S. H. Rennekar, *Organizer*
N. Sathitsuksanoh, *Organizer, Presiding*

1:15 Introductory remarks.

1:20 **CELL 282.** Comparative evaluation of industrial hemp varieties: Agronomical practices, biofuels, and bioproducts potential. **L. Das**, L. Dodge, J. Stevens, W. Li, D. Williams, H. Hu, C. Li, A. Ray, J. Shi

1:45 **CELL 283.** Medical cannabis products and Cannabinoids: Medicinal value through chemistry. **L.P. Kotra**

2:10 **CELL 284.** Withdrawn

2:35 **CELL 285.** Utilization of hemp fibers as reinforcements in biocomposites. W. Liu, M. Fei, **R. Qiu**

3:00 **CELL 286.** Chemical-free, green factory for lignin-containing nanocellulose production. **P. Tyagi**, S. Agate, H. Jameel, V. Nathani, L.A. Lucia, L. Pal

3:25 **CELL 287.** Quality management of hemp straw used in agro-materials. **B. Chabbert**, S. Rollet, S. Requile, A. Duborper, P. Rivard, P. Bono, A. Chamussy, A. Bourmaud, B. Kurek, C. Baley, P. Mortoire, A. Day

3:50 **CELL 288.** One-pot acid-catalyzed 5-hydroxymethylfurfural production from industrial hemp: from controversies to commodity chemicals. **N. Sathitsuksanoh**, S. Tulaphol, N. Gridanurak, L. Liu, S. Rennekar, T. Prasomsri

4:15 Concluding remarks.

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Sponsored by PROF, Cosponsored by AGFD, ANYL, BIOL, BIOT, CARB, CELL, CHED, CMA, COLL, COMP, ENVR, GEOC, I&EC, MEDI, MPPG, NUCL, ORGN, PHYS, PMSE, POLY, PRES, WCC and YCC

2019 ACS Sustainable Chemistry & Engineering Lectureship Awards: Symposium in Honor of Kevin Wu

Sponsored by I&EC, Cosponsored by CELL‡

Chemical Biology of Glycoproteins



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

N-Linked Glycosylation

Sponsored by CARB, Cosponsored by CELL

Bioenergy & Bioproducts

Green Chemistry

Sponsored by ENFL, Cosponsored by CELL

MONDAY EVENING

Section A

Orange County Convention Center
West Hall C

Sci-Mix

W. Thielemans, *Organizer*

8:00 - 10:00

90, 95, 102, 106, 109, 111, 122, 127, 144-146, 163, 176, 200. See previous listings.

502. See subsequent listings.

TUESDAY MORNING

Section A

Orange County Convention Center
Room W304A

Engineered Lignocellulosic Materials & Multiphase Systems: Anselme Payen Award Symposium in Honor of Orlando Rojas

Sustainable Materials in High Performance Applications

Cosponsored by ANYL and COLL

Financially supported by EPNOE Martin and Lora Kelley Family Foundation ACS Cellulose and Renewable Materials Division Department of Forest Biomaterials, NC State Elsevier Ronalds W. Gonzalez Stephen S. Kelley Daniel E. Saloni College of Natural Resources, NC State Eastman Chemical Company NonWoven Institute, NC State Sunkyu Park Springer Nature BV VTT Hasan Jameel Nathalie M. Lavoine Lucian Lucia Lokendra Pal Richard A. Venditti Yuan Yao



TECHNICAL PROGRAM

K. J. Edgar, S. S. Kelley, J. Zhu, J. O. Zoppe, *Organizers*
L. Bergstrom, *Presiding*

8:00 Introductory remarks.

8:05 **CELL 289.** Structural order in cellulose thin films prepared from trimethylsilyl cellulose. A. Jones, R. Resel, B. Schrode, P. Christian, C. Roethel, B. Kunert, N. Bedoya-Martinez, I. Salzmann, D. Reishofer, E. Kontturi, **S. Spirk**

8:30 **CELL 290.** Microstructure and properties of polysaccharide based cryogels. **D. Petri**

8:55 **CELL 291.** Nanocellulose-based superinsulating foams: Processing and properties. **L. Bergstrom**, V. Apostolopoulou-Kalkavoura, N. Lavoine, P. Munier

9:20 **CELL 292.** Cellulose fibril emulsifiers: Interesting and versatile. K. Lee, R. Murakami, **A. Bismarck**

9:45 Intermission.

10:00 **CELL 293.** Hierarchical films from cellulose. **T. Nypelo**, M. Liebi, R. Kádár, R. Bordes

10:25 **CELL 294.** Cellulose nanocrystal: A promising sustainable nanomaterial for advanced engineering applications. **M.K. Tam**

10:50 **CELL 295.** Thermoresponsive cellulose nanocrystals-xyloglucan hydrogels. **B. Cathala**, M. Talantikite, C. Moreau, N. Leray, A. Villares

11:15 **CELL 296.** Towards economical and sustainable production of wood-based nanomaterials. **J. Zhu**

11:40 Concluding remarks.

Section B

Orange County Convention Center
Room W304B

ACS Sustainable Chemistry & Engineering: Symposium in honor of Dr. Silvia Vignolini

Cosponsored by ANYL and I&EC
Financially supported by EPNOE
W. Thielemans, *Organizer*
B. Frka-Petesic, S. Vignolini, *Organizers, Presiding*

8:00 Intermission.

8:05 **CELL 297.** Impact of aspect ratio and its dispersity on the cholesteric pitch of cellulose nanocrystal suspensions. C. Honorato-Rios, **J. Lagerwall**

8:30 **CELL 298.** Surfactant-free emulsifiers based on cellulose nanocrystals. **W.Y. Hamad**



TECHNICAL PROGRAM

8:55 CELL 299. Magnetic and electric field alignment of cellulose nanocrystal suspensions. A. Fouques, B. Frka-Petesic, S. Vignolini, **L. Heux**

9:20 CELL 300. New processing and applications of cross-linked cellulose nanocrystal aerogels: Bone implants, delivery systems, and components for energy storage and production devices. D.A. Osorio, D. Levin, T. Or, J. Vapaavuori, B. Siefried, P. Moquin, K. Grandfield, J. Moran-Mirabal, **E.D. Cranston**

9:45 Introductory remarks.

10:00 CELL 301. Functional materials from cellulose: colours, magnetism and charge storage. **S.J. Eichhorn**

10:25 CELL 302. Helices from cellulose-based materials. **M. Godinho**, A. Almeida, L. Querciagrossa, P. Silva, J. Canejo, P. Almeida, C. Zannoni

10:50 CELL 303. Structural colors by block copolymer micellar self-assembly and nanocellulose colloidal networks. **O.T. Ikkala**, S. Vignolini, A. Gröschel

11:15 CELL 304. Liquid crystalline properties of chitin nanocrystals water suspensions. A. Narkevicius, L.M. Steiner, B. Frka-Petesic, Y. Ogawa, **S. Vignolini**

11:40 Concluding remarks.

Section C

Orange County Convention Center
Room W304C

Understanding Cellulose Crystallinity & Non-Crystalline Aggregated States of Cellulose

Cosponsored by ANYL
Financially supported by EPNOE Bruker Cotton Incorporated
U. P. Agarwal, A. D. French, S. H. Kim, *Organizers*
T. Larsson, *Organizer, Presiding*
T. Saito, *Presiding*

8:00 Introductory remarks.

8:05 CELL 305. Contributions of crystalline and non-crystalline cellulose occur in the same spectral regions: Evidence based on raman and IR spectroscopies and its implication for crystallinity measurements. **U.P. Agarwal**

8:30 CELL 306. Crystalline microstructure of cellulose nano crystals probed by scanning electron diffraction. **T. Willhammar**, D.N. Johnstone, Y. Liu, L. Bergstrom, P.A. Midgley

8:55 CELL 307. Heterogeneous dynamics in cellulose from molecular dynamics simulations. P. Chen, C. Terenzi, I. Furó, L. Berglund, **J. Wohlert**

9:20 CELL 308. Structure and properties of cellulose microfibril in G-layer of tension wood fiber in relation to characteristic hygro-mechanical properties of the tension wood. **H. Yamamoto**

9:45 Intermission.



TECHNICAL PROGRAM

10:00 CELL 309. Studying nanoscale crystalline order and mesoscale spatial arrangement of cellulose interspersed in amorphous matrix using vibrational spectroscopy. **S.H. Kim**, M. Makarem, C.M. Lee, K. Kafle, S. Huang, H. Yang, J.D. Kubicki

10:25 CELL 310. Cellulose microfibril structure and morphology *during* dilute acid and alkali thermochemical reactions of poplar. **S. Pingali**, H.M. O'Neill, L. Petridis, V. Urban, B.R. Evans, P. Langan, J. Smith, B.H. Davison

10:50 CELL 311. Correlating structure-properties of TEMPO-treated cellulose nanofibers. **G. Salazar-Alvarez**, S. Kumar, V. Guccini

11:15 CELL 312. Internal structural evolution of regenerated cellulose beads during drying. **H. Li**, T. Pettersson, L. Wagberg

11:40 Concluding remarks.

Section D

Orange County Convention Center
Room W304D

Failed Brilliance in Nanocellulose Science & Technology

Cosponsored by ANYL
Financially supported by EPNOE
E. Kontturi, *Organizer*
A. Bismarck, K. Lee, *Organizers, Presiding*

8:00 Introductory remarks.

8:05 CELL 313. Nanocellulose: What can go wrong? **E. Kontturi**, K. Lee, A. Bismarck

8:30 CELL 314. Chemical modification of nanoscaled cellulosic building blocks: How to define the versatility? **T. Tammelin**, M. Hakalahti, M.S. Peresin, E. Kontturi

8:55 CELL 315. Concept-driven trial and error to find out new functions of nanocellulose. **T. Kitaoka**

9:20 CELL 316. Nanocelluloses for enhanced oil recovery (EOR). **K. Syverud**, E. Heggset

9:45 Intermission.

10:00 CELL 317. Where does surface stabilisation end and bulk modification begin? T. Koso, E. Kontturi, **A. King**

10:25 CELL 318. Filled surface coating for PET with bamboo-ACC nanocellulose to allow to find a suitable container for the resin-adsorbable nanocellulose. **T. Kondo**, G. Ishikawa

10:50 CELL 319. Cellulose nanopaper-reinforced polylactide laminated composites: Is one nanopaper layer enough? M. Hery, A. Braz, J. Blaker, **K. Lee**

11:15 CELL 320. Self assembled nanocellulose-graphene oxide hybrids for water purification: Possibilities and limitations. **A. Mathew**, P. Liu, C. Zhu, S. Monti



TECHNICAL PROGRAM

11:40 Concluding remarks.

Section E

Orange County Convention Center
Room W304E

Advanced Chemistry of "Non-Traditional" Polysaccharides

Cosponsored by AGFD, ANYL, BIOL and CARB
Financially supported by EPNOE; Dupont Biomaterials
T. J. Heinze, C. Lenges, *Organizers*
M. Gericke, *Organizer, Presiding*

8:00 Introductory remarks.

8:05 **CELL 321.** Azide reduction by DTT and thioacetic acid: A novel approach to amino and amido polysaccharide. **C. Gao**, K.J. Edgar

8:30 **CELL 322.** Chemoenzymatic synthesis of artificial xylan polysaccharides with defined substitution patterns. D. Senf, C. Ruprecht, S. Kishani, L. Wagberg, **F. Pfrenge**

8:55 **CELL 323.** Enzymatic polymerization: A new process for engineered PolySaccharides. **C. Lenges**

9:20 **CELL 324.** Engineered PolySaccharides: α -1,3-Glucan esters showing UCST in organic solvents and thermoplastic properties. **T.J. Heinze**

9:45 Intermission.

10:00 **CELL 325.** Methylated hemicellulose as a surfactant prepared from sawdust. **H. Kamitakahara**, K. Miki, T. Takano

10:25 **CELL 326.** Xylan phenyl carbonates: An activated building block for modular synthesis of functional xylan derivatives. **L. Gabriel**, M. Gericke, T.J. Heinze

10:50 **CELL 327.** Engineered polysaccharides: Control of morphology & colloidal structure and applications in wood adhesives. C. Lenges, **M. Harvey**, N. Behabtu

11:15 **CELL 328.** Pectin aerogels for controlled release. S. Groult, G. Pricope, D. Peptanariu, D. Ciolacu, **T. Budtova**

11:40 Concluding remarks.

Exploring the Frontiers of Chemistry through NASA Research

Getting There: Advanced Materials for Space Travel

Sponsored by COMSCI, Cosponsored by ANYL, BIOL, BIOT, CELL, COLL, ENFL, I&EC, INOR, NUCL, PHYS, PMSE and POLY



TECHNICAL PROGRAM

Exploration of Carbohydrate/Protein Interactions/Recognition: The Latest Techniques & Achievements

Sponsored by CARB, Cosponsored by CELL

Opportunities and Challenges in Carbohydrate Synthesis B

Sponsored by CARB, Cosponsored by CELL and ORGN

Bioenergy & Bioproducts

Biofuel & Bioenergy

Sponsored by ENFL, Cosponsored by CELL

TUESDAY AFTERNOON

Section A

Orange County Convention Center
Room W304A

Engineered Lignocellulosic Materials & Multiphase Systems: Anselme Payen Award Symposium in Honor of Orlando Rojas

Lignocellulosic Materials & Multiphase Systems

Cosponsored by ANYL and COLL
Financially supported by EPNOE Martin and Lora Kelley Family Foundation ACS Cellulose and Renewable Materials Division Department of Forest Biomaterials, NC State Elsevier Ronalds W. Gonzalez Stephen S. Kelley Daniel E. Saloni College of Natural Resources, NC State Eastman Chemical Company NonWoven Institute, NC State Sunkyu Park Springer Nature BV VTT Hasan Jameel Nathalie M. Lavoine Lucian Lucia Lokendra Pal Richard A. Venditti Yuan Yao K. J. Edgar, J. Zhu, J. O. Zoppe, *Organizers*
S. S. Kelley, *Organizer, Presiding*

1:15 Introductory remarks.

1:20 CELL 329. Biomimetic mineralization of 3D printed alginate/TEMPO-oxidized cellulose nanofibril scaffolds. R.E. Abouzeid, R. Khiari, D. Beneventi, **A. Dufresne**

1:45 CELL 330. Celebrating Orlando (Rojas) in Orlando (Florida). **J. Genzer**

2:10 CELL 331. Designing nanocellulose-based architectures by exploiting water interactions. **T. Tammelin**



TECHNICAL PROGRAM

2:35 CELL 332. Use of model cellulose substrates to determine molecular interactions. **L. Wagberg**

3:00 CELL 333. Thermodynamics of Adsorption at Nanocellulose Surfaces. S. Lombardo, **W. Thielemans**

3:25 CELL 334. Effect of polymer/surfactant complexation on colloidal depletion forces. B. Lele, **R.D. Tilton**

3:50 Intermission.

4:05 CELL 335. Interfacial assembly and structuring of renewable nanoparticles for advanced materials. **O.J. Rojas**

5:05 Concluding remarks.

Section B

Orange County Convention Center
Room W304B

Ionic-Liquids Processing of Polysaccharides

Cosponsored by ANYL and CARB
Financially supported by EPNOE
M. Hummel, A. King, *Organizers*
S. J. Eichhorn, J. Scott, *Organizers, Presiding*

1:15 Introductory Remarks.

1:20 CELL 336. Use of ionic liquids in industrial processes. A. Suurnäkki, K. Kovasin, **N. von Weymarn**

1:45 CELL 337. Metal chloride deep eutectic solvents for biomass fractionation: Experimental and computational approach. **L. Das**, A. Landera, A. George, B. Simmons, J. Gladden

2:10 CELL 338. Structural characterization of cellulose-based composite fibers from ionic liquid [DBNH]OAc. **D. Sawada**, H.R. Zahra, M. Trogen, H. Sixta, M. Hummel

2:35 CELL 339. Derivatization and functionalization of chitin in ionic liquid. **J. Kadokawa**

3:00 CELL 340. Chitosan-cellulose composite fibers from Ioncell-F process as the precursor of carbon fiber. **H.R. Zahra**, D. Sawada, Y. Ma, N. Byrne, H. Sixta, M. Hummel

3:25 CELL 341. Carbon fibers made from multi-biopolymer precursor fibers spun from ionic liquid solution. **M. Hummel**, M. Trogen, H.R. Zahra, D. Sawada, H. Sixta, N. Byrne

3:50 Concluding remarks.

Section C

Orange County Convention Center
Room W304C



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

Understanding Cellulose Crystallinity & Non-Crystalline Aggregated States of Cellulose

Cosponsored by ANYL
Financially supported by EPNOE Bruker Cotton Incorporated
A. D. French, S. H. Kim, T. Larsson, *Organizers*
U. P. Agarwal, *Organizer, Presiding*
W. Y. Hamad, *Presiding*

1:15 Introductory Remarks.

1:20 **CELL 342.** Solid state NMR and crystallinity of cellulose. **L. Heux**

1:45 **CELL 343.** Cellulose crystallinity determined by two-dimensional Rietveld analysis: Principles, limitations, and prospects. **C. Driemeier**

2:10 **CELL 344.** Atomic Resolution of Cellulose Structure Enabled by Dynamic Nuclear Polarization Solid-State NMR and Database Development. A. Kirui, Z. Ling, X. Kang, M. Dickwella Widanage, F. Mentink-Vigier, A.D. French, **T. Wang**

2:35 **CELL 345.** Morphological and crystalline properties of airbrush spray-deposited enzymatic cellulose thin films. W. Ohm, A. Rothkirch, P. Pandit, V. Koerstgens, P. Mueller-Buschbaum, R. Rojas Escontrillas, S. Yu, C. Brett, D. Söderberg, **S. Roth**

3:00 **CELL 346.** Grazing incidence X-ray scattering reveals texturing in primary cell walls. **S. Rongpipi**, D. Ye, W. Barnes, S. Kiemle, A. Woll, C. Zhu, C. Anderson, D. Cosgrove, E. Gomez, E. Gomez

3:25 **CELL 347.** Chirality and bound water in the hierarchical cellulose structure. **A. Paajanen**, S. Ceccherini, T. Maloney, J. Ketoja

3:50 Concluding Remarks.

Section D

Orange County Convention Center
Room W304D

Failed Brilliance in Nanocellulose Science & Technology

Cosponsored by ANYL
Financially supported by EPNOE
E. Kontturi, *Organizer*
A. Bismarck, K. Lee, *Organizers, Presiding*

1:15 Introductory remarks.

1:20 **CELL 348.** Ways you can fail with cellulose nanocrystals produced from phosphoric acid hydrolysis. O.M. Vanderfleet, D.A. Osorio, **E.D. Cranston**

1:45 **CELL 349.** Why haven't plastic packaging been replaced by cellulose? **T. Larsson**, R. Karlsson, L. Wagberg



TECHNICAL PROGRAM

2:10 CELL 350. Water-stable (or not) nanocellulose porous beads for controlled release applications. **T. Abitbol**, M. Lundin-Johnson, A. Millqvist-Fureby

2:35 CELL 351. Oriented deposition of bacterial nanocellulose induced by nematic ordered cellulose templates with unique surface energy distribution. **S. Yokota**, K. Miura, T. Kondo

3:00 CELL 352. Challenges on specific surface area analysis of cellulosic materials. **A. Kondor**, A. Mautner, K. Lee, A. Bismarck, D. Williams

3:25 CELL 353. Chitosan sol gel thin thin films: Preparation, and interaction with biological materials. **S. Spirk**

3:50 Concluding remarks.

Section E

Orange County Convention Center
Room W304E

Advanced Chemistry of "Non-Traditional" Polysaccharides

Cosponsored by AGFD, ANYL, BIOL and CARB
Financially supported by EPNOE; Dupont Biomaterials
M. Gericke, C. Lenges, *Organizers*
T. J. Heinze, *Organizer, Presiding*

1:15 Introductory remarks.

1:20 CELL 354. Seaweed polysaccharide based materials: From chemical derivatization to functional composite hydrogels and advanced applications. **M. Gericke**, M. Witzler, D. Büchner, A. Enkelmann, P. Ottensmeyer, G. Schneider, E. Tobiasch, M. Schulze, T.J. Heinze

1:45 CELL 355. Extraction and modification of hemicellulose to produce high value super absorbent gels. **R.A. Venditti**, W. Geng, J. Pawlak, H. Chang

2:10 CELL 356. Enzymatic polysaccharides: Review of applications in paper coatings. **N. Behabtu**, J. Fisher, C. Grinsell, W. Ripmeester

2:35 CELL 357. Application of chitosan-simplexes: From biogenic paper wet-strength to flame retardancy. **M.A. Biesalski**, F. Schäfer, S. Moehle-Saul

3:00 CELL 358. Enzymatic polymerization: Engineered polySaccharides and unique properties in coating systems. C. Lenges, N. Behabtu, M. Harvey, **K. Kim**

3:25 CELL 359. Sustainable thermoplastic composites: Enzymatic polysaccharide additives to enhance performance. **C. Lenges**, **N. Behabtu**

3:50 Concluding remarks.



TECHNICAL PROGRAM

Exploration of Carbohydrate/Protein Interactions/Recognition: The Latest Techniques & Achievements

Sponsored by CARB, Cosponsored by CELL

Exploring the Frontiers of Chemistry through NASA Research

Living There: Science for the Future of Manned Space Exploration

Sponsored by COMSCI, Cosponsored by ANYL, BIOL[‡], BIOT, CELL, COLL, ENFL[‡], I&EC[‡], INOR[‡], NUCL[‡], PHYS[‡], PMSE[‡] and POLY[‡]

Exploring the Frontiers of Chemistry through NASA Research

Living There: Science for the Future of Manned Space Exploration

Sponsored by COMSCI, Cosponsored by ANYL, BIOL[‡], BIOT, CELL, COLL, ENFL[‡], I&EC[‡], INOR[‡], NUCL[‡], PHYS[‡], PMSE[‡] and POLY[‡]

Opportunities and Challenges in Carbohydrate Synthesis B

Sponsored by CARB, Cosponsored by CELL and ORGN

WEDNESDAY MORNING

Section A

Orange County Convention Center
Room W304A

Nanocellulose: From Fundamentals to Function

Cosponsored by AGFD, ANYL and BIOL
Financially supported by EPNOE CelluForce Performance Biofilaments Spectra Research Corporation
T. Abitbol, S. A. Kedzior, E. Niinivaara, M. S. Reid, *Organizers*
S. Kedzior, *Presiding*

8:00 Introductory Remarks.

8:05 CELL 360. Mechanochemical phosphorylation of polymers with solid phosphorylating agents for application as flame retardants. **B. Fiss**, L. Hatherly, R. Stein, T. Friscic, A.H. Moores

8:30 CELL 361. Effects of degree of polymerization, surface chemistry, and surface charge density on cellulose nanocrystal thermal stability. **O.M. Vanderfleet**, M.S. Reid, J. Bras, L. Heux, J. Godoy, M.K. Panga, E.D. Cranston



TECHNICAL PROGRAM

8:55 CELL 362. Gold nanoparticles and thermoresponsive polymer end-grafted cellulose nanocrystals. **F. Lin**, J. Putaux, B.R. Jean

9:20 CELL 363. Polymer modification of nanocellulose in water: A versatile approach to new materials. **E.E. Malmstrom**, R. Telaretti, T. Kaldéus

9:45 Intermission.

10:00 CELL 364. One-component nanocomposites based on polymer-decorated cellulose nanocrystals. **S. Wohlhauser**, J.O. Zoppe, C. Weder

10:25 CELL 365. Controlling the dispersion properties of nanocellulose systems by surface modification. **T. Kaldeus**, E.E. Malmstrom

10:50 CELL 366. Functional cellulose nanocrystals: Grafting with conjugated polymers. **A. Chang**, K.R. Carter

11:15 CELL 367. Physico-chemical factors relevant to the chemical modification of nanofibrillated cellulose. **K.S. Salem**, L. Pal, L.A. Lucia, H. Jameel

11:40 Concluding remarks.

Section B

Orange County Convention Center
Room W304B

Bioactive Delivery: Frontiers in Biomaterials

Cosponsored by ANYL, BIOL and CARB

Financially supported by EPNOE

A. Ayoub, B. S. Ghotra, J. M. Goddard, L. A. Lucia, *Organizers*

A. AYOUB, *Presiding*

8:00 Introductory remarks.

8:05 CELL 368. In situ imaging and characterization of bioactive compounds and surfactants in an emulsion system using Raman microscopy. **L. He**

8:30 CELL 369. Recent advances in injectable hydrogels and electrospinning for drug delivery. **S.V. Madihally**

8:55 CELL 370. Electrospinning cargo-containing complex coacervates from synthetic and natural polyelectrolytes. X. Meng, J. Sun, S.L. Perry, **J.D. Schiffman**

9:20 CELL 371. Carbon dots as bioactivity inducers in polymeric biomaterials. **M. Hakkarainen**

9:45 Intermission.

10:00 CELL 372. Novel protein transduction domains as bioactives. **G.N. Tew**



TECHNICAL PROGRAM

10:25 CELL 373. Bioactive composites of cellulose nanofibrils and recombinant silk proteins. **D. Soderberg**, M. Hedhammar, N. Mittal, R. Jansson, M. Widhe, T. Bensselfelt, K. Hakansson, F. Lundell

10:50 CELL 374. Wound Healing and Melanogenesis Potential of EGF-Loaded Nano-Pillared Chitosan-Gelatin Films. **S. Altuntas**, H. Dhaliwal, **A.E. Radwan**, F. Buyukserin, M. Amiji

11:15 CELL 375. Polymer biomaterial surface modification: the key to integration. H. Mahjoubi, E. Buck, P. Manimunda, R. Chromik, M. Murshed, R. Farivar, L. Stone, **M. Cerruti**

11:40 Concluding remarks.

Section C

Orange County Convention Center
Room W304C

Bio-Based Gels & Porous Materials

3D printing & Rheology of Cellulose & Nanocellulose

Cosponsored by ANYL, BIOL and COLL
Financially supported by EPNOE
T. Budtova, F. Liebner, *Organizers*
B. Cathala, J. Moran-Mirabal, *Presiding*

8:00 Introductory Remarks.

8:05 CELL 376. 3D printable nanocellulose aerogels via a green crosslinking approach and a facile evaporation procedure. **H. Françon**, T. Bensselfelt, H. Granberg, P.A. Larsson, L. Wagberg

8:30 CELL 377. 3D bacterial cellulose biofabrication using superhydrophobized molds: Fundamentals and opportunities. **L. Garcia Greca**, J. Lehtonen, B.L. Tardy, M. Rafiee, A. Karakoc, B. Mattos, O. Rojas

8:55 CELL 378. Droplet microfluidic templating of ultraporous cross-linked cellulose nanocrystal microparticles. D. Levin, S. Saem, D. Osorio, A. Cerf, E.D. Cranston, **J. Moran-Mirabal**

9:20 CELL 379. Rheology of cellulose/1,5-diazabicyclo[4.3.0]non-5-enium propionate solutions and shaping into aerogel beads. L. Druel, P. Niemeyer, B. Milow, **T. Budtova**

9:45 Intermission.

10:00 CELL 380. Photo-crosslinked porous cellulose nanofibrils (CNF) based composite gel. **M. Hossen**

10:25 CELL 381. Rheology and morphology of ultra-low solid content hydrogels of TEMPO-CNF/mixed-linkage beta-glucan bionanocomposites. **S. Arola**, M. Ansari, A. Oksanen, S. Hatzikiriakos, H. Brumer

10:50 CELL 382. Rheological properties of wheat arabinoxylan/cellulose nanocrystals bio-hydrogels. **M. Talantikite**, C. Antoine-Assor, C. Moreau, N. Beury, B. Cathala



TECHNICAL PROGRAM

11:15 CELL 383. Monovalent salt induced gelation of oxidised cellulose nanofibrils and starch networks. **Z. Hossain**, J. Schmitt, M. da Silva, V. Calabrese, J. Scott, K. Edler

11:40 Concluding remarks.

Section D

Orange County Convention Center
Room W304D

Valorization of Renewable Resources & Residuals into New Materials & Multiphase Systems

Cosponsored by AGRO and ANYL
Financially supported by EPNOE
M. L. Auad, O. J. Rojas, *Organizers*
J. Campos-Teran, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 CELL 384. Cascade processing of softwood bark with hot water extraction, pyrolysis and anaerobic digestion. **P.O. Kilpelainen**, R. Korpinen, J. Raitanen, K. Rasa, S. Rasi, T. Jyske

8:30 CELL 385. Versatile assembling of bio-based nanomaterials into functional superstructures. **B. Mattos**, B.L. Tardy, L. Garcia Greca, W.E. Magalhães, O. Rojas

8:55 CELL 386. Self-assembled networks of short and long chitin nanoparticles for oil/water interfacial super-stabilization. **L. Bai**, S. Huan, W. Xiang, R.W. Nugroho, O. Rojas

9:20 CELL 387. Phase separated chitin nanocrystal suspensions. **J. Majoinen**, L. Bai, W. Xiang, B.L. Tardy, O. Rojas

9:45 Intermission.

10:00 CELL 388. Hybrid hydrogels from xylan/HEMA and SBA-15 as scaffolds for fibroblast attachment and growth. **G. Toriz**, L. G Uriostegui, E. Delgado, P. Gatenholm

10:25 CELL 389. Using Fique residual biomass for nanocellulose/Ag NPs hybrid hydrogels synthesis. L.A. Díaz-Serrano, S. Ovalle Serrano, C. Blanco-Tirado, **M.Y. Combariza**

10:50 CELL 390. Role of chitin nanocrystals in aqueous foam stabilization. **W. Xiang**, L. Bai, J. Majoinen, L. Liu, O. Rojas

11:15 CELL 391. Minerals in sugarcane bagasse and straw as observed by X-ray microtomography and microfluorescence. **C. Driemeier**, D.R. Negrao, L.Y. Ling

11:40 Concluding Remarks.

Section E

Orange County Convention Center
Room W304E



TECHNICAL PROGRAM

Wood-Based Polymers: From Functional Structures to Applications

Lignin

Cosponsored by ANYL
Financially supported by EPNOE Lenzing AG
M. Ek, T. Nypelo, S. Spirk, *Organizers*
I. Filpponen, J. O. Zoppe, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 CELL 392. Lignin engineering for high-value applications. **M. Balakshin**, E. Capanema, O. Rojas

8:30 CELL 393. Lignin phenol-formaldehyde resins with suitable bonding strength synthesized from “less reactive” hardwood lignin fractions. **T. Lourençon**, W.E. Magalhães, G.B. de Muniz, T. Virtanen, A. Jääskeläinen, T. Liitiä, S. Alakurtti, M. Hughes, T. Tamminen

8:55 CELL 394. Tunable polymer systems containing well-characterized derivatives from lignin. **C. Gioia**, G. Lo Re, M. Lawoko, L. Berglund

9:20 CELL 395. Elucidating lignin structure and relationships from naturally variant *Populus trichocarpa*. **N. Bryant**, A.J. Ragauskas

9:45 Intermission.

10:00 CELL 396. Characterization and synthesis of next generation of lignin-based polyurethanes. **X. Meng**, P. Singh, C. Wyman, C. Cai, A. Ragauskas

10:25 CELL 397. 2-Methoxyhydroquinone from vanillin as bio-based active material for redox-flow batteries. **W. Schlemmer**, M. Sahin, P. Nothdurft, E. Mourad, P. Frühwirth, G. Riess, M. Schmalegger, G. Gescheidt-Demner, R. Fischer, S. Freunberger, W. Kern, S. Spirk

10:50 CELL 398. Hydroxystilbene dehydrogenation polymers and copolymers with monolignols. **H. Kim**, J. Rencoret, S.D. Karlen, J. del Río, J. Ralph

11:15 CELL 399. Synthesis of lignin-porphyrin nano-particles to perform fluorescence enhancement at high water fraction with broad pH range and heavy metals sensor applications. **H. Tse**, S. Leu, Y. Chi Shun

11:40 Concluding remarks.

Exploration of Carbohydrate/Protein Interactions/Recognition: The Latest Techniques & Achievements

Sponsored by CARB, Cosponsored by CELL

WEDNESDAY AFTERNOON

Section A



TECHNICAL PROGRAM

Orange County Convention Center
Room W304A

Nanocellulose: From Fundamentals to Function

Cosponsored by AGFD, ANYL and BIOL
Financially supported by EPNOE CelluForce Performance Biofilaments Spectra Research Corporation
T. Abitbol, S. A. Kedzior, M. S. Reid, *Organizers*
E. Niinivaara, *Organizer, Presiding*

1:15 Introductory Remarks.

1:20 CELL 400. Energy efficient nanocellulose foam coating on cellulosic textiles for water filtration membranes. **A. Mautner**, M. Fortea-Verdejo, A. Bismarck

1:45 CELL 401. Withdrawn

2:10 CELL 402. Foaming nanocellulose for coating applications. **M. Fortea-Verdejo**, A. Mautner, A. Bismarck

2:35 CELL 403. Dewatering of nanocellulose dispersions: Efficiency and property preservation. M. Henriksson, **A.B. Fall**, K. Hakansson, A. Karppinen, E. Heggset

3:00 Intermission.

3:15 CELL 404. High shear rheology of nanocellulosics. **M. Bortner**, J.P. Youngblood, B. Sutliff

3:40 CELL 405. Effect of chemical composition on the rheological behavior of cellulose nanofibrils suspensions obtained from different sources. **M.C. Iglesias**, **M.S. Peresin**

4:05 CELL 406. Edible cellulose-based colorimetric timer. **A.G. Dumanli**, G. Kamita, S. Vignolini

4:30 CELL 407. Recyclable deep eutectic solvent for the production of cationic nanocelluloses. **P. Li**, J.A. Sirvio, B. Asante, H. Liimatainen

4:55 Concluding remarks.

Section B

Orange County Convention Center
Room W304B

Bioactive Delivery: Frontiers in Biomaterials

Cosponsored by ANYL, BIOL and CARB
Financially supported by EPNOE
A. Ayoub, B. S. Ghotra, J. M. Goddard, L. A. Lucia, *Organizers*
A. AYOUB, *Presiding*

1:15 Introductory remarks.



TECHNICAL PROGRAM

1:20 CELL 408. Withdrawn

1:45 CELL 409. Cellulose nanofibrils from wood for drug molecule immobilization and release. **J. Bras**, H. Durand, C. Sillard, P. Jaouen, E. Zeno

2:10 CELL 410. Strain activated covalent crosslinking in synthetic and naturally derived polymers. **J. Klier**, Y. Tran, S. Peyton

2:35 CELL 411. High-throughput production of physiologically relevant tissue equivalents. **S.N. Nazhat**

3:00 Intermission.

3:15 CELL 412. Synthesis of biodegradable nonmigratory active packaging via reactive extrusion. **J.E. Herskovitz**, J.M. Goddard

3:40 CELL 413. Responsive polymeric assemblies for protein delivery. **S. Thayumanavan**

4:05 CELL 414. Modified macrophages as cell-based delivery tools and therapeutic entities for cancer study and treatment. **M.E. Farkas**

4:30 CELL 415. Polysaccharides and lignin based hydrogels with potential pharmaceutical use as a drug delivery system produced by a reactive extrusion process. W. Farhat, **R.A. Venditti**, N. Mignard, M. Taha, F. Becquart, A. Ayoub

4:55 Concluding remarks.

Section C

Orange County Convention Center
Room W304C

Bio-Based Gels & Porous Materials

Gels in Medical Applications

Cosponsored by ANYL, BIOL and COLL
Financially supported by EPNOE
T. Budtova, F. Liebner, *Organizers*
C. R. Freire, D. O. Klemm, *Presiding*

1:30 Introductory Remarks.

1:35 CELL 416. Antimicrobial molecules impregnation of nanocellulose-based structures in supercritical carbon dioxide. **C. Darpentigny**, J. Bras, G. Nonglaton, B.R. Jean

2:00 CELL 417. Nanocellulose hydrogels for blood typing diagnostics. **R. Curvello**, L. Mendoza, H. McLiesh, R. Tabor, **G. Garnier**

2:25 CELL 418. Nanocellulose membranes loaded with antioxidant phenolic compounds formulated as ionic liquids: from preparation to in vitro anti-inflammatory assessment. E. Morais, N. Silva, S. Santos, B. Neves, I. Almeida, P. Costa, I. Correia-Sá, S. Ventura, **A. Silvestre**, M. Freire, C. Freire



TECHNICAL PROGRAM

2:50 CELL 419. Process-controlled design of multilayered nanocellulose materials for regenerative medicine and membrane technologies. **D.O. Klemm**, F. Kramer, K. Petzold-Welcke, T. Richter, W. Fried

3:15 Intermission.

3:20 CELL 420. Enzymatic synthesis of hydrogels based on thiolated chitosan and chicoric acid for chronic wound application. **I.S. Stefanov**, J. Hoyo, T. Tzanov

3:45 CELL 421. Organogels of surface modified nanocellulose for applications in crystallizing pharmaceuticals. **M. Banerjee**, S. Saraswatula, L. Willows, B. Brettmann

4:10 CELL 422. Alginate-chitosan scaffolds modified by gold nanoparticles for cardiac tissue engineering. D. Vaquero-Hernández, E. Francisco-Solano, D. Gomez-Maldonado, N. Beltrán, **J. Campos-Teran**

4:35 CELL 423. Nanocellulose hydrogel for organoids culture. **R. Curvello**, M. Dannappel, R. Firestein, J. Rosenbluh, R. Tabor, G. Garnier

5:00 Concluding remarks.

Section D

Orange County Convention Center
Room W304D

Valorization of Renewable Resources & Residuals into New Materials & Multiphase Systems

Cosponsored by AGRO and ANYL
Financially supported by EPNOE
J. Campos-Teran, O. J. Rojas, *Organizers*
M. L. Auad, *Organizer, Presiding*

1:15 Introductory Remarks.

1:20 CELL 424. Withdrawn

1:45 CELL 425. Lignin containing nanocellulose fibrils: A promising biomaterial for performance enhancement in polymeric systems. **N. Yan**

2:10 CELL 426. Simple, greener and robust routes to make esterified lignin. **L. Liu**, Q. Hua, S. Renneckar

2:35 CELL 427. Multifunctional transparent wood for thermal energy storage applications. **C. Montanari**, Y. Li, L. Berglund

3:00 Intermission.

3:15 CELL 428. Photopolymerization of acrylated lignin monomers: Implications for lignin utilization in additive manufacturing by stereolithography. **K. Rajan**, S.C. Chmely, D.P. Harper, N. Labbé, D.J. Carrier

3:40 CELL 429. Liquefaction of Kraft lignin with selective oxyalkylation of phenolic hydroxyls for polyurethane application. **X. Zhang**, Y. Kim, E. Hassan, T. Eberhardt, R. Shmulsky



TECHNICAL PROGRAM

4:05 CELL 430. Processable soft materials obtained from biobased microbial glycolipids. **N. Baccile**, G. Ben Messaoud, S. Roelants, F. Fernandes, C.V. Stevens, L. VanRenterghem, W. Soetaert

4:30 CELL 431. Plastics with high unmethylated Kraft-Lignin contents surpass polyethylene in tensile strength. **S. Sarkanen**, Y. Chen

4:55 Concluding Remarks.

Section E

Orange County Convention Center
Room W304E

Wood-Based Polymers: From Functional Structures to Applications

Hierarchies & Assembly, Films & Fibers

Cosponsored by ANYL
Financially supported by EPNOE Lenzing AG
I. Filpponen, T. Nypelo, J. O. Zoppe, *Organizers*
M. Ek, S. Spirk, *Organizers, Presiding*

1:15 Introductory Remarks.

1:20 CELL 432. Sensory profile of spruce galactoglucomannans and birch glucuronoxylans in food. S. Kirjoranta, A. Knaapila, P. Kilpeläinen, **K.S. Mikkonen**

1:45 CELL 433. Enhancing mechanical performance of cellulose materials with designed structural complexity. **J. Ketoja**, A. Ivanova, A. Tanaka, I. Nurminen, P. Kääriäinen

2:10 CELL 434. Pickering emulsions stabilized from biomass nanoparticles: role of composition and emulsification parameters. **C. Jimenez Saelices**, F. Vasquez, S. Tapin-Lingua, D. Da Silva, Z. Mouloungui, R. Valentin, I. Capron

2:35 CELL 435. Wet-expandable cellulose-based capsules. **K. Mystek**, P.A. Larsson, A. Svagan, L. Wagberg

3:00 Intermission.

3:15 CELL 436. High throughput characterization of bio-based fibres and fibre interfaces using microrobotics. **P. Kallio**

3:40 CELL 437. Sulfated wood nanofibers produced using reactive deep eutectic solvent. **J.A. Sirvio**, M. Visanko

4:05 CELL 438. Bio-based activated carbon fibers for use as supercapacitor electrodes. **S. Breitenbach**, C. Unterweger, C. Fürst, A.W. Hassel

4:30 CELL 439. In situ sonosynthesis of photo-catalytic TiO₂ nanoparticles on cellulose fibers. E. Sánchez-Ramos, A. Andrade, G. Toriz, C.B. Ramirez-Lopez, **E. Delgado**

4:55 Concluding remarks.



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

Exploration of Carbohydrate/Protein Interactions/Recognition: The Latest Techniques & Achievements

Sponsored by CARB, Cosponsored by CELL

THURSDAY MORNING

Section A

Orange County Convention Center
Room W224G

Nanocellulose: From Fundamentals to Function

Cosponsored by AGFD, ANYL and BIOL
Financially supported by EPNOE CelluForce Performance Biofilaments Spectra Research Corporation
S. A. Kedzior, E. Niinivaara, M. S. Reid, *Organizers*
T. Abitbol, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 CELL 440. Observations of phase separation in cellulose nanocrystals. **E. Facchine**, O. Rojas, S.A. Khan

8:30 CELL 441. High resolution self-assembled patterns on flexible nanocellulose film. **M.S. Gestranus, I. Otsuka**, H. Sami, R. Borsali, T. Tammelin

8:55 CELL 442. Development of domains and stratification in chiral nematic cellulose nanocrystal films. **K.W. Klockars**, B.L. Tardy, M. Borghesi, A. Tripathi, L. Garcia Greca, O. Rojas

9:20 CELL 443. Cellulose nanocrystals to stabilize water-in-water Pickering emulsions and emulsion gels. **I. Capron**, T. Nicolai, K. Peddireddy, L. Benyahia

9:45 Intermission.

10:00 CELL 444. Direct cryo writing of aerogels inspired by the plant cell wall by 3D printing of aligned cellulose nanocrystals. **D. Kam**, M. Chasnitsky, C. Nowogrodski, I. Braslavsky, T. Abitbol, S. Magdassi, O. Shoseyov

10:25 CELL 445. Effect of drying flux inhomogeneities on the development of coffee rings from cellulose nanocrystals and visual designs perspective.. **K. Klockars**, N. Yau, **B.L. Tardy**, J. Majoinen, T. Kämäräinen, K. Miettunen, E. Boutonnet, J. Beidler, O. Rojas

10:50 CELL 446. Orientation and alignment of cellulose nanofibrils in shear and extensional flows. **K. Vijayakumar**, D. Söderberg, F. Lundell

11:15 CELL 447. Melt extrusion of polypropylene nanocomposites reinforced with TEMPO-oxidized pulp. **A.N. Gaduan**, K. Lee

11:40 Concluding remarks.



TECHNICAL PROGRAM

Section B

Orange County Convention Center
Room W224H

Additive Manufacturing of Bio-based & Renewable Materials

Cosponsored by AGRO, ANYL and BIOL
Financially supported by EPNOE
M. Bortner, G. Siqueira, *Organizers, Presiding*

8:00 Introductory remarks.

8:05 CELL 448. Stretchable and conductive nanocellulose-based inks for the one-step fabrication of wearable sensors. **M. Binelli**, R. Van Dommelen, G. Siqueira, J. Pratiwi, A. Studart, D. Briand

8:30 CELL 449. 3D printed soft and porous materials for functional applications. **G. Siqueira**, M. Hausmann, Y. Nagel, T. Zimmermann, G. Nyström

8:55 CELL 450. Thermo-responsivity and tunable optics of a PNIPAM/cellulose nanofibrillar hydrogel for 3D printing. **X. Sun**, S. Agate, L.A. Lucia, M. McCord, L. Pal

9:20 CELL 451. Versatile approach to 3D printed cellulose-reinforced composites. **M. Hausmann**

9:45 Intermission.

10:00 CELL 452. Conductive 3D printed structures based on nanocellulose for electro-responsiveness and controlled drug release. R. Ajdary, N. Zanzanizadeh Ezazi, S. Huan, H. Santos, **O. Rojas**

10:25 CELL 453. 3D printing of mechanically responsive cellulose nanocrystal thermoplastic urethane composites. **M. Bortner**, J. Foster, J. Fallon

10:50 CELL 454. Potential of ligno-cellulosic materials in DIW and FFF additive manufacturing technologies. **K. Torvinen**, P. Lahtinen, K. Immonen, H. Orelma

11:15 CELL 455. Photo-patterned properties in bio-inspired cellulose nanofibrils (CNF) nanocomposites. W. Yu, **J. Guo**, A. Walther

11:40 Concluding remarks.

Section C

Orange County Convention Center
Room W225A

Bio-Based Gels & Porous Materials

Nanostructuration of Gels & Aerogels & their Use as Sensors



TECHNICAL PROGRAM

Cosponsored by ANYL, BIOL and COLL
Financially supported by EPNOE
T. Budtova, F. Liebner, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 CELL 456. Preparation of porous nanocellulose structures via ambient pressure drying and their characterization. **W. Sakuma**, S. Yamasaki, S. Fujisawa, T. Saito, A. Isogai

8:30 CELL 457. Ultra-light and flexible nanochitin aerogel prepared from ice templating. **L. Liu**, L. Bai, Y. Fan, O. Rojas

8:55 CELL 458. Cotton aerogels from fabric waste for high-value engineering and medical applications. **H.M. Duong**, D.K. Le, Q.B. Thai, N. Phan-Thien, B. Gu, H. Cheng, T.P. Luu

9:20 CELL 459. Following nanostructure development of isotropic and anisotropic cellulose II gels (and aerogels) at the high-flux SAXS beamline at Elettra. **F. Liebner**, S. Plappert, H. Rennhofer, S. Bernstorff, H. Lichtenegger

9:45 Intermission.

10:00 CELL 460. Biographene infused protein hydrogels interlocked in paper for biocatalysis and sensing applications. **M. Puglia**, C.V. Kumar

10:25 CELL 461. Controllable 3D hollow double-wrinkled chitosan/polyaniline hydrogels for highly sensitive pressure sensors. **Y. Du**, X. Lei, A. Lu, X. Shi

10:50 CELL 462. Probing solvent and temperature effects on the chiral self-assembly and gelation of ferrocene-diphenylalanine. **G. Zhang**, Y. Wang, W. Qi

11:15 CELL 463. Withdrawn

11:40 Concluding remarks.

Section D

Orange County Convention Center
Room W225B

Valorization of Renewable Resources & Residuals into New Materials & Multiphase Systems

Cosponsored by AGRO and ANYL
Financially supported by EPNOE
J. Campos-Teran, O. J. Rojas, *Organizers*
M. L. Auad, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 CELL 464. Peculiar XPS spectra on oxidized and carboxylated celluloses. **L. Johansson**, J. Campbell, H. Orelma, A. Shchukarev, O. Rojas



TECHNICAL PROGRAM

8:30 CELL 465. Fabrication of superhydrophobic and highly porous aerogels via solid templating of cellulose-silica composite nanofibers. **S. Khan**

8:55 CELL 466. Protein-functionalized cellulose fibrils and nanopapers derived from tunic wastes. **F. Quero**, G. Opazo, A. Quintro, J. Fernandez, Y. Zhao, A. Mautner, M. Flores

9:20 CELL 467. Synthesis of polyphenol-based nano- and microparticles from tannic acid. **T. Kämäräinen**, M. Ago, L. Garcia Greca, B.L. Tardy, M. Müllner, L. Johansson, O. Rojas

9:45 Intermission.

10:00 CELL 468. A fully green wood adhesive based on hemicelluloses derived from pulp processes. **L. Fogelstrom**, E. Norström, F. Khabbaz, J. Brucher, E.E. Malmstrom

10:25 CELL 469. Esterification-induced lignin conversion towards aromatic acids. **Z. Tong**, H. Bao

10:50 CELL 470. New chemistry to modify natural lignin: synthesis of lignin-based functional polymers. **H. Chung**, H. Liu

11:15 CELL 471. Renewable thermosetting resins based on refined technical lignin: fractionation, modification and valorization. **M. Jawerth**, M.K. Johansson, M. Lawoko

11:40 Concluding Remarks.

Section E

Orange County Convention Center
Room W230D

Wood-Based Polymers: From Functional Structures to Applications

From Biomass to Materials: Global Challenges

Cosponsored by ANYL
Financially supported by EPNOE Lenzing AG
M. Ek, I. Filpponen, T. Nypelo, S. Spirk, J. O. Zoppe, *Organizers*
W. Fischer, T. Nypelö, *Presiding*

8:00 Introductory Remarks.

8:05 CELL 472. Potential valorization of trace element-contaminated willow for bioethanol production. **I. Ziegler-Devin**, Z. Menana, L. Chrusciel, M. Chalot, V. Bert, N. Brosse

8:30 CELL 473. Converting CO₂ to biofuels with photosynthetic microalgae immobilized in cellulose nanofibrils. **V. Rissanen**, M. Jämsä, S. Kosourov, J. Ketoja, Y. Allahverdiyeva, T. Tammelin

8:55 CELL 474. Towards sustainable high performance thermoplastics: Synthesis, characterization, and enzymatic hydrolysis of xylochemical based polyesters. **S. Curia**, A. Biundo, G.M. Guebitz, J.F. Stanzione

9:20 CELL 475. FLIPPR²: Future lignin and pulp processing research in Austria. **T. Timmel**



TECHNICAL PROGRAM

9:45 Intermission.

10:00 CELL 476. Marine pollution: Exposing some of the myths and facts. **M. Kogler**, S. Rahbaran, K. Schuster, S. Kulka

10:25 CELL 477. Efficient removal of Arsenic (III) by novel micro and nano dialdehyde cellulose-cysteine complex extracted from wood pulp cellulose. **H. Chen**, S. Sharma, P.R. Sharma, H. Yeh, B.S. Hsiao

10:50 CELL 478. Enhance adsorption of microcystin-LR on nanocellulose/ β -cyclodextrin polymer surfaces. **D. Gomez-Maldonado**, S. Lombardo, I. Vega Erramuspe, I. Filpponen, A. King, W. Thielemans, M.S. Peresin

11:15 CELL 479. Preparation of cellulose nanocrystal sensors for antibody-antigen binding of model cancer biomarkers. **D. Gomez-Maldonado**, P. Saha, U.M. Noori, W.R. Ashurst, M.S. Peresin, **V.A. Davis**

11:40 Concluding remarks.

THURSDAY AFTERNOON

Section A

Orange County Convention Center
Room W224G

Nanocellulose: From Fundamentals to Function

Cosponsored by AGFD, ANYL and BIOL

Financially supported by EPNOE CelluForce Performance Biofilaments Spectra Research Corporation

T. Abitbol, S. A. Kedzior, E. Niinivaara, M. S. Reid, *Organizers*

M. Reid, *Presiding*

1:15 Introductory Remarks.

1:20 CELL 480. Bionanomaterials derived from carboxy cellulose nanofibers- Al^{+3} composite for effective removal of fluoride from water. **S. Sharma**, P.R. Sharma, K.I. Johnson, B.S. Hsiao

1:45 CELL 481. Removal of emerging pollutants from water using cellulose nanofibrils derived from deep eutectic solvents. **T. Selkälä**, T. Suopajärvi, J.A. Sirvio, H. Liimatainen

2:10 CELL 482. Withdrawn

2:35 CELL 483. Surface-carboxylated nanocellulose as a crystalline polysaccharide catalyst for acetal hydrolysis and acid–base tandem reaction. **K. Kanomata**, Y. Hirayama, Y. Tamura, T. Kitaoka

3:00 Intermission.

3:15 CELL 484. Nanocellulose aerogels for CO₂ capture. Y. Li, K. Martin, J. Wassgren, **K.R. Carter**

3:40 CELL 485. GISAS study of spray deposited metal precursor ink on a cellulose template. **C. Brett**, N. Mittal, W. Ohm, D. Söderberg, S. Roth



TECHNICAL PROGRAM

4:05 CELL 486. Tailored PISA-latexes for modification of nanocellulosics: Investigating compatibilizing and plasticizing effects. **J. Engstrom**, F. Hatton, T. Benselfelt, C. Freire, C. Vilela, A. Boujemaoui, C. Cobo Sanchez, G. Lo Re, L. Wagberg, F. D'Agosto, M. Lansalot, A.E. Carlmark, E.E. Malmstrom

4:30 CELL 487. Large-scale processing of nanocellulose into films and coatings: Challenges and prospects. **V. Kumar**, H. Kangas

4:55 Concluding Remarks.

Section B

Orange County Convention Center
Room W224H

Additive Manufacturing of Bio-based & Renewable Materials

Cosponsored by AGRO, ANYL and BIOL
Financially supported by EPNOE
M. Bortner, G. Siqueira, *Organizers, Presiding*

1:15 Introductory remarks.

1:20 CELL 488. 3D printed wood. **D. Kam**, M. Layani, O. Shoseyov, S. Magdassi

1:45 CELL 489. 3D printed nanocellulose scaffolds designed for biomedical applications. **S. Sultan**, A. Mathew

2:10 CELL 490. 3D Bioprinting of soft tissues using nanocellulose-based cell instructive bioinks. **E. Karabulut**, L. Strid Orrhult, P. Gatenholm

2:35 CELL 491. Isosorbide-based low viscosity resins for additive manufacturing applications. **J.H. Vergara**, D. Bolarin, J. La Scala, G.R. Palmese

3:00 Intermission.

3:15 CELL 492. 3D-printing of nano-polysaccharide/collagen composite bioink. **M. Loste-Berdot**, A. Denneulin, D. Beneventi, J. Bras, D. LeCorre-Bordes

3:40 CELL 493. Evaluating the processing of keratin-based copolymer systems into 4D responsive materials. M. Plowman Holmes, S. Scott, **W.J. Grigsby**

4:05 CELL 494. Confinement and alignment of miscible amorphous lignin in polypropylene and polyethylene by 3D-printing and melt-spinning. **N.A. Nguyen**, C. Bowland, J.K. Keum, A.X. Staub, L.T. Kearney, J.L. Long, A.K. Naskar

4:30 CELL 495. Cellulosic structures for magnetoactive and electroactive printed applications. **E. Lizundia**, C. Costa, P. Martins, S. Lanceros-Mendez

4:55 Concluding remarks.

Section C



TECHNICAL PROGRAM

Orange County Convention Center
Room W225A

Bio-Based Gels & Porous Materials

Gels, Aerogels & Carbogels

Cosponsored by ANYL, BIOL and COLL
Financially supported by EPNOE
T. Budtova, F. Liebner, *Organizers*
R. Liu, A. Silvestre, *Presiding*

1:15 Introductory Remarks.

1:20 **CELL 496.** Self-healing, *in situ* forming chitosan-hydroxypropyl polysaccharide-based hydrogels with tunable modulus. **J. Chen**, B.L. Nichols, K.J. Edgar

1:45 **CELL 497.** Composite silk-glycolipid hydrogels: symbiosis or simple coexistence? **A. Lassenberger**, N. Baccile

2:10 **CELL 498.** Gelation of sodium alginate aqueous solution. **R. Liu**, H. Kang

2:35 **CELL 499.** Effect of depletion forces on the morphological structure of carboxymethyl cellulose and micro/nano cellulose fiber suspensions. S.F. Souza, M. Mariano, M.A. de Farias, **J. Bernardes**

3:00 Intermission.

3:15 **CELL 500.** Thermally reversible hemicellulose-based networks: Synthesis and characterization. **R.A. Venditti**, W. Farhat, A. Ayoub, F. Becquart, N. Mignard

3:40 **CELL 501.** Photo-degradable bio-based gels as platforms for electrical conductivity. **S. Agate**, L.A. Lucia, L. Pal

4:05 **CELL 502.** Nanocellulose hydrogels for electrophoresis. L. Mendoza, T. Gunawardhana, W. Batchelor, **G. Garnier**

4:30 **CELL 503.** Enzymatic actuation of gelatin bilayers. **L. Hanzly**, J.R. Barone

4:55 Concluding remarks.

Section D

Orange County Convention Center
Room W225B

Valorization of Renewable Resources & Residuals into New Materials & Multiphase Systems

Cosponsored by AGRO and ANYL
Financially supported by EPNOE
M. L. Auad, J. Campos-Teran, O. J. Rojas, *Organizers*
I. Vega Erramuspe, *Presiding*



TECHNICAL PROGRAM

1:15 Introductory Remarks.

1:20 **CELL 504.** Piezoelectricity of cellulose: Myths and facts. **S. Kim**

1:45 **CELL 505.** Propargylation and azidation of chitosan-cellulose pearls as a template for clickable substrates. **I. Vega Erramuspe**, D. Gomez-Maldonado, I. Filpponen, M.L. Auad, M.S. Peresin

2:10 **CELL 506.** Mesomorphic behavior of cellulose nanocrystal films prepared from different electrolyte solutions. **S. Jin**, R.J. Spontak, S. Khan, O. Rojas

2:35 **CELL 507.** Elephantidae manure and biogas residue as potential raw material for the extraction of cellulose. **K. Weiland**, A. Mautner, J. Lizasoain Arteaga, A. Bauer, A. Bismarck

3:00 Intermission.

3:15 **CELL 508.** Upcycling of paper mill sludge into cellulose fibres by ionic liquid dissolution and dry-jet wet spinning. **S.J. Eichhorn**, C. Adu, C. Zhu, A. Koutsomitopoulou, K. Potter, M. Jolly

3:40 **CELL 509.** Hybrid films of cellulose nanofibers and lignin particles for advanced applications. **E. Pasquier**, J. Bras, O. Rojas

4:05 **CELL 510.** Hydrophobic and antibacterial textile fibres prepared by covalently attaching betulin to cellulose. **T. Huang**, C. Chen, D. Li, M.K. Ek

4:30 **CELL 511.** Multilayered nanocellulose based systems for skin regeneration. **C.R. Freire**, D. Fonseca, C. Vilela, A. Silvestre

4:55 Concluding Remarks.

Section E

Orange County Convention Center
Room W230D

Wood-Based Polymers: From Functional Structures to Applications

Films & Fibers

Cosponsored by ANYL
Financially supported by EPNOE Lenzing AG
M. Ek, T. Nypelo, J. O. Zoppe, *Organizers*
I. Filpponen, S. Spirk, *Organizers, Presiding*

1:15 Introductory Remarks.

1:20 **CELL 512.** Surface modification of CNF films by roll-to-roll nanoimprinting and plasma deposition. **A. Khakalo**, T. Mäkelä, H. Orelma, T. Tammelin

1:45 **CELL 513.** Hybridization of nanocelluloses for improved nanopaper properties. **F.F. Mayer**, A. Mautner, K. Lee, A. Bismarck



TECHNICAL PROGRAM

2:10 CELL 514. Is it possible for lignin molecules to become oriented during processing? **M. Cho**, F.K. Ko, S. Renneckar

2:35 CELL 515. Multilayer density analysis of cellulose thin films. **C. Sampl**, K. Niegelhell, K. Kontturi, R. Resel, U. Hirn, S. Spirk

3:00 Intermission.

3:15 CELL 516. Aqueous processing of all cellulose blend thin films. **M. Weißl**, M. Hobisch, C. Sampl, L. Johansson, K. Hettrich, E. Kontturi, B. Volkert, S. Spirk

3:40 CELL 517. Self-assembled filaments from deacetylated chitin nanofibers and sodium alginate obtained by interfacial complexation. **R. Grande**, L. Bai, L. Wang, W. Xiang, A.J. Carvalho, O. Rojas

4:05 CELL 518. Janus-type nanorods by surface-initiated polymer grafting from the reducing end-groups of cellulose nanocrystals. **K. Heise**, M. Kostianen, E. Kontturi

4:30 CELL 519. Visualizing acid hydrolysis of cellulose nanofibers by hydrogen chloride gas. **P. Spiliopoulos**, T. Pääkkönen, S. Spirk, E. Kontturi

4:55 Concluding Remarks.

CHED

Division of Chemical Education

A. Cannon, D. Bromfield-Lee and I. Levy, *Program Chairs*

SUNDAY MORNING

Section A

Orange County Convention Center
Room W315A

Chemistry Teachers Day Program

S. C. Rukes, *Organizer*
M. Mury, *Presiding*

8:00 Registration.

8:30 Introductory Remarks.



TECHNICAL PROGRAM

8:35 CHED 1. Chemistry and the final frontier: Student designed sustainable payloads at the edge of space. **L.J. Doody**

9:05 CHED 2. Elements of paper science: Material for teaching chemistry. **D. Keller**

9:50 CHED 3. Viral videos as teaching tools. **R.M. Burks**

10:20 Intermission.

10:30 CHED 4. What's in a name? Possibly death and taxes! **R. Hartshorn**

10:55 CHED 5. Geography of the periodic table. **C.J. Giunta, J.L. Marshall**

11:20 CHED 6. AACT and the IYPT. **S.C. Rukes**

11:35 Concluding Remarks.

Section B

Orange County Convention Center
Room W312A

Strategies Promoting Success of Two-Year College Students

Cosponsored by CTA

A. M. Palmer, *Organizer*

L. J. Anna, V. L. Miller, K. S. Owens, *Organizers, Presiding*

A. Palmer, *Presiding*

8:30 Introductory Remarks.

8:35 CHED 7. Mobile Galaga-style game as a teaching supplement for Chemistry. **V. Flaris**

8:55 CHED 8. Crossing disciplines with threshold concepts in chemistry. **K.S. Owens, A.J. Murkowski**

9:15 CHED 9. Increasing motivation and retention for general chemistry generation Z students in University of Puerto Rico-Bayamón (UPRB). **H. Felix, W. Ortiz, M. Chevres, J. Olavarria, O.M. Primera**

9:35 Intermission.

9:45 CHED 10. Challenges and successes with implementing a revised authentic curriculum in an introductory chemistry course at a community college. **B. Ngo, V.I. Jaramillo**

10:05 CHED 11. Innovate & invest: Building a successful organic chemistry program at a two-year regional campus. **R.J. Yoder**

10:25 CHED 12. Fostering transfer student success in chemistry through inter-institutional curriculum alignment. **H. Oonge, L.B. Sessions, T.A. Dorman, Z. Li**



TECHNICAL PROGRAM

10:45 CHED 13. Establishment of a grad-school modeled research group at a community college: who would have thought? **R. Silvestri**

11:05 Concluding Remarks.

Section C

Orange County Convention Center
Room W312B

NMR Spectroscopy in the Undergraduate Curriculum

Financially supported by Bruker BioSpin, JEOL, MESTRELAB Research, Anasazi Instruments
D. P. Soulsby, A. S. Wallner, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 CHED 14. Teaching heteronuclear fluorine spectroscopy in the undergraduate teaching laboratory. **R.A. Dohoney**, S.M. Schelble

8:55 CHED 15. Broadening the undergraduate NMR experience: An in-class activity focused on NMR spectra containing NMR-active heteronuclei. **S.S. Rocks**

9:15 CHED 16. Electrophilic fluorination of aromatics: The use of ^{19}F -NMR spectra for the analysis of mixtures. **M.L. Druelinger**, D.L. Dillon

9:35 Intermission.

9:50 CHED 17. NMR spectroscopy as a component of an advanced organic laboratory project. C.J. Hull-Crew, M.N. Trujillo, A.D. Outlaw, C.M. Clements, A.A. Zeller, L.J. Taylor, K.A. Stewart, **A.M. Schoffstall**

10:10 CHED 18. Experimental approach to teaching hybridization: Hybridization does not determine internal bond angles. **D.D. Clarke**

10:30 Concluding Remarks.

Section D

Orange County Convention Center
Room W311A

Active Learning in Organic Chemistry

J. L. Muzyka, *Organizer*
A. Leontyev, *Organizer, Presiding*

8:30 Introductory Remarks.



TECHNICAL PROGRAM

8:35 CHED 19. Using clickers for peer instruction in weekly discussion sessions of a large-enrollment course of organic chemistry. **D. Cruz-Ramirez de Arellano**

8:55 CHED 20. Using clicker questions and small group discussions to foster an active learning environment in the organic chemistry lecture.. **S.P. Hickey**

9:15 CHED 21. Role of iOS and Android mobile apps in teaching and learning of organic chemistry. **G. Naik**

9:35 Intermission.

9:40 CHED 22. Short videos as a tool to teach problem solving in a Large Undergraduate Organic Chemistry Class: A multi-semester study of student attitudes and approaches. **R.R. Srinivasan, J. Su, W. Kong**

10:00 CHED 23. Using short videos to regularly review common misconceptions: A change inspired by the cWCSC *Active Learning in Organic Chemistry*. **R. DeCicco**

10:20 CHED 24. Flippin Fridays: Active learning in organic chemistry. **D.T. Esterline**

10:40 CHED 25. Full vs. partial flip: A comparison of two active learning pedagogies in organic chemistry. **G.E. Rudd, M. Anzovino**

11:00 CHED 26. Hybrid learning in large and small organic chemistry lectures. **C.G. McDaniel**

11:20 Intermission.

11:25 CHED 27. Evaluation of a peer-led team learning-blended classroom reform on student success in large organic chemistry courses. **J. Mutanyatta-Comar**

11:45 CHED 28. Using "*mechanism as a class*" activities to move students from novice toward expert thinking. **K.N. Cossey**

12:05 CHED 29. Peer instruction and peer review in an upper-level organic reaction mechanism class. **K. Masters**

Section E

Orange County Convention Center
Room W311B

Advances in e-Learning, Digital Learning & Online Education

D. A. Canelas, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 CHED 30. Activating blended learning approaches in two freshmen chemistry courses. **M. Wijtmans, D. Scholten, S. Dekker, C. Vos, M. Siderius, J. van Muijlwijk-Koezen**



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

8:55 CHED 31. Comparison of course modalities for a fundamental chemistry course using novel multimedia instruction. **N. Lapeyrouse**, C. Yestrebky

9:15 CHED 32. Engaging students with multiple problem-solving pathways for complex problems. **E. Yuriev**, J. Burton, S. Devine, K. Vo, S. Maher, C. Thompson, M. Scanlon

9:35 Intermission.

9:45 CHED 33. Interactive e-book introduces new ways to teach and learn general chemistry. **L.R. Stepan**, M.J. Bojan, P. Maslak

10:05 CHED 34. Impact of distance learning & hybrid teaching cCWCS workshop on our chemistry online course. **S. Svojanovsky**

10:25 CHED 35. Teaching chemistry with evolving virtual platforms: Celebrations and challenges. **D.A. Canelas**

10:45 Concluding Remarks.

Section F

Orange County Convention Center
Room W311C

International Perspectives on Chemistry Education & Olympiads

Cosponsored by IAC

A. Leontyev, A. Nakamura, *Organizers*
W. E. Schatzberg, *Organizer, Presiding*
R. M. Kelly, A. Leontyev, *Presiding*

8:30 Introductory Remarks.

8:35 CHED 36. Comparison of similarities and differences in chemistry undergraduate education between US and Indian institutions: Experiences from a Fulbright US Scholar program. **S. Raje**

8:55 CHED 37. Same or not the same: Chemistry learning, teaching, and researching abroad. **R. Romero Chacon, S. Sandi-Urena**

9:15 CHED 38. Interactive strategies implementation to promote attention, interest and generation of explanations in large enrollment general chemistry courses. **B. Fernandez Solano**, S. Sandi

9:35 CHED 39. Incorporating international scientific research into teaching high school science. **B.M. Volbers**, J. Toth, D. Lacks, R. Sankaran, J. Zhou, L. Xie

9:55 Intermission.

10:05 CHED 40. Internet in a Box meets LibreText: Bringing OER web content to the chemistry classroom in regions without broadband.. **R.E. Belford**, A. Holt, M.A. Walker, D.S. Larsen



TECHNICAL PROGRAM

10:25 CHED 41. Student perception of multiple-choice General Chemistry exams and its influence in the teaching-learning process at the University of Costa Rica. **E.N. Jimenez-Alvarado**

10:45 CHED 42. Upcoming international conferences in chemistry education in 2019. **W.E. Schatzberg**

11:05 Intermission.

11:15 CHED 43. Chemistry Olympiad training: Finding balance between scientific education, motivation and excitement. **C.A. Saber**

11:35 CHED 44. Costa Rican chemistry olympiad: Opportunity to motivate high school female students into STEM careers. **L.Y. Robles**, I.F. Cespedes-Camacho, R. Coy-Herrera, A. Sanchez-Kopper

11:55 Concluding Remarks.

Section G

Orange County Convention Center
Room W311D

Underrepresented Minority Groups in Chemistry Education

R. E. Gibbons, G. Rocabado, *Organizers, Presiding*

8:30 Introductory Remarks.

8:50 CHED 45. Harnessing oral and gustatory senses for the chemical education of students with visual impairments.. **B.F. Shaw**

9:10 CHED 46. Peer mentoring, faculty advising, and incorporation into research as tools for improving retention and student outcome in the sciences. **N.E. Leadbeater**

9:30 CHED 47. Novel supplemental instruction model for supporting underrepresented STEM students at an open access institution. **C.L. Anfuso**, B. Shepler, R. Simmons, C. Achat-Mendes, J. Awong-Taylor, J. Curry Savage, S. Dekhane, J. Hurst-Kennedy, C. Johnson, T. Leader, K. Pinzon, E. Sudduth

9:50 Intermission.

10:10 CHED 48. Being black and being a chemistry person: Parallel development of students' identities. **G.J. O'Dell**, N.S. Stephenson, J.H. Carmel

10:30 CHED 49. Understanding the relationship between attitude and achievement in organic chemistry classrooms using reciprocal causation modeling for Hispanic female students. **G. Rocabado, J.E. Lewis**

10:50 CHED 50. Exploring students' self-efficacy and its relationship with the teaching and learning of chemistry in a very diverse general chemistry course. **S. Villafane-Garcia**

11:10 Discussion.



TECHNICAL PROGRAM

11:40 Concluding Remarks.

Section H

Orange County Convention Center
Room W311E

Undergraduate Research Papers

J. V. Ruppel, N. L. Snyder, *Organizers*
C. V. Gauthier, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 CHED 51. The remarkable reaction between a terbium(III) complex and aqueous HCl, and it's equally remarkable reversibility. **A.S. Daniels**, K. Schulen, L.A. Ligon, J.J. Stace

8:45 CHED 52. Europium(III) coordinated to tetracycline derivatives as potential bioprobes. **T. Cabrerros**, G. Muller

8:55 CHED 53. Structural characterization of hemoglobin-nitrosoalkane complexes. **K.Y. Prather**, S. Powell, V.E. Herrera, N.T. Nguyen, G.B. Richter-Addo

9:05 CHED 54. Alkoxy-substituted diphenyl-porphyrin synthesis utilizing palladium-catalyzed C-O cross coupling. **D.V. Shchirov**, C.F. Dixon, J.V. Ruppel

9:15 CHED 55. Polynuclear ruthenium organometallic complexes induce DNA damage in cells repaired by the nucleotide excision repair pathways. **O. Fast**, B. Gentry, L. Strouth, M. Niece, F.A. Beckford, S.M. Shell

9:25 CHED 56. Toward efficient molecular catalysis: An investigation into soft-donor biomimetic complexes. **C. Phipps**

9:35 Intermission.

9:45 CHED 57. Metal decorporation: Building blocks for amino acid-derived chelants. **B.M. Jones**, B.I. Jackson, K.J. Friedrich

9:55 CHED 58. Synthesis of flavonols for CO release. **R. Dean**, A. Petrillo, W.E. Lynch, B.P. Quillian, S. Zingales

10:05 CHED 59. Improving the synthesis of selenium- and tellurium-containing tryptophan amino acid analogs. **M.C. Barber**, D.M. Hatch, R. Martí-Arbona, L.A. Silks

10:15 CHED 60. Understanding the iron(III)-induced sol-gel transition of gum arabic suspensions. **B. Hacha**, M. Columbia

10:25 CHED 61. Cooperative catalytic hydrolysis using a dinuclear metalloenzyme mimic. **T.B. Best**, A. Lajmi, M. Gulsby, L. Carroll, S. Peyer

10:35 CHED 62. Synthesis of variable sized silver for the binding of drug derivatives. **A.N. Eubanks**, P.J. Rosado

10:45 Intermission.



TECHNICAL PROGRAM

10:55 CHED 63. Preparation of surface-grafted poly(3-hexylthiophene) brushes using an easily cleavable self-assembled monolayer. **K. Campbell**, P. Lundin

11:05 CHED 64. Plasmon-free surface-enhanced Raman spectroscopy on TiO₂-graphene oxide inverse opal substrates. **L.E. Perez**, E.J. Atkinson

11:15 CHED 65. Withdrawn

11:25 CHED 66. Semi-empirical method parameter optimization for rovibrational spectra calculations on small interstellar hydrocarbons. **J. Arend**, J.P. Layfield

11:35 CHED 67. Optimization polarizing agents for scalar overhauser DNP at 14.1 T. **N. Harmon**, T. Dubroca, E. Megiel, J. van Tol, S. Hill

11:45 CHED 68. Mechanism of decomposition of protonated methionine: A computational study. **D. Devore**, J. Johnston, P.B. Armentrout

11:55 Concluding Remarks.

SUNDAY AFTERNOON

Section A

Orange County Convention Center
Room W315A

Chemistry Teachers Day Program

S. C. Rukes, *Organizer*
M. Mury, *Presiding*

1:00 Introductory Remarks.

1:05 CHED 69. **Award Address** (James Bryant Conant Award in High School Chemistry Teaching sponsored by the Journal of Chemical Education and ChemEd X). Elements of a thermodynamically favorable classroom. **D.C. Wood**

1:55 CHED 70. Take home labs: Taking science beyond the classroom. **A. Modic**

2:35 Intermission.

2:45 CHED 71. Supporting and assessing molecular-level sensemaking. R. Stowe, **J. Carmel**

3:35 CHED 72. Simple, hands-on activities from ChemEdX. **E. Posthuma-Adams, T.S. Kuntzleman**

Section B

Orange County Convention Center
Room W312A



TECHNICAL PROGRAM

Strategies Promoting Success of Two-Year College Students

Cosponsored by CTA

A. M. Palmer, *Organizer*

L. J. Anna, V. L. Miller, K. S. Owens, *Organizers, Presiding*

A. Palmer, *Presiding*

1:30 Introductory Remarks.

1:35 CHED 73. Correlation of study skills and student success in general chemistry. **A.M. Palmer**, O. Kutai

1:55 CHED 74. How high impact practices build attachment to increase persistence. **B.M. Fetterly**

2:15 CHED 75. Trying on teaching for student success: The Learning Assistant Program at a two-year college. **C.P. Schick**

2:35 Intermission.

3:25 CHED 76. Never underestimate the power of a strong sense of belonging. **A.J. Sanders**, E. Buyuktanir

3:45 Concluding Remarks.

Section C

Orange County Convention Center

Room W312B

NMR Spectroscopy in the Undergraduate Curriculum

Financially supported by Bruker BioSpin, JEOL, MESTRELAB Research, Anasazi Instruments

D. P. Soulsby, A. S. Wallner, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 CHED 77. Sharing NMR data in the cloud: Expanding the opportunities for learning in the undergraduate laboratory. **D.P. Soulsby**

1:55 CHED 78. Microwave-promoted reduction of aldehydes and ketones: Incorporation of benchtop NMR into multi-outcome experiment. **M. Zhang**, R.W. Morrison

2:15 CHED 79. Utilizing 2D NMR in the characterization of unknown organic compounds in second-year organic chemistry. **A. Anderson-Wile**, T.C. Celius

2:35 Intermission.

2:50 CHED 80. NMR analysis of essential oils: An adaptable (and fragrant!) laboratory experiment. **L.E. Parmentier**, **K. Jansen Labby**



TECHNICAL PROGRAM

3:10 CHED 81. ¹H NMR investigation of acid-catalyzed enolization of acetophenones. **N.M. Wachter**, H. Tarbox

3:30 CHED 82. Beginners Guide to qNMR: Introduction of qNMR to undergraduates. **J. Araneda**, S. Riegel, T. Chu

3:50 Concluding Remarks.

Section D

Orange County Convention Center
Room W311A

Active Learning in Organic Chemistry

J. L. Muzyka, *Organizer*
A. Leontyev, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 CHED 83. NMR spectroscopy as a predictor of reactivity: A guided inquiry experience in an organic chemistry lab. **I. Larraza**, S. Jahjah, M. Harrison

1:55 CHED 84. Progressive Learning in the Laboratory of Organic Chemistry II. A new perspective in Costa Rica. **C.A. Arias**

2:15 CHED 85. Towards student success: A multistep synthesis based organic chemistry teaching laboratory. **G. Pour**, A. Reed, R. Sapia

2:35 Intermission.

2:45 CHED 86. Exam wrappers in organic chemistry. **S. Zingales**

3:05 CHED 87. Increasing student engagement in organic chemistry courses: Project based opportunities. **A. Frazer**, E. Loe, R. Murray

3:25 CHED 88. Practice makes . . . great organic students: Giving the power of learning back to the students. **K.N. Cossey**

3:45 CHED 89. Minimizing PowerPoints, maximizing discussions in organic chemistry class meetings. **K. Masters**

4:05 Intermission.

4:15 CHED 90. Investigating student misconceptions in solving spectroscopy problems (NMR & IR) in undergraduate organic chemistry laboratory courses. **M. Chatterjee**

4:35 CHED 91. How do learner beliefs about knowledge affect performance in an active-learning organic chemistry class? **D.A. Canelas**, M. Barger, A. Perez, L. Linnenbrink-Garcia

4:55 CHED 92. Electronic and steric effects: Gateway to making organic chemistry resonate with students. **M. Ilies**



TECHNICAL PROGRAM

5:15 Concluding Remarks.

Section E

Orange County Convention Center
Room W311B

Advances in e-Learning, Digital Learning & Online Education

D. A. Canelas, *Organizer*
M. Gallardo-Williams, *Presiding*

1:30 Introductory Remarks.

1:35 **CHED 93.** Development of an online non-majors laboratory course on the science of food and cooking. M.L. Mislevy, I.J. Rhile

1:55 **CHED 94.** Incorporation of a project-based lab curriculum into hybrid and online chemistry labs for non-science majors. U. Swamy, J. Vihlen, J. Carmel

2:15 **CHED 95.** Realistic immersive virtual reality organic chemistry laboratory experiences. M.T. Gallardo-Williams, C. Dunnagan

2:35 Intermission.

2:45 **CHED 96.** On-line and on-the-ground science of food and drink. R.M. Hyde

3:05 **CHED 97.** Integration of Hypothes.is social annotations systems into LibreText. R.E. Belford, D.S. Larsen

3:25 Concluding Remarks.

Section F

Orange County Convention Center
Room W311C

Green and Sustainable Chemistry Theory & Practice: Chemistry for New Frontiers

Cosponsored by CEI
Financially supported by ACS Green Chemistry Institute; I&EC Green Chemistry Subdivision
E. J. Brush, J. E. Wissinger, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 **CHED 98.** Incorporating green chemistry into organic chemistry laboratory curriculum: Strategies, challenges and successes. I.B. Nejad



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

1:55 CHED 99. Green chemistry at Seton Hall University: A new department-wide initiative. **D.A. Laviska**, R.L. Augustine, W.R. Murphy, S.K. Tanielyan, **C.E. Marzabadi**

2:15 CHED 100. Improving students' chemistry self-efficacy and motivation through a digital learning activity on phosphate sustainability. **O. Gulacar**, S. Burke, A. Nabavizadeh, C. Zowada, I. Eilks

2:35 CHED 101. Ligand-free palladium-nanoparticle catalyzed Suzuki and Heck cross-coupling reactions: Creating a modernized and greener laboratory experience for undergraduate organic chemistry curricula. **C.C. Rounds**, M. Jaskula-Dybka, N. Filian, D.P. Jamieson

2:55 Intermission.

3:05 CHED 102. High school - college collaboration using the ACS Science Coaches program: A successful model. S.P. Kosmas, **M.A. Benvenuto**

3:25 CHED 103. Exposing high school students to sustainability concepts: An engaging green chemistry think tank. **S. Foster**, G. Bonomo, M. Gillett-Kunnath, K. Ruhlandt-Senge

3:45 CHED 104. Chemical principles in public policy, and vice versa. **J.D. Soper**

4:05 Intermission.

4:15 CHED 105. Teaching Green Chemistry along with Polymers: A natural combination! **W.R. Winchester**, D.G. Kovacs

4:35 CHED 106. Green chemistry commitment: Progress report and future directions. **A.S. Cannon**, I.J. Levy, D. Ward

Section G

Orange County Convention Center
Room W311D

Underrepresented Minority Groups in Chemistry Education

R. E. Gibbons, G. Rocabado, *Organizers, Presiding*

1:30 Introductory Remarks.

1:40 CHED 107. Nelson Diversity Surveys: Quantifying underrepresented groups in STEM faculty at research universities, disaggregated by race/ethnicity, by rank, and by gender. **D.J. Nelson**

2:20 CHED 108. Introducing diversity in a chemistry classroom. **K.R. Ries**, Z.L. Mensinger

2:40 Intermission.

2:55 CHED 109. Breaking the language barrier: Equitable assessment in general chemistry. **E.N. Lee**, M. Orgill

3:15 CHED 110. Specifications grading with a diverse chemistry student population. **M. Anzovino**, **D. Behmke**, T. Gluick, **M.S. Morton**, M. Tsoi, O. Villanueva, C.M. Woodbridge



TECHNICAL PROGRAM

3:35 Intermission.

3:45 CHED 111. Birds of a feather: An exploratory study of the effects of similarity with peer-leaders. V.L. Rhodes, E.S. Pietri, L. Ashburn-Nardo, **P. Varma-Nelson**

4:05 CHED 112. Who is underrepresented? **R.E. Gibbons**, G. Rocabado

4:25 Discussion.

4:55 Concluding Remarks.

Section H

Orange County Convention Center
Room W311E

Undergraduate Research Papers

C. V. Gauthier, N. L. Snyder, *Organizers*
J. V. Ruppel, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 CHED 113. Development of new carbohydrate analogs for studying the role of galectins in tumor migration. **E.J. McLaren**, N.L. Snyder

1:45 CHED 114. Synthesis and evaluation of fused tricyclic ring scaffolds with antibiotic adjuvant activity in Methicillin-resistant *Staphylococcus aureus* (MRSA). **N. Cutrona**, R. Berndsen, N. Kirby, H.B. Miller, M.S. Blackledge

1:55 CHED 115. Design and synthesis of dipeptide-boronic acid gelators. **A.S. York**

2:05 CHED 116. Force generation and encapsulation of fluorophores in swellable organically modified silica. **R. Reffner**, P.A. Bonvallet, R. Silvestri

2:15 CHED 117. Antimicrobial properties of menthol and its derivatives. **K.L. Scrudgers**, N. Beres

2:25 Intermission.

2:35 CHED 118. Semi-synthesis of (–)-melodinine K via chemical and biological routes. **T.M. Tran**, M. Walia, A. Gardner, C. Teijaro, R.B. Andrade, S. O'Connor

2:45 CHED 119. Rapid synthesis of N,N-di-(4-chlorobenzyl)-N-methylamine. **T.A. Skinner**, L.I. Bobyleva, M.M. Bobylev

2:55 CHED 120. Optimization of initial steps in the synthesis of poly(2,5-bis(3-(heptyloxy)propyl)-1,4-phenylene vinylene) (PHOPPV). **Y. Tran**, J. Nguyen, C.A. Young

3:05 CHED 121. Synthesis and characterization of angled aromatic diimides. **K.A. Stellmach**, D.D. Cao



TECHNICAL PROGRAM

3:15 CHED 122. Synthesis of isoquinoline alkaloids via Suzuki coupling reaction mediated by microwave chemistry. **C. Gettridge**, F.L. Payton, B. Kang, T. Luster

3:25 Intermission.

3:35 CHED 123. Efficient and sustainable synthesis of novel four-armed cores for dendrimers and other branched macromolecules. **C.T. Burgin**, A.M. Baliya

3:45 CHED 124. Microwave assisted, gold-catalyzed Ritter-type reaction of benzylic alcohols. **J. Scott**, I. Levesque, S. Acosta, R.G. Iafe

3:55 CHED 125. Isomers of tricyanofuran-type metastable-state photoacids: A mixed theoretical and experimental approach. **J.E. Arias**, D. Richardson, E. Romero, P.K. Patel, K.Y. Chumbimuni Torres

4:05 CHED 126. Heterocyclic ferrocenyl chalcones salts derivatives as potential anticancer and antioxidant candidates. **G. Duran Camacho**, S. Delgado-Rivera, A. Baerga-Ortiz, I. Montes-Gonzalez

4:15 Concluding Remarks.

SUNDAY EVENING

Section A

Orange County Convention Center
West Hall C

General Posters

7:00 - 9:00

CHED 127. Biennial Conference on Chemical Education: A place to share information about the teaching and learning of chemistry. **J.M. Sophos**, J. Carmel, R.S. Cole, S.J. Donnelly, I.J. Levy, S.R. Mooring, B. Murray, M. Orgill, A. Putti, C. Sorensen-Unruh, D.G. Sykes, V.M. Williamson

CHED 128. Celebrating the international year of the periodic table with [P][Er][I][O][D][I][C] [Po][Es][Y] [Co][N][Te][S][T]. **Q. Dougherty**, **L. Atlas**, **V. Ganss**, H. Gordon, D. McGibbon, A.H. Kjellson, **I.J. Levy**

CHED 129. Analysis of 125 STEM scholarship websites; Looking for common themes and identifying successful ways to promote STEM careers. **G.D. Phelan**

CHED 130. Exploring STEM teaching: Being a learning assistant at a two-year college. **C.P. Schick**, K. Reimer, S.L. Bontems

CHED 131. EASE: A pre-matriculation intensive research experience to promote student success and retention in STEM. **K.N. Crowder**, D.M. Baker

CHED 132. Importance of contextualized STEM education in the 'fake news' era. **B.D. Fahman**



TECHNICAL PROGRAM

- CHED 133.** Improving STEM retention at a liberal arts college: Retention analysis of Scots Science scholars. **A.D. Gibson**, M. Siopsis
- CHED 134.** UTM STEM Academy: A summer bridge program for UTM S-STEM scholars. **R. Montgomery**, B. Bradley, J. DeVito, M. Gibson, P.A. Shelton, R. Witmer
- CHED 135.** National Science Foundation programs that support chemistry education. **J.E. Lewis, D. Rickey**
- CHED 136.** Exploring students' attitudes and identities in a non-STEM majors chemistry laboratory. **J. Vihlen**, N.S. Stephenson, U. Swamy, J.H. Carmel
- CHED 137.** Green chemistry commitment. **I.J. Levy**, A.S. Cannon, D. Ward
- CHED 138.** Content analysis of green chemistry concepts in organic chemistry textbooks and laboratory manuals. **A. Leontyev**
- CHED 139.** Explorations of the synthesis of 2,5-Dimethyl-1-phenylpyrrole derivatives in undergraduate organic chemistry laboratory. **C. Wu, X. Fan**
- CHED 140.** Does supplemental instruction help students learn organic chemistry? **J.A. Jenson**, T. Cornett, R.L. Claus, H. Bascal
- CHED 141.** Esterification reaction using heterogeneous catalyst: Development of a laboratory experiment for undergraduate analytical/organic chemistry students. **L. Brown**, M. Cox, B. Mondal, A.S. Manchanda
- CHED 142.** Project based opportunities in organic chemistry education. **A. Frazer**, E. Loe, R. Murray
- CHED 143.** Is flipping the second semester organic chemistry classroom an effective way to increase student learning? **K.S. Taylor**, D.W. Holley, B. Smith
- CHED 144.** Acid/base extraction coupled with chemical ionization mass spectrometry as an introductory organic chemistry laboratory experiment. **T.W. Nalli**, T.L. Collier
- CHED 145.** Development of a mastery-based tool to reinforce the retention of skills and concepts in organic chemistry. **W.E. Brenzovich**, W.G. Hollis, E.E. Hardy
- CHED 146.** Modern technology in the organic chemistry classroom: online components and clickers and apps, oh my! **S.K. Hamilton**
- CHED 147.** Overcoming challenges teaching online organic chemistry. **B. Weintraub**
- CHED 148.** Use of the Pope Engagement Index to measure cognitive load of organic chemistry modeling activities. **J. Calvert**, V. Williamson, C. Terrell, A. Randolph, K.J. Linenberger Cortes
- CHED 149.** Teaching using distributed active learning for long-term retention in the organic chemistry lecture. **L.G. Habgood, J. Patrone, J.S. Queen**
- CHED 150.** Design and implementation chemistry curriculum for police officers and fire fighters. **P.K. Yuen**, C. Lau, A. Yuen



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- CHED 151.** Communicating chemistry to the public through art in a senior chemistry seminar course. **E. Osborne**
- CHED 152.** Flipping the switch: Insights gained on how to retain chemistry majors. **A.J. Casanova**, N.S. Stephenson, J.H. Carmel
- CHED 153.** Retaining and preparing student scholars. **J.M. Esson**, D. Robertson, A. Nenciu
- CHED 154.** Attempting to find the most accurate clustering method for chemistry education research: Simulating 3.6 million cluster analyses. **J. Harshman**, A. McDevitt, Q. Cui, A. Kolarkar
- CHED 155.** Providing context for the undergraduate chemistry degree in an upper level elective course titled: History of Chemistry, A Materials Perspective. **G.D. Claycomb**
- CHED 156.** Investigative comparison between drinking water quality and socioeconomic status in Los Angeles County. **H. Hakopian, M. Hasan, V.I. Jaramillo**
- CHED 157.** Molecules and *machine learning (ML)*: Images classified by ML used as *input to an augmented reality app* for chemistry education. **D. Behmke**, E. Brannock, D. Kerven, R. Lutz, J.E. Barker Paredes, R. Pennington, D. Doghaimat, N. Tyner, C. Maldonado, J. Anderson, T. Moses
- CHED 158.** Psychometric investigation of the Revised Approaches to Teaching Inventory (R-ATI). **T.C. Pentecost**, R. Komperda, R. Pearson
- CHED 159.** Three-dimensional visualization of kinase inhibitors: Correlating foundational concepts to therapeutic application. **S.R. Kurup**
- CHED 160.** Design and implementation of a bacteriophage lysin protein project in an advanced biochemistry lab. **M. Harrison**, C. Mageeney, A. Awuah, A. Budzilowicz, C. Cena, C. Curcio, S. Grant, N. Kuchinos, A. Rothman, S. Sampura, O. Townsend
- CHED 161.** Developing a drug displacement assay for the undergraduate laboratory. **D. Chavez**, C. Arpin, N. Barnett, J. Diaz, M.M. McDonald
- CHED 162.** Implementation of nucleic acid chemistry in undergraduate teaching and research. **L. Xue**
- CHED 163.** Development and use of a tool to assess students' understanding of biochemical pathway dynamics and regulation. **J.A. Loertscher**, B.J. Heyen, J.E. Lewis, V.M. Thorsell, T.A. Murray, S. Villafane-Garcia
- CHED 164.** Teaching mathematical methodology in general chemistry. **P.K. Yuen**, C. Lau, A. Yuen
- CHED 165.** Application of the Gay-Lussac Law to determine absolute zero for undergraduate chemistry. **A. Dukart**, D. Viernes
- CHED 166.** Incorporating food chemistry into GOB (general, organic, and biochemistry). **S.E. Hubbard**
- CHED 167.** How general chemistry and physical chemistry students use enthalpy and entropy to reason about dissolving and precipitation. **T.N. Abell**, S. Bretz
- CHED 168.** Use of an online simulation to help students understand gas behavior. **B. Martinez**, R.D. Sweeder, D.G. Herrington, J.R. Vandenplas



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- CHED 169.** Research and design of an atomic structure experiment for general chemistry I laboratory. **C. Lilly, B. Levengood**
- CHED 170.** Effect of online exam review session video format on student exam performance in general chemistry courses. **A. Alanazi, D.B. King**
- CHED 171.** Tracking improvements from interactive vs. lecture-style delivery of a large General Chemistry course: Topic-by-topic & student-by-student. **A.G. Caster, A. Sower, M. Seger, R.L. Falconer**
- CHED 172.** Detection of lead and other metals: Comparison of “dye” preparative methods vs commercial kits for the general chemistry laboratory. **D.P. Rillema, H. Nguyen**
- CHED 173.** Chemistry with friends: Investigating students’ social interaction networks in an active learning general chemistry course. **N.F. Mendez, N.S. Stephenson, J.H. Carmel**
- CHED 174.** Molecular CaseNet: Developing case studies using molecular representations for use in introductory chemistry and biochemistry. **K.J. Linenberger Cortes, S. Dutta, H.V. Jakubowski, M. Lenahan, D. Marcey, P. Marsteller, C. Terrell**
- CHED 175.** Using an assessment design and critique activity to investigate secondary chemistry teachers’ assessment beliefs and practices. **A.G. Schafer, E.J. Yeziarski**
- CHED 176.** Forensic Science: A useful blend of mystery and science to intrigue young kids. **A.A. Ellsworth**
- CHED 177.** Intersections and interconnections among groups in a pre-service teacher development program. **S.D. Wiediger, J.S. Krim, K. Barry, S.M. Locke, L. Cummings, T. Voepel**
- CHED 178.** Investigating the impacts of zoo-inquiry projects on student learning in introductory chemistry laboratories. **J. Kamitono, D. Donnelly, E.C. Person**
- CHED 179.** Learning simple concepts of X-Ray Powder Diffraction through a Project based Learning(PBL) approach suitable for Undergraduate Chemistry Students.. **T.O. Salami, K.S. Parrish**
- CHED 180.** Coke and Mentos fountain: Probing popular claims. **T.S. Kuntzleman, N. Doctor**
- CHED 181.** Comparing the effects of context-based vs. traditional POGIL activities on students’ exam performance. **G. Ibarrola Recalde, D.B. King**
- CHED 182.** Withdrawn
- CHED 183.** Implementation of the quantization and probability representations inventory at institutions across the United States. **Z. Allred, S. Bretz**
- CHED 184.** Use of a panel of nursing professionals to evaluate the authenticity of the use of electronic laboratory notebooks as pre-professional preparation in a general, organic, and biochemistry laboratory course. **A.J. Dood, L.M. Johnson, J.M. Shorb**
- CHED 185.** Investigating students’ thinking about the connections among kinetics, thermodynamics, and reaction coordinate diagrams. **M. Croisant, S. Bretz**



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

CHED 186. Students' responses to making mistakes in the undergraduate chemistry teaching laboratory. **S. Fullington**

CHED 187. Increasing organic chemistry students' communication and professional skills from INCLD: International Network for Chemistry Language Development. **M.T. Wentzel**, B. McCollum, L.A. Morsch, I.J. Ripley

CHED 188. Inventory to measure student thinking about reaction coordinate diagrams. **M.B. Atkinson**, M. Croisant, S. Bretz

CHED 189. Correlation between clicker use and student performance. **D.B. King**

CHED 190. Helping students construct understanding of kinetics with an online simulation. **R.D. Sweeder**, **D.G. Herrington**, **J.R. Vandenplas**

CHED 191. Viscosity, density, and refractive indices of binary mixtures of styrene with chloroform, 1,4-dioxane, dimethyl sulfoxide, N,N-dimethylformamide, and tetrahydrofuran. **H. Bascal**

CHED 192. Applications of Raman spectroscopy to study dyes and molecular conformations. **C. Ortiz**, **E.M. Marzluff**

CHED 193. Novel apparatus and data processing for teaching thermal analysis. **V.O. Jones**, B.H. Milosavljevic

MONDAY MORNING

Section A

Orange County Convention Center
Room W315A

Chemistry & Our Common Future: 2019 George C. Pimentel Award Symposium in Honor of Cathy Middlecamp

Symposium in Honor of Cathy Middlecamp

Cosponsored by CEI[†]
M. A. Fisher, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 CHED 194. 4 + 3: A moral imperative for chemistry professors. **G.M. Bodner**

8:55 CHED 195. Advances in incorporating sustainability into chemistry education and the role of the ACS Committee on Environmental Improvement. **S.O. Obare**

9:15 CHED 196. Environmental advocacy in action: The green chemistry commitment. **I.J. Levy**

9:35 Intermission.

9:45 CHED 197. Introducing undergraduate students to environmental chemistry and sustainability: From turrets to sheep to Baraboo. **N.J. Pienta**



TECHNICAL PROGRAM

10:05 CHED 198. Engaging students in the learning of chemistry “for the benefit of Earth and its people.” Lessons learned from Cathy Middlecamp. **J.M. Iriarte-Gross**

10:25 CHED 199. Reflections on transforming chemistry education, one faculty member at a time. **C. Maguire**

10:45 Intermission.

10:55 CHED 200. Award Address (George C. Pimentel Award in Chemical Education sponsored by Cengage Learning and the ACS Division of Chemical Education). The universe is made up of stories, not of atoms. **C.H. Middlecamp**

11:45 Concluding Remarks.

Section B

Orange County Convention Center
Room W312A

Training Professional Teaching Assistants

C. S. Bagwill, D. Sokic-Lazic, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 CHED 201. Lessons learned when revamping TA training in the Department of Chemistry at Purdue University. **F.K. Lang**, G.M. Bodner

8:55 CHED 202. Training professional graduate laboratory teaching assistants through role playing. **C.S. Bagwill, D. Sokic-Lazic**, J. Monahan

9:15 CHED 203. Can graduate students defy perceptions of trade-offs between research and teaching? **E. Shortlidge**, S. Eddy, E. Goodwin

9:35 CHED 204. Collaboratively designing teaching assistant training programs to address institution-specific needs. **J.C. Schwabacher**, A. Coleman, V.M. Berns, S.N. Knezz

9:55 Intermission.

10:10 CHED 205. Holistic approaches to training involving pedagogy, career skills & community building. **V. Dragisich**

10:30 CHED 206. Using active learning approaches to provide authentic training of teaching assistants for high enrollment general chemistry courses. **L. Stoll**, L. Lamont, S. Block, B.J. Esselman

10:50 CHED 207. Mixed messages: GTA perceptions of instructional expectations influenced by cross-tiered professional development. **E. Saitta**, W.D. James, M. Wilcox, J. Chini

11:10 Intermission.

11:25 Panel Discussion.



TECHNICAL PROGRAM

Section C

Orange County Convention Center
Room W312B

Process-Oriented Guided Inquiry Learning (POGIL)

R. S. Moog, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 CHED 208. POGIL and the POGIL Project. **R.S. Moog**

8:55 CHED 209. Adapting chemistry POGIL activities for your classroom: Modifying existing chemistry POGIL activities to meet the needs of a variety of student learners. **A. Annina**

9:15 CHED 210. Building attachment through POGIL to aid in student persistence. **B.M. Fetterly**

9:35 Intermission.

9:45 CHED 211. Supplementing POGIL classrooms with undergraduate learning assistants. **M.D. Perry**, B. Barth, E.C. Bucholtz, N. Sanguantrakun

10:05 CHED 212. Process skill development is predictive of student success in introductory STEM classes. **M.A. Horn**, H. Wilson-Ashworth, R. Qudisat, C. Warr

10:25 CHED 213. Pedagogies of engagement: Characteristics associated with implementation of POGIL, PBL, and PLTL in postsecondary chemistry courses. **J.R. Raker**, S. Srinivasan, K.L. Murphy

10:45 Panel Discussion.

Section D

Orange County Convention Center
Room W311A

Chemistry Education Research: Graduate Student Forum

D. V. Xue, *Organizer*
T. N. Abell, R. E. Gibbons, *Organizers, Presiding*
D. Xue, *Presiding*

8:30 Introductory Remarks.

8:35 CHED 214. E.Q.U.I.P.M.E.N.T: Education through questioning, using inquiry, and projects to maintain engagement and nourish thinking. **C. Felton**



TECHNICAL PROGRAM

8:55 CHED 215. Blending Learning applied in course about electrochemical surface treatment. **J. Zhang**, P. Yang, D. Wang, M. An, P. Cong, X. Ji, B. Wang

9:15 CHED 216. Multi-institutional qualitative analysis of course-based undergraduate research experiences. **K. Klay**, E.M. Bowers, J.H. Tomasik, D.J. Lecaptain, K.A. Cissell, K. Good, B.S. Harkness, T. Sivy, D.S. Karpovich, J. VanHouten, A. Mueller

9:35 Intermission.

9:45 CHED 217. Perceived roles of organic chemistry peer leaders: An analysis of reflection journal entries. **A.M. Clark**, J.R. Raker

10:05 CHED 218. Exploration of chemistry graduate teaching assistants' conceptions about teaching and participation in the teaching role. **E.K. Zotos**, A. Moon, G.V. Szymczak Shultz

10:25 CHED 219. Providing an authentic instructional experience through the development of rehearsal concept modules for a mixed reality teaching simulator. **A.A. Geraets**, J. Chini, E. Saitta

10:45 CHED 220. Analyzing the role of social influence for instructional practice within three chemistry departments. **J.D. McAlpin**, K.B. Downs, B.N. Earl, S.E. Shadle, J.P. Ziker, B.A. Couch, A.K. Lane, M.N. Stains, L.B. Prevost, J. Skvoretz, J.E. Lewis

11:05 CHED 221. How does active learning classroom affect STEM faculties in tertiary STEM Classes? **S. Gao**, J. Harshman

11:25 CHED 222. Community and Assessment: How membership in a community of practice influenced the assessment practices of a biochemistry instructor. **S. Feola**, J.A. Loertscher, V.M. Thorsell, P. Lemons, J.E. Lewis

Section E

Orange County Convention Center
Room W311B

There's an App for That

E. A. Aleman, K. Stone, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 CHED 223. Using clickers for more than just "clicking" things. **R. Quinones**

8:55 CHED 224. Interdisciplinary exploration of augmented reality to enhance student learning in organic synthesis. **J.E. Barker Paredes**, R. Pennington, D. Behmke, D. Kerven, R. Lutz, E. Brannock

9:15 CHED 225. Targeted App Design: Creating specific applications to address student-learning needs by content area. **J. Burkett**

9:35 CHED 226. Using molecular modeling Apps to provide interactive content examples in physical chemistry lectures. **E.A. Aleman**



TECHNICAL PROGRAM

9:55 Intermission.

10:05 CHED 227. Gradescope.com as a tool for rapid, information-rich feedback on student work. **M.A. Kubasik**, A.S. Harper-Leatherman, A.R. Van Dyke, L.A. McSweeney

10:25 CHED 228. Chemical Valence, an iOS app: Understanding molecular structure through visualization and knowledge integration. **L.B. Lewis**, M. Schira Hagerman, S. Kokoszka, A. Clark

10:45 CHED 229. Active lectures featuring “notes with gaps” and live audience polling with Poll Everywhere. **K.L. Peterson**

11:05 CHED 230. Pivoting peer review outside of the classroom using Turnitin. **K. Stone**, E.A. Aleman

11:25 Concluding Remarks.

Section F

Orange County Convention Center
Room W311C

Green Chemistry Student Chapters: Stories of Success

Cosponsored by SOCED
Financially supported by ACS Green Chemistry Institute; I&EC Green Chemistry Subdivision
M. C. Enright, J. MacKellar, *Organizers*
D. Constable, M. Enright, *Presiding*

8:30 Introductory Remarks.

8:50 CHED 231. Green chemistry activities at Tennessee Technological University. **J. Ralston**, A.J. Carroll

9:00 CHED 232. Small everyday actions! Big impact! UCA's efforts toward sustainable chemistry in Central Arkansas. **E.N. Tran, J. Schneider, A. Abdulrahim, W. Higgins, J. Dodson**, G.R. Naumiec, F.M. Yarberr

9:10 CHED 233. Transforming lives through green chemistry. **S.M. Pérez Lajara, D.I. Oyola Soto**, L.I. Santiago

9:20 CHED 234. Green chemistry at Heidelberg University. **K.L. Scruders, M. Cohn**, C. Ihrig, K. Malone, K.M. Iwanek, C. Morrison, N. Beres

9:30 Intermission.

9:40 CHED 235. Started from the bottom, now we're green! **M.J. Mio**, D.N. Maxwell, C.M. Johns

9:50 CHED 236. SAACS Green Chemistry Promotion at UAB. **L. Buchan, R. Andersen**

10:00 CHED 237. Operation G.R.E.E.N.. I. Montes-Gonzalez, **J.J. Maldonado Mendez, D.Y. Díaz Rohena**, Y. Rosario, **L.I. Penabad Peña**, J. Rosa Rosado, **A.E. Soto, R.J. Garcia Del Valle**, G. Colon, **E. Pagán Colón, C.A. Maysonet Navarro, H.L. Pabón Colón**



TECHNICAL PROGRAM

10:10 Intermission.

10:20 CHED 238. Green Chemistry Student Chapters: Success stories of Midland College Chemistry Club. P. Conlin, M. Holeman, S. Aina, J. Dimas, **A. Lum**, J. Anderson, P. Kesavan

10:30 CHED 239. Getting crafty: Artistic applications of green chemistry. **M. Youmans**, M. Pavlac, N. Fitzpatrick, D. Defazio, H. Arcure, A. Black

10:40 CHED 240. ACS UPR-Aguadilla green chemistry division: Searching for environmental action using the be-know-do model. **J. Goyco**, E. Rivera-Rosario, C. Nieves-Marrero, B.J. Ramos-Santana

10:50 Intermission.

11:00 CHED 241. Successful integration of green activities into our chapter's existing demo program. **L. Harris**, M. Stubbert, J. Wilhelm, C. Wilhelm, D. Corey, M.R. Wilhelm, J.L. Tischler

11:10 CHED 242. Green, White and Blue: Green chemistry at the University of New England. **J. White**, Y. Wang

11:20 CHED 243. (gc)²: Gordon College's green chemistry education to students of all ages. **Q. Dougherty**, **V. Ganss**, L. Atlas, A.H. Kjellson, H. Gordon, D. McGibbon, I.J. Levy

11:30 Concluding Remarks.

11:50 Discussion.

Section G

Orange County Convention Center
Room W311D

PolyEd: Incorporating Polymer Chemistry in Undergraduate & High School Curricula

Cosponsored by POLY
E. S. Sterner, *Organizer*
E. S. Sterner, *Presiding*

8:30 Introductory remarks.

8:40 CHED 244. Polymer outreach and in-reach through research with high school teachers. **K.A. Cavicchi**

9:00 CHED 245. Engaging students in polymer science through maker challenges. **C.A. Nichol**, C. Crawford, F. Gozuacik, S. Reyes, J. Polan

9:20 CHED 246. Polymer Science lessons and laboratory activities developed for high school classrooms by RET participants at the University of Southern Mississippi. **K.L. Wingo**, S.E. Morgan, J. Brownlow

9:40 CHED 247. Using a sustainability theme to introduce fundamentals of polymer chemistry to high school students. **D.E. Fagnani**, A.O. Hall, B.N. Barbu, K.N. Sekoni, A.J. McNeil



TECHNICAL PROGRAM

10:00 CHED 248. 3 in 1 polymer semiconductor STEM education kit to engage students in hands-on polymer inquiry activities. M. Kaushal, **M.G. Walter**

10:20 CHED 249. Material science and shape memory in the classroom. **L. Ruttig**, T. Lai, K.A. Cavicchi

10:40 Intermission.

10:50 CHED 250. OPALL: The Open Polymer Active Learning Laboratory at Georgia Tech. **P.S. Russo**, X. Zhang, P. Verma, P. Balding, G. Parkinson, L. Le, A.A. Advincula, C. Kozma, D. Thompson, I. Watt, A.M. Blake, D. Snyder, D. Roach, C. Smith, G.P. Carrazana, R. Volkovinsky

11:10 CHED 251. “Plastic” surgery: Giving a new face to common plastics. **R.L. Lewis**, **R. Hooper**, S. Nazarenko, V. Vasagar, R. Ramakrishnan, K. Reynolds

11:30 CHED 252. Seeing the flexibility of polymers. **J. Sorrell**, Y.C. Simon, B. Davis

11:50 CHED 253. Exploring the use of PLA films for oil spill cleanup: A sustainable classroom experiment. **J.E. Wissinger**, J.A. Byers, C. Knutson, R. Andrisen, M. Thompson, J. Belter

12:10 CHED 254. Emulsion templated polyimide aerogels. **M. Hill Langston**, E. Farrell, S.C. Jana

Section H

Orange County Convention Center
Room W311E

Undergraduate Research Papers

C. V. Gauthier, J. V. Ruppel, N. L. Snyder, *Organizers*
T. Hamilton, *Presiding*

8:30 Introductory Remarks.

8:35 CHED 255. Detection of hydrogen sulfide with a coumarin-based fluorescent probe. **Z. Baker**, K. Peterson

8:45 CHED 256. Qualitative and quantitative elemental analyses of total gunshot residue with TXRF. **N.C. Homburger**, M. Oliva, J. Berger, L. Huang

8:55 CHED 257. Method development for GC-MS detection of dimethylsulfone. **C. Wigder**, D.K. Wicht

9:05 CHED 258. Analysis of different steel alloys in order to identify their convenience to constitute molds for the Costa Rican plastics market. **L.G. Corea**

9:15 CHED 259. Studing the rate of redox reactions on gold-modified pyrolytic carbon electrodes. **E.M. Ness**, J.E. Kelm, J.C. Lytle, J. Parker, D.R. Rolison, J.W. Long

9:25 Intermission.



TECHNICAL PROGRAM

- 9:35 CHED 260.** Detection of lubricants using Raman microspectroscopy and ratio comparisons. **A. Fergus**, C. Vadell-Orsini, M. Maric, C. Bridge
- 9:45 CHED 261.** Enhancing the magnetic properties of iron-based spin-crossover complexes bearing hydrogen bonding groups through hydrogen bonding solvents. **M.J. Demmings**, A. Rabon, M.C. Young
- 9:55 CHED 262.** Fluorescence human serum lipoprotein profiling via anion-exchange high performance liquid chromatography. **N. Nguyen**, R. Chandra
- 10:05 CHED 263.** Applications of naturally-sourced waste ingredients in cosmetics. **K. Westergaard**, K. Gilcrease, T. Filipova
- 10:15 CHED 264.** Synthesis and characterization of bioderived polyureas for controlled ammonia release. **J.M. Migliore**, T. White, T.E. Long
- 10:25 CHED 265.** 3D printed microfluidics for hands-on undergraduate laboratory experiments. **M.T. Vangunten**, U.J. Walker, H.G. Do, K.N. Knust
- 10:35** Intermission.
- 10:45 CHED 266.** Vapor-phase pyrolysis of 4-methylguaiacol in a flow reactor. A. Nguyen, C. Luong, **E.B. Ledesma**
- 10:55 CHED 267.** Implementing POGIL strategies in an online general chemistry course. **H. Patel**, P.L. Daubenmire
- 11:15 CHED 268.** Measuring chemistry students' cognitive load on working memory: The development of an inventory of load-inducing topics in biochemistry. **K. Amir Hakim**, N.P. Grove
- 11:25 CHED 269.** Evaluation of the effectiveness of PreK-12 Green Chemistry workshops. **K. Ly**, J. Swanson, T. Filipova
- 11:35 CHED 270.** How participation in REU programs transforms undergraduate students' understanding of the nature of science. S. Dufort, **P.A. Mabrouk**
- 11:45** Concluding Remarks.

The Tenure-Track & Beyond: Academic Career Perspectives from Young Chemists

Sponsored by YCC, Cosponsored by CHED and PROF

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Sponsored by PROF, Cosponsored by AGFD, ANYL, BIOL, BIOT, CARB, CELL, CHED, CMA, COLL, COMP, ENVR, GEOC, I&EC, MEDI, MPPG, NUCL, ORGN, PHYS, PMSE, POLY, PRES, WCC and YCC

MONDAY AFTERNOON



TECHNICAL PROGRAM

Section A

Orange County Convention Center
Room W315A

**Chemistry & Our Common Future: 2019 George C. Pimentel Award Symposium in Honor of Cathy Middlecamp
Symposium in Honor of Cathy Middlecamp**

M. A. Fisher, *Organizer*
J. M. Iriarte-Gross, *Presiding*

1:30 Introductory Remarks.

1:35 CHED 271. Orchestrating our future through chemistry with Cathy Middlecamp. **Z.M. Lerman**

1:55 CHED 272. All are called to the periodic table. **P.L. Daubenmire**

2:15 CHED 273. Teaching and learning chemistry in the Arctic: Student research on microbes in a warming environment.
L. Nicholas-Figueroa

2:35 Intermission.

2:45 CHED 274. Leading us over the education horizon: Cathy Middlecamp as a harbinger of change in higher education.
J. Labov

3:05 CHED 275. Systems thinking: Camping in the middle of science, sustainability, and society. **P.G. Mahaffy**

3:25 CHED 276. Chemistry and our common future: Educating the heads, hands, and hearts of chemistry majors. **M.A. Fisher**

3:45 Concluding Remarks.

Section B

Orange County Convention Center
Room W312A

Enhancing Chemical Education with 3-D Printing

P. Bernard, J. D. Mendez, L. A. Porter, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 CHED 277. 3D-printed macroscopic model of an atomic force microscope that can be used to produce true force-distance curves. D. Gruber, T.J. Perez, B. Layug, M. Ohama, L. Tran, L.A. Rojas, A.X. Garcia, G. Liu, **W.J. Miller**



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

1:55 CHED 278. OMIS: The Open Millifluidic Inquiry System for small scale chemical synthesis and analysis. **R.J. Lesuer**

2:15 CHED 279. Designing and optimizing 3D printable microfluidic devices for utilization in undergraduate laboratory classes. **A. Alagic**, T. Tabibi, J. Norys

2:35 CHED 280. “MakerLab” approach: Student engagement and inquiry-based problem solving via digital design and 3D printing. **L.A. Porter**

2:55 Intermission.

3:05 CHED 281. Drawing chemical models with 3D printer pens. **P. Bernard, J.D. Mendez**

3:25 CHED 282. From MakerBots to new generation color inkjet modeling: Six years of 3D printing in support of chemical education at Stetson University. **W.T. Grubbs**, S. Ryan

3:45 CHED 283. Getting started with digital design and 3D printing: A beginner’s guide for chemical educators. **L.A. Porter**

4:05 Discussion.

Section C

Orange County Convention Center
Room W312B

Process-Oriented Guided Inquiry Learning (POGIL)

R. S. Moog, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 CHED 284. POGIL-PCL project: Guided inquiry experiments for the physical chemistry laboratory. **A. Grushow**, S.S. Hunnicutt, M. Muniz, R.M. Whitnell

1:55 CHED 285. Research-like experience for undergraduate biochemistry students: How much sugar is in this milk? **K. Willian**

2:15 CHED 286. Redesigning first semester Organic Chemistry labs to align with the POGIL teaching pedagogy. **M.A. Vanalstine-Parris**

2:35 Intermission.

2:45 CHED 287. Development of the POGIL Activity Clearinghouse (PAC). C. Fish, A. Mahoney, S. Garrett-Roe, A. Grushow, S.S. Hunnicutt, B. Fetterly, M.P. Garoutte, E.M. Kowalski, A.E. Martin, R. Pongdee, **M.S. Reeves**, C.M. Teague

3:05 CHED 288. Development of an observation protocol for teaching in interactive classrooms (OPTIC). **R. Frey**, U. Halliday, S. Radford, S. Wachowski



TECHNICAL PROGRAM

3:25 Panel Discussion.

Section D

Orange County Convention Center
Room W311A

Chemistry Education Research: Graduate Student Forum

D. V. Xue, *Organizer*
T. N. Abell, R. E. Gibbons, *Organizers, Presiding*
D. Xue, *Presiding*

1:30 Introductory Remarks.

1:35 **CHED 289.** Analysis of student reasoning about Michaelis-Menten enzyme kinetics. **J.G. Rodriguez**, M.H. Towns

1:55 **CHED 290.** Promoting student argumentation in undergraduate general chemistry. **K. Mauger-Sonnek**, R.S. Cole

2:15 **CHED 291.** Analyzing the relationship between assignment design and reasoning patterns in students' writing about organic mechanisms. **F.M. Watts**, J.A. Schmidt-McCormack, G.V. Szymczak Shultz

2:35 **CHED 292.** Assessing students' understanding of the nature and purpose of models in chemistry contexts. **K. Lazenby**, N.M. Becker

2:55 Intermission.

3:05 **CHED 293.** Student understanding in acid-base concepts in chemistry. **N.A. Kilpatrick**, S.R. Mooring

3:25 **CHED 294.** Embracing student challenges in general chemistry lab activities. **C. Keen**, H. Sevia

3:45 **CHED 295.** Towards student success: A skill based biochemistry teaching laboratory. **A. Reed**, T. Molden, Y. Gerasimova

4:05 **CHED 296.** Determination of Xylitol in sugar free gum by GC-MS with direct aqueous injection: A laboratory experiment for chemistry students. **D. Samarasekara**, S. Rajapaksha, D. Mlsna, T. Mlsna

4:25 Concluding Remarks.

Section E

Orange County Convention Center
Room W311B

New Frontiers for Chemical Education: Digital & Online Tools for Learning



TECHNICAL PROGRAM

M. McCartney, *Organizer*
J. Houck, T. S. Ritchie, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 CHED 297. Seventeen years of CheMagic.com. **O.S. Rothenberger, J.W. Webb**, T.A. Newton

1:55 CHED 298. Using digital tools to engage students in prerequisite review for organic chemistry. **J. Houck**, J. Robert

2:15 CHED 299. Open education resource lab manual for undergraduate lab courses. **J. Caras**, D. Harris

2:35 Intermission.

2:45 CHED 300. Chem compute science gateway: Web-based computational chemistry for undergraduates. **M.J. Perri**, M. Akinmurele, R.M. Whitnell, M.S. Reeves

3:05 CHED 301. Chem101: Drag and drop dimensional analysis for active learning assessments and practice in first-year chemistry. **J.B. Weinberg**

3:25 Intermission.

3:35 CHED 302. Internet of Chemistry Things: A chemistry elective course using cheap micro-computers and sensors to engage students and develop problem-solving skills. **R.E. Belford**, E.C. Bucholtz

3:55 CHED 303. Searching for chemical information using PubChem. **S. Kim**, A. Gindulyte, E. Bolton

4:15 CHED 304. Learning platform for lab courses to improve student preparedness, increase TA engagement, and improve TA mentoring. **J. Caras**

4:35 Concluding Remarks.

Section F

Orange County Convention Center
Room W311C

UN Sustainable Development Goals: Unique Opportunities for the Chemical Enterprise

Cosponsored by CEI
Financially supported by ACS Green Chemistry Institute; I&EC Green Chemistry Subdivision
E. J. Brush, J. E. Wissinger, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 CHED 305. Linking the UN sustainable development goals to green and sustainable chemistry: Unique opportunity for chemistry education. **E.J. Brush**



TECHNICAL PROGRAM

1:55 CHED 306. Systems thinking: A vital contribution to strengthening the role of chemistry in achieving the UN Sustainable Development Goals. **S.A. Matlin, P.G. Mahaffy**

2:35 CHED 307. Green chemistry addressing the UN sustainable development goals. **J.C. Warner**

3:15 Intermission.

3:30 CHED 308. Moore's law for chemistry. **M. George, P. Licence, M. Poliakoff**

3:50 CHED 309. International perspective on incorporating sustainability education into science education during the UN Decade of Education for Sustainable Development. **G.M. Bodner**

4:10 CHED 310. Withdrawn

4:50 CHED 311. Symposium workshop exploring new opportunities in green and sustainable chemistry education: UN sustainable development goals. **E.J. Brush, J.E. Wissinger**

Section G

Orange County Convention Center
Room W311D

PolyEd: Incorporating Polymer Chemistry in Undergraduate & High School Curricula

Cosponsored by POLY
E. S. Sterner, *Organizer*
E. S. Sterner, *Presiding*

1:30 Introductory Remarks.

1:35 CHED 312. Withdrawn

1:55 CHED 313. Incorporating polymer chemistry into an undergraduate instrumental analysis course. **M. Rasmussen**

2:15 CHED 314. Integrating polymer laboratory experiments across the curriculum. **J.W. Krumpfer**

2:35 CHED 315. Photoinitiated radical polymerization in the organic chemistry teaching laboratory; exploration of inorganic fillers on polymer strength. **I.J. Ripley, L. Gillett, M.T. Wentzel**

2:55 CHED 316. Nylon three ways: The impact of mechanism on polymer properties. **E.S. Sterner**

3:15 Concluding Remarks.

Section H

Orange County Convention Center
Room W311E

Undergraduate Research Papers



TECHNICAL PROGRAM

C. V. Gauthier, J. V. Ruppel, *Organizers*
N. L. Snyder, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 CHED 317. Manipulation of transmembrane pinholin protein in lipid mimetics: Applications in understanding the bacteriophage lytic cycle. **M. Anderson**

1:45 CHED 318. Elucidating the efficacy of a novel quinone in the treatment of *BRCA2*-mutant breast cancer. **L. PALmquist**, H.L. Dixon, K. Hutchinson, M.C. Srougi

1:55 CHED 319. Identification of microbial genus specific DNA fragments in tumor tissue, as a source for production of volatile organic compounds as breast cancer specific biomarkers. **H. Mattheisen**, A. Chen, H. Yokota

2:05 CHED 320. Fatty acid effects on CINC-1 and VEGF signaling in rat hepatoma cells. **A. Fee**, A. Stoeckman

2:15 CHED 321. Towards engineering a fully continuous CRISPR diversifier. **C.J. Tou**, S.O. Halperin, D.V. Schaffer, J. Dueber

2:25 Intermission.

2:35 CHED 322. Bacterial adhesion to heart valve biomaterials. **B. Norling**, K. McKenzie, L. McKinley, A. Stoeckman, K.E. Rohly

2:45 CHED 323. Mapping the binding of fibronectin and plasminogen to the immunodominant adhesin domain of *Mycoplasma genitalium*. **J.D. Mahlum**, A. Yang, G.E. Wood, P.A. Totten, B.J. McFarland

2:55 CHED 324. Biochemical analysis of three clinically-relevant variants of human fumarase. **B. Gemechu**, S. Ali, Z. Almajed, I. Couvertier, H. Dame, O. Damore, M. Feeley, N. Grimaud, O. Huber, L. Johnsky, B. Karki, J. Khaksari, A. Mendes, M. Nasser Mohi Eddin, A. Oranczak, K. Ortega, D. Parsons, A. Samman Nick Silva, M. Berkmen

3:05 CHED 325. Investigations of protein conformational changes of caspases as a signal for apoptosis. **L.K. Love, S. Hethcox**, M. Davis Mcgibony

3:15 CHED 326. Design and synthesis of aminoflavonols as M1 mAChR agonists to treat Alzheimer's Disease. **S. Jarrell**, R. Mans, S. Zingales

3:25 Intermission.

3:35 CHED 327. ¹H-NMR T1 and T2 relaxation times of aqueous solutions with varying concentrations of acetylcholine chloride and its metabolites. **A. Sivils**, C. Breaux

3:45 CHED 328. Evaluation of immune response of a library of cationic surface modified cellulose nanocrystals for biomedical application as potential vaccine adjuvants. **B. Tuga**, A. Rabideau, C. Smith, K. Ckless, R. Sunasee

3:55 CHED 329. Mechanism of the enzymatic synthesis of furan-containing compound, hydroxymethylfurfural. **C. Brown**

4:05 CHED 330. Development of lectin-based biosensors for the detection of flaviviruses. **N. Mercer**, K.T. Hamorsky



TECHNICAL PROGRAM

4:15 CHED 331. Utilization of maltotetraose during a nine generation serial repitching experiment. **A.D. Smith**, W. Deutschman

4:25 CHED 332. Computational study of PRL-3 in complex with the selective inhibitor of nuclear export selinexor. **C.J. Hansen**, M. Thompson Odom

4:35 Concluding Remarks.

Section I

Orange County Convention Center
West Hall C

Undergraduate Research Posters

Agricultural & Food Chemistry

Cosponsored by AGFD and SOCED
N. Di Fabio, J. Roberts, *Organizers*

12:00 - 2:00

CHED 333. Comparison of chemical constituents of various species of basil. **B. Cavanaugh**, **B. Gajmer**, **A.B. Waghe**

CHED 334. In vitro antibacterial activities of basil species: *Ocimum sanctum*, *Ocimum tenuiflorum*, and *Ocimum basilicum*. **B. Gajmer**, **B. Cavanaugh**, **A.B. Waghe**

CHED 335. Response of *Megacopta cribraria* to insect exposed soybeans plants in a Y- track olfactometer. **R. Ortiz**

CHED 336. Nutrient, pH and salinity of Guanajibo and Yagüez rivers mouths soils. **E. Rodriguez-Santana**, M.A. Rivas-Vazquez, A.M. Gonzalez-Mederos

CHED 337. Effect of ozone on barley malt quality. **S.L. Miller**, D.J. Oostendorp, A. MacLeod, K. Miller

CHED 338. Microbial and sensory quality of dried fruit processed in low enthalpy geothermal food dehydrator. **C. Sanchez Paredes**, O.d. Velázquez Madrazo, P. Severiano Pérez, R.A. Sanabria Aguirre, Y. Carmona López, E. Pérez González, M. Salinas Vázquez, H.M. Aviña Jiménez

CHED 339. Novel compounds extracted from endophytes isolated from *Populus nigra*. **J.M. Taylor**, M.D. Halling

CHED 340. Isolation of natural insecticides from yew trees. **C.T. Morante**, A. Hoffman

CHED 341. Investigation of guava extracts on enamel demineralization. **K. Hutsell**, C. Breaux

CHED 342. Synthesis and analysis of 6-acetyl-1,2,3,4-tetrahydropyridine, a major contributor to 'mousy' off-flavor in sour and wild beers. L. Benedict, **L. Krout**, M. Hausman, Z. Bodah

CHED 343. Quantification of flavor components in Scotch whisky and aged corn whiskey. **M.R. Owens**, Z.S. Davis



TECHNICAL PROGRAM

- CHED 344.** Investigation into the potentially devastating diastatic activity of the hop. L. Benedict, **N. Mesloh**, M. Ackerman, Z. Bodah
- CHED 345.** Characterization of reaction products of simple carbonyls with ammonium sulfate in secondary organic aerosol mimics. **R. Holappa**, **D. Grace**, J.R. Sharp, M.M. Galloway
- CHED 346.** Effect of induced mutations on the ability of rye grass to bind lead. **A. Bakerson**, D.J. Schauer
- CHED 347.** Factors impacting the desorption of heavy metals by *Coriandrum sativum*. **N. Adams**, D.J. Schauer
- CHED 348.** Phenolic content and antioxidant properties of fifteen commercially available basil essential oils. **R.J. Meyer**, E.D. Niemeyer
- CHED 349.** Evaluation of *Acer sp.* for the biosorption of lead from water. **A. Roschyk**, D.J. Schauer
- CHED 350.** Variations in total phenolic content and antioxidant capacity in 22 commercially available basil (*Ocimum basilicum L.*) cultivars. **E.M. Bajomo**, L. Ford, M.S. Aing, E.D. Niemeyer
- CHED 351.** Effects of brewing methods on levels of antioxidants in coffee. **K. Wiczorkowski**, J.K. Vohs
- CHED 352.** Biogas digester effluent as fertilizer for organic farming and its effect on plant growth and vitamin content. **M.E. Lee**, S.K. St Angelo
- CHED 353.** Immobilizing acetolactate decarboxylase to eliminate diacetyl from beer. **J.R. Pugh**, R.A. Hunter
- CHED 354.** Elemental, phenolic, and stable isotopic fingerprinting of wines from the Chesapeake Bay growing region. **P. Conner**, R.K. Larsen
- CHED 355.** Isolation and characterization of lemongrass components using various extraction techniques. **S. Jordon**, L.B. Lewis, C. Bieler
- CHED 356.** Analysis of volatile aroma compounds in homebrewed ale beer samples using SPME/GC-MS. **J. Goyco**, E. Molina
- CHED 357.** Batch to batch variation of flavonoids and alpha-acids in craft beers. **A. Foringer**, J.A. Lupica, P. Tandler
- CHED 358.** Standardizing a protocol for determining the caloric content of beer. **A. Marcy**, C.K. Saner
- CHED 359.** Determination of pesticides in raw, roasted, and brewed coffee using QuEChERS method with GC-MS. N.R. Lien, **Z. Kitzhaber**
- CHED 360.** Utilizing hops in the scientific investigation of the relationship between international bitterness units and standard reference method. **A. Hudson**, C.K. Saner
- CHED 361.** Withdrawn

Section I



TECHNICAL PROGRAM

Orange County Convention Center
West Hall C

Undergraduate Research Posters

Analytical Chemistry

Cosponsored by ANYL and SOCED
N. Di Fabio, J. Roberts, *Organizers*

12:00 - 2:00

CHED 362. Plasma temperature determination of Martian laser-induced breakdown spectroscopy (LIBS) data. **J.P. Stetzler**, R. Chinni

CHED 363. Quantitative evaluation of the ecological and biological make-up of Silver Lake in light of increase urban development pressures and climatic shifts. **T.J. Roberts**, R.M. Hyde

CHED 364. Forensic analysis of organic gun-shot residue on bullet casings. **B. Shaikoski**, B. Pauley, M. Rich, C. Hanson

CHED 365. Analysis of heavy metal accumulation in wolf spiders with graphite furnace atomic absorption spectroscopy. L.A. Tom, M.H. Persons, **S.A. Daigle**, T.M. Bitner

CHED 366. Utilizing HPLC and GC-MS in brewing. **S. Speak**, M.B. Jacobs

CHED 367. Development and evaluation of alkyne functionalization on metal surfaces. **M. Silas**, E.C. Landis

CHED 368. Attachment and ordering of alkyne self-assembled monolayers on nanoporous gold surfaces. **A. Sevigny**, E.C. Landis

CHED 369. Binding of alkyne monolayers on gold surfaces. **Z. Li**, E.C. Landis

CHED 370. Development of novel surface chemistry for the fabrication of electrochemical aptamer-based sensors. **A.I. McDarby**, R.J. White

CHED 371. Study of perfume degradation by solid-phase microextraction – gas chromatography mass spectrometry. **B. Utley**, M. Sabo, J. Hall-Yates

CHED 372. Determination of pesticide residues in vegetable samples. **E. Bullington**, C.H. Lisse

CHED 373. Electrodeposition of Cu₂O from O₂ saturated deposition solution as an attempt for enhancement of Cu₂O electrical conductivity. **C.H. Fortna**, A. Fillinger

CHED 374. Quantification of nitric oxide released from a wound healing patch. **A. Sugrue**, K. Scrudders, N. Beres

CHED 375. Essential oil and headspace aroma composition of *Illicium c.f. ekmanii* Smith from the Dominican Republic using HD, SPME, and GC-MS. **K. Soun**, M. Bida, A. Guerrero, T.E. Pagano



TECHNICAL PROGRAM

- CHED 376.** Determination of lithium in Andean mummy hair using LA-ICP-MS. D. Blumenstiel, M. McDonald, B. Arriaza, **D.D. Amarasiriwardena**
- CHED 377.** Isolation of active compounds of medicinal plants. **S. Paske**, K. Nell, B.P. Nell
- CHED 378.** Classification of Caddo pottery sherds using SEM-EDS. **L. Hazeslip**, R. Mauldin, M. Corley, D.P. McKinnon
- CHED 379.** Development and validation of a method using QuEChERS and liquid chromatography-mass spectrometry for determination of atrazine and its metabolites in crayfish. K.E. Yacoo, D.J. Dayfield, D.N. Maxwell, V.C. Torres, A. Almouseli, **K.S. Lambert**, **I. Sayed**, C.R. Fiorido, **K.M. Marji**, **K.M. Marshall**, **M. Azam**, R.M. Belanger, E. Roberts-Kirchhoff, K.R. Evans
- CHED 380.** Quantitation of atrazine in crayfish tissue to investigate the effects of atrazine exposure. **K.E. Yacoo**, D.J. Dayfield, **D.N. Maxwell**, **V.C. Torres**, **A. Almouseli**, K.S. Lambert, I. Sayed, C.R. Fiorido, K.M. Marji, K.M. Marshall, M. Azam, R.M. Belanger, E. Roberts-Kirchhoff, K.R. Evans
- CHED 381.** Characterization of pharmaceutical polymorphs by variable temperature NMR. **S. Stuchell**, A. Viggiano, R. Iulucci
- CHED 382.** Lipid extraction and characterization from bee pollen. **C. Rohrbaugh**, G.P. Foy
- CHED 383.** Isolation of potential antifungal compounds in *Aloe cameronii*. **A. Colah**, **L. Raess**, R.L. Bretz
- CHED 384.** Factors influencing the modified Scott test for cocaine using substances that result in a false positive. **M. Klem**, N. Kiwiet
- CHED 385.** Measuring the antibacterial efficacy of silver nanoparticles and essential oils on *Staphylococcus epidermidis* using GCMS. **A. Aspin**, T. Toggweiler, K.A. Cissell
- CHED 386.** Health risk assessment for benzene exposure from candles. **C. Gall**, A.J. MacPherson
- CHED 387.** Evaluation of chemical ionization methods for standard-free quantitative analysis of alkaloids in poison frogs. **K. Gleason**, **A.H. Kemp**, R.W. Fitch
- CHED 388.** Method development for the detection and comparison of potential trace compounds in different sources of *Trigonella foenum-graecum* seed powder using RP-HPLC. **N. Hartwig**, E. Price
- CHED 389.** Using noble metal nanoparticles with SERS to characterize colorants in cultural artifacts. **A. Davis**, M. Schiza
- CHED 390.** Puerto Rican craft beer characterization. **A. Rodriguez-Nieves**, **A. Quintana-Martinez**, **E.N. García**, N. Martinez-Santos, K. Durand-Freda, L. Santos-Pimentel, J. Rivera-Colón, D. Martín-Díaz, E. Rodriguez-Santana, K. López-Sánchez, D. Reyes-Hermina, G. Sanchez-Nieves, A.M. Gonzalez-Mederos
- CHED 391.** Probing the root exudation of harmala alkaloids from Syrian rue. **C.M. Borton**, J. Weidenhamer, B.K. Mohney
- CHED 392.** 3D printed cuvette adapters for customizable UV-Vis spectroscopy. **J.V. Waldman**, H.D. Whitehead, G. LeBlanc
- CHED 393.** Analysis of west Tennessee riverways for nitrogen, phosphorus, and potassium. **A. Orr**, R. Montgomery



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- CHED 394.** Analysis of sucrose, glucose, and fructose present in maple sap and syrup. **M. Meyers**, C. Chant
- CHED 395.** Investigating the potential of self-assembling peptide systems for uric acid electrochemical sensing applications. **J.L. Myers**, **S.J. Brown**, J.E. Smith-Carpenter, A.S. Harper-Leatherman
- CHED 396.** Improved electrochemical performance of fused filament fabrication 3D printed electrodes using hydroxide treatment methods. **M. Sheaff**, D.M. Wirth, H.D. Whitehead, G. LeBlanc
- CHED 397.** Natural products analysis: Identifying endophytic fungi which produce beta-bisabolol. **T. Haines**, R. Iulucci
- CHED 398.** Study of fluorescence and electrochemiluminescence quenching of luminescens by explosives. **D.R. Ogburn**, K.D. Sienerth
- CHED 399.** Determination of BPA in vaping mouthpieces using spectrofluorometry. **J. Cook**, S.E. Hubbard
- CHED 400.** Withdrawn
- CHED 401.** Fluorescence quantitation of albumin and very low density lipoprotein via anion-exchange high performance liquid chromatography. **A. Akhtar**, **N.Y. Kong**, R. Chandra
- CHED 402.** Healthy lake-happy city. **J.W. Tallman**
- CHED 403.** Revisiting the quaternary rhyolites of the mineral mountains: New $^{40}\text{Ar}/^{39}\text{Ar}$ geochronology, paleomagnetic, and geochemical data. **H. Peacock**, T. Rivera, G. Rae-Downing, P. Lippert, S. Kirby, B. Jicha
- CHED 404.** Analysis of volcanic ash from Mount St. Helens and Kilauea eruptions: Comparison and contrast of elemental content by ICP-OES. **J. McElroy**, **M. Whalum**, M.J. Kendrick-Murphy
- CHED 405.** Ultrasensitive detection of cancer biomarkers using multi-photon nonlinear laser wave-mixing spectroscopy. **S. Crawford**, T. Inouye, J. Liang, F. Venturini, J. Suprpto, S. Pradel, W.G. Tong
- CHED 406.** Gold aerogels incorporating carbon nanotubes for biosensing applications. **C.E. Zarra**, A.S. Harper-Leatherman
- CHED 407.** Jet fuel analysis and four-component mixtures as fuel models. **J. Fries**, **R. Gober**, J. Cowart, D.J. Luning Prak
- CHED 408.** Cytochrome *c* adsorbed to peptide SAM modified evaporated gold electrodes. T. Yawitz, **K. Patterson**, B. Onkst, R.A. Clark
- CHED 409.** Particle formation in an aerosol chamber: Trimethylamine, dimethyl sulfide, and oxidants. **T.J. Cress**, R. Drover, C. Michael, P. van Rooy, D. Cocker, A. Foote, K. Purvis-Roberts, P.J. Silva
- CHED 410.** Measurement of urinary sulfate concentration in horses by conductometric titration. **S.A. Andrews**, L.D. Schultz
- CHED 411.** Development of a quality control lab for a microbrewery. G. LeBlanc, **M. Symcox**, K.D. Symcox
- CHED 412.** Analysis of drug-protein interactions by high performance affinity chromatography. **M. Weigand**, A.G. Woolfork, D.S. Hage



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- CHED 413.** Weathering patterns of alternative “green” ignitable liquids. **N. Rohrbaugh**, K.L. Opel
- CHED 414.** Investigation of the hyperaccumulation ability of Mammoth sunflowers using ICP-OES. **S. Beauchamp**, M.J. Kendrick-Murphy
- CHED 415.** ATR-FT-IR analysis of organic gunshot residue to infer caliber type and distance from firing event. **J.D. Leon**, A.C. Suroviec
- CHED 416.** Performance of accelerated solvent extraction in comparison to other methods in the extraction of active compounds from bee propolis. **J. Charland**, J. Farshi, **E.E. Mojica**
- CHED 417.** Determination of halogens in pharmaceutical market products using laser-induced breakdown spectroscopy. **S. Nsiah**, D. Rusak
- CHED 418.** Characterization and antioxidant activities of different solvent fractions of a bee pollen sample from the Philippines. **J. Farshi**, E.E. Mojica
- CHED 419.** Heavy metal content of dog food using MP-AES. **B. Evans**, R. Montgomery
- CHED 420.** Raman spectroscopy of different metformin tablets. **E. Krupoff**, L. Reilly, E.E. Mojica
- CHED 421.** Raman spectroscopic studies of nitro containing compounds. **L. Reilly**, E.E. Mojica
- CHED 422.** Analysis of over-the-counter antihistamines using Raman spectroscopy and density functional theory (DFT) calculations. **L. Wyan**, E.E. Mojica
- CHED 423.** Fatty acids profile of some breast milk samples from the Philippines. **E. Oberlender**, A. Gabriel, E.E. Mojica
- CHED 424.** Evaluating the water quality of Newton Creek, New York City. **G. Iannone**, E.E. Mojica
- CHED 425.** Synthesis and evaluation of a chiral ionic liquid derived from an aspartame cation for potential applications in chromatographic separations. I. Kimaru, **O. Culbertson**
- CHED 426.** Correlation analysis determines mechanistic pathway and the presence of general base catalysis. **A.C. Lonski**, M.J. D'Souza
- CHED 427.** Synthesis of general molecularly imprinted polymers for aspirin and naphthalene derivatives. **P.A. Dome**, L. Demoranville
- CHED 428.** Nutraceutical properties of several commercial herbal tea samples. **V. Carranza**, E.E. Mojica
- CHED 429.** Multivariate analysis of global fuel spectral data sets. **C. Orrison**, S. Downes, J. Cooper
- CHED 430.** Extraction and analysis of volatile biomarkers in oral disease using solid-phase microextraction (SPME). **E. Feldman**, **E. Horta**, **S. Ide Bolet**, K. Crump, J.S. Brown
- CHED 431.** Blood alcohol testing using SPME and head-space gas chromatography. **T. Rinehart**, R. Montgomery



TECHNICAL PROGRAM

- CHED 432.** Quantitative analysis of polyvinyl alcohol-polyethylene (PVOH-PE) copolymers and polyvinyl pyrrolidone-polyvinyl acetate (PVP-PVAc) copolymers and blends using Fourier transform infrared spectroscopy and elemental analysis. R.P. D'Amelia, L. Huang, **J. Mancuso**
- CHED 433.** High-field NMR spectroscopy and mass spectrometry for the quality control of *Epimedium grandiflorum* dietary supplements. **I.O. Okeke**, M. Malet-Martino
- CHED 434.** Extraction and quantification of cocaine and its metabolites in coffin fly pupae. **S. Sarginson**, K.L. Opel
- CHED 435.** Preparation and characterization of magnetic nanoparticles functionalized with molecularly imprinted polymers (Fe₃O₄@TEOS@MIP) for the extraction of ibuprofen from water samples. **N. Middelmeer**, Y. Mei-Ratliff
- CHED 436.** Synthesis of a fluorescent and colorimetric chemosensor for detection of trivalent cations. **A.R. Garza, C. Quintero**, S. Plummer Oxley
- CHED 437.** NMR investigation and characterization of leucine based surfactants bound to various amine counterions. **M. Aleksich**, F.H. Billiot, K.F. Morris, E. Billiot
- CHED 438.** Effect of number density on aromatic seeded aerosols as measured through thin film spectroscopy. **J. Rishi**, N. Bishop, J. Sebree
- CHED 439.** Comparative analysis of rose volatiles in essential oils via GC-MS. **J. Chong**, P.J. Iles, M. Alvarez, R.V. Valcarce, L.D. Giddings, J. Mesa De La Cruz
- CHED 440.** Paper based assay of copper ion using egg white as natural reagent. **W. Nzobigeza**, S. Kradtap
- CHED 441.** Determining the nutrient health of the Oconee River. **D. Cook**, C.H. Lisse
- CHED 442.** Separation of TGF-beta1 in a microchannel using isotachopheresis. **F. Matthews**, M. Hossan, S. Gamagedara
- CHED 443.** Simple method for preparing customizable pyrolyzed resin carbon electrodes using 3D printing. **D.L. Glasco**, K.N. Knust
- CHED 444.** Construction of an electron impact mass spectral library for the automated analysis of poison frog alkaloids. **J.M. Smith, M.M. Reid, A.H. Kemp**, R.W. Fitch
- CHED 445.** Analyzing triphenyltin chloride in air using a high performance liquid chromatography based, NIOSH-sanctioned method. **J. Reed**, B. Hopkins
- CHED 446.** Analysis of branched polyethylenimine (BPEI): Linking structure, molecular weight, pH, and electrostatic properties by using a particle charge detector. **T. Ma**, V. Wong
- CHED 447.** Hydrogen peroxide generation at Cu₂O photocathode. **A.T. McCabe**, A. Fillinger
- CHED 448.** Chemical characterization of Kentucky honeys. **C.M. Fitzpatrick, R. Jenkins**, B.G. Vanness
- CHED 449.** Characterization of materials in Western African artifacts. **K. Dodds**, J.M. Esson
- CHED 450.** Characterization of a paper-based analytical device for heparin. **B. Giedeman**, J.M. Esson



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- CHED 451.** A chemical investigation of arsenic in 19th century women's garments. **N. Shandor**, S. Brayton, J.N. Richardson
- CHED 452.** Development of quantitative HPTLC-densitometry methods for the analysis of amiodarone HCl and irbesartan using a model approach for the transfer of TLC screening methods. **K. Nguyen**, J.A. Sherma
- CHED 453.** Chemical characterization of compounds found in herbal cigarette smoke as a first step in bioactivity analysis. **K. Dunnivant**, C. Bowers
- CHED 454.** Determination of BPA in infant oral hygiene products using fluorescence spectrophotometry. **M. Mayfield**, S.E. Hubbard
- CHED 455.** Determination of tulathromycin in fish tissue by liquid chromatography with UV detection. **E. Lavadour**, A.G. Cavinato
- CHED 456.** Experimental and theoretical study of the electrochemistry of metals deposited on indium tin oxide modeled using the Cottrell equation. **L. Rankin**, J. Kegerreis, J.N. Richardson
- CHED 457.** Electrochemical synthesis of urea in ionic liquid catalytic system with CO₂. **W.J. Winchester**, Z. Wang, K. Riley, M. Reed, P. Ling, A. Osborne, L. Dykes
- CHED 458.** Photocatalytic degradation of pharmaceuticals in acid and base solutions. L.A. Tom, **T.M. Bitner**, S.A. Daigle
- CHED 459.** Rapid approach for measurement of aptamer-protein binding constant using quantitative polymerase chain reaction (q-PCR). **J. Carter**, **H. Breen**, A.G. Cavinato
- CHED 460.** Method development and determination of metal complex pK_a's by NMR and visible spectroscopy. **B. Vinson**, T.K. Ellis, J. Henrikson
- CHED 461.** Spectrophotometric determination of iron(II) and iron(III). **M. Otayfah**, D.A. Habboush
- CHED 462.** Spectrophotometric study of the reaction of nitrite with indole. **F. Alrasheedi**, D.A. Habboush
- CHED 463.** Blocking electrochemical collisions of single bacteria: Dependence of current transient shapes on species and supporting electrolyte concentration. **S. Jenkins**, S.N. Thorgaard
- CHED 464.** Spectrophotometric titration of CrO₃ with KOH. **D.S. Yeboah**, **R.B. Yozzo**, D.A. Habboush
- CHED 465.** Determination of tetrodotoxin in the California newt, *Taricha torosa*, by high performance ion-pair liquid chromatography coupled with fluorescence detection: Geographic and environmental considerations. **D. Hu**, G.M. Bucciarelli, L.B. Kats, D.B. Green
- CHED 466.** Mercury concentration in water fowl in Wisconsin. **S. Frisque**, M.D. Schuder
- CHED 467.** Measurement of sulfate in swine urine by conductometric titration and ion chromatography. **H.C. Stephen**, **S.A. Andrews**, L.D. Schultz
- CHED 468.** Spectroscopic characterization of aged historic inks for their rapid detection and remediation. **T. Huntington**, D. Rothfels, R.P. Jensen, N.A. Swartz



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- CHED 469.** Synthesis and analysis of primary amine functionalized silica sol-gels. **J. Fortwengler**, C.H. Lisse
- CHED 470.** Comparison of the elemental content of commercial tattoo inks with native Maori body dyes from New Zealand. **M.K. Smelley**, **S. Warren**, M.J. Kendrick-Murphy
- CHED 471.** Identification of *Homarus americanus* neuropeptides and precursor-related peptides: The use of off-line high pH fractionation prior to LC/MS analysis. **C.M. Call**, C.D. Rivera, P.S. Dickinson, A. Christie, E.A. Stemmler
- CHED 472.** Determination of the chicken organ odor profiles (COOPs) from the decomposition of chicken thighs using gas chromatography mass spectrometry (GCMS). **M. Boes**, **A. Frantz**, A. Flotteron, T.N. Lewis, M. Sabo
- CHED 473.** Examination of the elemental content of coral from the Gulf of Mexico. **J. Fleming**, **S.E. Ison**, M.J. Kendrick-Murphy
- CHED 474.** Characterizations of bacterial isolates from cationic nanoparticle solution and their interactions with cationic nanoparticles. **S.D. Frand**, S. Yang, J.E. Kuether, R. TapiazHernandez, Y. Zhang, R.J. Hamers, V. Feng
- CHED 475.** Synthesis and characterization of carbon nitride electrodes for the reduction of oxygen. **J. Nisly**, R.W. Schaeffer, N. Hellgren
- CHED 476.** Segmented flow droplet formation using low-cost microfabrication techniques. **J.D. Maturano**, J.P. Grinias, A. Kaplintz, M. Padalino, J. Davis
- CHED 477.** Investigation of native New Jersey macroalgae for use in producing biodiesel. **E. Bell**, V. Contractor, M. Mongelli, **C. Gaviria**
- CHED 478.** Designing and optimizing 3D printable microfluidic devices. **T. Tabibi**, A. Alagic
- CHED 479.** Withdrawn
- CHED 480.** Designing and optimizing 3D printable microfluidic valve. **J. Norys**, A. Alagic
- CHED 481.** HPLC analysis of the light-induced reaction between lumazine and dGMP for applications in photodynamic therapy. **R.C. de Dios**, C. Collyer, L.M. Mier
- CHED 482.** Chemometric analysis of biodiesel-diesel blended fuels using a moderately polar gas chromatography column. **A. Riddell**, **H. Tsiagras**, K. Ramos, A.M. Hupp
- CHED 483.** Comparison of photochemical decomposition products and efficiency of two commercially available sunscreens. K. LaiHing, **D.C. Jenkins**, R. James
- CHED 484.** GC-MS/MS analysis of archaeological smoking pipe residues and plant materials. **L. Schulz**, **G. Tolan**, S. Carmody, J. Russ
- CHED 485.** Biomarker analysis of ceramic beakers from the Early/Middle Mississippian cultures. **U. Aziz**, M.A. Martin, D. Dye, J. Russ
- CHED 486.** Monitoring the products of the reaction between the potential photodynamic therapy agent, lumazine, and dAMP using HPLC. **C. Collyer**, R.C. de Dios, L.M. Mier



TECHNICAL PROGRAM

CHED 487. Optimization of the analysis of raw materials in a veterinary topical analgesic. **S.J. Haskin, A.J. Lisle, J. Erickson, K. Peterson**

CHED 488. Qualitative analysis of the ions within the metalloproteins of humans and horseshoe crabs. **K. Sylvester, D. Young, S.J. Rolle**

CHED 489. Deuterium-hydrogen exchange reactions under microwave reaction conditions. **E. Nevarez, M.C. Ramos, A. Martinez, E. De La Fuente, X. Chen**

CHED 490. High performance liquid chromatography method for the quantitative determination of acetaminophen in commercial drugs and to study degradation of the drugs under extreme conditions. **C. Sircher, A.K. Korir**

CHED 491. Using MALDI-MS and LC-MS to analyze 4-hydroxy-2-nonenal (4HNE) adduction to electron transfer flavoprotein (ETF). **P. Kremer, E. Schaible, C.M. Byron**

CHED 492. Immobilization of porphyrins in sol-gel matrices. **M. Schellman, C.H. Lisse**

CHED 493. Forensic ink analysis with miniaturized UV-Vis spectrometry. **M. Morrill, L. Huang, M. Chambers**

CHED 494. Further studies of chalcone-like derivatives and analysis of substituent effects on UV-Vis, IR absorption and NMR chemical shifts of the vinylic protons. **D. Nguyen, A. Zeng, M. Young, P. Gordon**

CHED 495. Determining the magnitude of color perception in soil analysis. **H. Martin, K.L. Opel**

CHED 496. Development of an analysis method of forensically significant reduced-size STRs by MALDI-TOF-MS. **A. Osenbach, K.L. Opel**

CHED 497. Evaluation of PCR product purification methods for analysis of forensically important SNPs by MALDI-TOF-MS. **A. Kendrick, K.L. Opel**

CHED 498. Photo activation study of three isomers of N-pyridyl mesosubstituted porphyrin. **L. Sanz, K. Chamarti, M. Ballester, V. Castro, B. Van Hoozen**

CHED 499. Porphyrin basicity on 5, 15 diphenyl and 5, 15 di (4-cyanophenyl) substituted porphyrins. **M. Ballester, K. Palreddy, A. Tracey**

CHED 500. Effects of contaminants on the reliability of presumptive and confirmatory tests for blood. **F. Deichert, K.L. Opel**

CHED 501. Quantitative determination of fusel alcohols, esters, di-methyl sulfide, and vicinal diketones in craft beer during a nine generation serial re-pitching experiment. **B. Bruggeman, W. Deutschman**

Section I

Orange County Convention Center
West Hall C

Undergraduate Research Posters

Biochemistry



TECHNICAL PROGRAM

Cosponsored by BIOL and SOCED
N. Di Fabio, J. Roberts, *Organizers*

12:00 - 2:00

CHED 502. Influence of genipin on the activity and presence of amylin in SH-SY5Y and RIN-5F cells. **G. Manuel**, T. Clemons

CHED 503. Construction of *mnth* knockout in *Escherichia coli* strain CSH104 using CRISPR/Cas9 and verification of manganese concentration using atomic absorption spectroscopy. **M.N. Nguyen**

CHED 504. Copper modulation to effect yeast lifespan. **Z.J. Sherlock**, M. Bestwick

CHED 505. Exploring the differences among statins in enhancing the metabolic labeling of prenylated proteins using isoprenoid probes. **P. Thao**, M.D. Distefano

CHED 506. Quantitative determination of amino acid concentration and kinetic studies of degradation in *Arthrospira platensis*. **T.D. Williams**, C.K. Saner, C. Hartwig

CHED 507. Exotic butter formulation to enhance bacterial resistance and UV protection. **R. Persaud**

CHED 508. Coconut and medium chain triglycerides infused with plant powders to combat bacteria. **M. Ames**, A. Melkonian, K. Melkonian, J.I. Rizzo

CHED 509. Beeswax and honey as a novel antibacterial surface. **J.T. Fatum**, A. Melkonian, K. Melkonian, J.I. Rizzo

CHED 510. Finding potential cures for visceral leishmaniasis. **J.T. Fatum**, T. Lee, K.V. Tienhoven, N. Yarlett, Z. Dai

CHED 511. Absorption of toxic nitrate and phosphate ion concentrations via native graminoid and forb-perennial species. **M. Strickley**, R.L. Bretz

CHED 512. Investigating the role of the bulge and pentaloop for *htrA* RNA thermometer melting behavior. **Y. Tan**, R.M. Mitton-Fry

CHED 513. Characterization of tyrosine 141 in Y-family DNA polymerase kappa. **J. Andrade**, S. Lone

CHED 514. Synthesis, characterization, and cell toxicity of nitrosylated tris-(ethylenediamine) cobalt (III) complex. **E.A. Cronin**, J.A. Lupica, M. Dunphy, J.A. Bauer

CHED 515. Levels of *sall4* expression as a function of location in the body of an axolotl. **M. Franey**, M.A. Fisher

CHED 516. Biochemical changes in the shikimate and phenylpropanoid pathways in the bioenergy crop, shrub willow, due to nitrogen stress. **J.R. Holowko**, M. Serapiglia

CHED 517. Physiological and biochemical responses in shrub willow clones to nitrogen stress. **B. Koons**, S. Long, R. Minocha, L. Smart, M. Serapiglia

CHED 518. Recombinant expression of conotoxins in *Escherichia coli*. **R.P. Baskin**, H. Safavi-Hemami, C. Hackney, L. Ellgard



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- CHED 519.** Extraction, purification, and characterization of a possible Prodigiosin. **A. Wagler**, D.C. Bromfield-Lee
- CHED 520.** Purification and isolation of natural compounds: Actinomycetes found in ancient soil. **C. Raul**, A. Hoffman
- CHED 521.** Characterization of GP133: A human orphan g-protein coupled receptor. **W.H. Sellers**, T. Frielle
- CHED 522.** Analysis of a hibiscus-mango blonde craft beer during fermentation. **K. Vedan**, M.A. Steiger
- CHED 523.** Improving bioavailability by selective pruning of glycosylated molecules: The crystal structure of a Rrhamnosidase from novosphingobium sp. PP1Y. **B. Terry**, M.H. Sazinsky
- CHED 524.** Effect of over-expression of an engineered RAD18 variant on repair outcomes at CRISPR/Cas9 induced double stranded breaks. **A. Palacios**, A. Gupta, T. Nambiar, A. Ciccia
- CHED 525.** Biosynthesis of new diketopiperazine natural products from unnatural amino acids. **R. Lopez**, A. Lane
- CHED 526.** Effectiveness of apocynin-based antioxidant agents. **G. Gray**, E.J. Merino
- CHED 527.** Building a genetic library of biofuel producing proteins using rational design and random mutagenesis techniques. **L. Kim**, J. Freeman
- CHED 528.** Use of agar and natural butters as antibacterial surfaces. **J.B. Coughlin**, T. Rosenking, K. Melkonian, J.I. Rizzo
- CHED 529.** Characterization of adenosine deaminase from *Mycobacterium tuberculosis*. **W. Osae**, C.A. Sarisky
- CHED 530.** Solid-phase peptide synthesis, purification, and analysis of short peptides for potential antimicrobial applications. **T.C. Montoya**, M.J. Crawford
- CHED 531.** Allosteric aptamer scaffolds for detection of miR-92a. **J. Anderson**, N. Hughes, N. Nguyen, M. Moss, M.F. Ali
- CHED 532.** Candidate RNAi screen to identify novel regulators of membrane turnover in *C. elegans*. **K. Mahurkar**, C.P. Olsen
- CHED 533.** Responses of protein kinase and zinc finger protein of leishmania under different stresses. **H. Song**, N. Carter, L. David, P. Wilmarth, S. Tannouri
- CHED 534.** Exploration of flavin-based self-quenching using newly designed allosteric aptamers. **M. Moss**, N. Nguyen, J. Anderson, N. Hughes, M.F. Ali
- CHED 535.** Converting glycosidases to glycosynthases: Developing catalysts for synthesis of peptidoglycan fragments. **T.J. Blakely**, J.E. Hanson
- CHED 536.** Analyzing the binding of a zinc-finger protein to its target DNA. **S. Delaney**, C. Chant
- CHED 537.** Investigating the effect of manganese mutation rate in *E.coli* strain CHS101 and CSH104. **A. Edobor**, **C.P. Quinonez**, **A. Avalos**, **S. Rodriguez**, P. Lee



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- CHED 538.** Macromolecular crowding effects on detergent solubilized porcine liver cytochrome P450 reductase. **J. Miller**, D.W. Seybert
- CHED 539.** Probing the *Mycobacterium tuberculosis* Rv3802 with covalent and non-covalent inhibitors. **C.M. Schreidah**, C.M. Goins, D.R. Ronning
- CHED 540.** Elimination of 2-ethynylpyridine polymerization using E11Q, a mutation of bacteriophage T4 lysozyme. **W.D. Turner**, S. Thomas, E. Cureau, T. Leeper
- CHED 541.** Determining the activation energy of the light-dependent assembly of the oxygen evolving complex. **E. Napier**, A. Garmany, J. Board, D. Kolling
- CHED 542.** Withdrawn
- CHED 543.** Investigation of G-quadruplex structure formation within pre-miR-1249. **M. Then**, M. Mihailescu
- CHED 544.** Role of conserved heme residues in the oxygen-sensing mechanism of the SmFixL protein from *S. meliloti*. M. Reynolds, **D. McCann**, **E. Dispenziere**
- CHED 545.** Prevention of oxidative damage from Mn²⁺ on *Escherichia coli*: A closer look at strains CSH104, CSH101, and CSH102. **C. Flores**, M.K. Parmar, M. Minasyan, P. Lee
- CHED 546.** Investigating Tat-SF1 interactions with HIV-1 RNA. **J. Trautman**, A. North, S. Roszczenko, K.H. Fogarty, H.B. Miller
- CHED 547.** Kinetics studies of archaeal PurO and PurH1-related cyclohydrolases. **M. Johnson**, C.A. Sarisky
- CHED 548.** Effects of macromolecular crowding on rabbit muscle aldose reductase. **B. Roman**, D.W. Seybert
- CHED 549.** Effect of Anthocyanin-rich purple corn extract on the healthspan of *Caenorhabditis elegans*. **D. Shaw**
- CHED 550.** Effect of amino acid concentration on metabolism in cells lacking P27kip1. **S. Sullivan**, R.J. Sheaff
- CHED 551.** Investigating human glyoxalase-I inhibition by a glutathione-methyleneoxindole conjugate as a means of anti-cancer therapeutics. **E. Perry**, E.J. Brush
- CHED 552.** Determination of the zonula occludin-1 phosphorylation pathway: Tight junction disassembly in diabetic retinopathy. **M. Kreiser**, R.L. McCann
- CHED 553.** Identification of novel indoleamine-2,3-dioxygenase inhibitors as potential immunotherapy additives. **R. Bacani**, O.J. Alao, J.C. Dicesare, R.J. Sheaff
- CHED 554.** Development of maltose binding protein purification for cytochrome c. **M. Simpson**, H. Prieto
- CHED 555.** Effects of novel naphthoquinone derivatives on topoisomerase activity. **A. Rowe**, O.J. Alao, J.C. Dicesare, R.J. Sheaff
- CHED 556.** Analyzing the role of Tat-SF1 in HIV-1 RNA stability and export. **M. Hulver**, A.E. Goodwin, H.B. Miller



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- CHED 557.** Cooperativity and competition in the binding of intercalators and groove binders to DNA. **S.A. Winkle, N. Rodriguez,** D. Gomez, J. Singh, G. Valdes
- CHED 558.** Preventative treatment of oxidative damage using green tea catechins. **M.J. Bossert,** K.M. Halligan, J.M. Fautch
- CHED 559.** Difference of tRNA gene distribution between three low-GC bacteria. **G. Sebastiao,** R.L. Moore
- CHED 560.** Development of artificial cartilage hydrogel using silk fibroin solution and polyvinyl alcohol. **A. Borik,** K.M. Halligan
- CHED 561.** Identification of functionally important residues in histone H2A.Z in *Saccharomyces cerevisiae*. **O. Geesaman**
- CHED 562.** Generation and identification of opioid metabolites using CYP102A1 mutants. **R. Liliedahl,** D.C. Haines
- CHED 563.** Implications of RecA binding in *Mycobacterium tuberculosis*. **K. Rickman,** R.L. Moore
- CHED 564.** Quantification and source tracking of fecal indicator bacteria from beaches and drains of the Saginaw Bay Watershed in Bay County, Michigan. **T. Vogel,** O. Bishop, B. Hart, T. Sivy
- CHED 565.** Structural determinants of substrate selection in erythromycin resistance methyltransferases. **G. Munezero,** A. Amanor, C. Schoose, J. Dunkle
- CHED 566.** Developing an assay for fluorescent visualization of in vitro mitochondrial DNA transcription. **K.A. Bruce,** M. Bestwick
- CHED 567.** Increasing the health of human dermal cell function through the topical application of a nitric oxide delivering emulsion. **C. Henderson,** J.P. Yapor, Y. Zang, M.M. Reynolds
- CHED 568.** Protein encapsulation inside the HK97 virus-like particle. **B. Ceessay,** D. Patterson
- CHED 569.** Quantitative DNA analysis of fecal contamination levels and sources from Saginaw Bay Watershed sites in Michigan's Thumb. **O. Bishop,** T. Vogel, B. Hart, T. Sivy
- CHED 570.** Development of an intranasal alginate-based drug delivery system containing β -casein for the treatment of Alzheimer's disease. **D.J. Sanchez Rodriguez,** L. Aponte Cruz, M.P. Alvarez
- CHED 571.** MMP-9 cleavage of self-assembling amyloid peptides. **J. Bell,** J.E. Smith-Carpenter
- CHED 572.** Investigating the effectiveness of the antioxidant catechin hydrate on artemisinin activity *in vitro*. **W. Zander,** C. Hartwig, C.K. Saner
- CHED 573.** Kinetic characterization of recombinant human peptidylarginine deiminase type 2. **M. Malgarini,** R. Sharma, D. Barko
- CHED 574.** Effects of unpredictable chronic stress on the epigenome of the Zebrafish brain. **N.A. Weirath,** V. Huang, F. Lubin
- CHED 575.** Components of *Cinnamon verum* (cinnamon) and *Salvia officinalis* (Sage) in 4T1 breast cancer cells. **M. Nicholson,** J. Tudman, A.J. Reinhart, G. Gray



TECHNICAL PROGRAM

- CHED 576.** Elucidating the physiological conditions of human protein arginine methyltransferase 7. **K.R. Miller**, S.G. Clarke
- CHED 577.** Separation of nucleic acids by ion pair reversed phase high performance liquid chromatography. **Z. McLeod**, M. Bestwick
- CHED 578.** Cloning, overexpression, purification and characterization of rapidly growing mycobacterial L,D-transpeptidases. **K. Melinosky**, **R. Parker**, L. Basta
- CHED 579.** Alteration in enzymatic activity due to a mutation in bacteriophage lysozyme. **E. Cureau**, S. Thomas, W.D. Turner, T. Leeper
- CHED 580.** Identifying drug combinations to specifically target cancers with deregulated p27kip1. **D. Raval**, A. Kalantari, R.J. Sheaff
- CHED 581.** Synthesis of a macrocyclic mimic of hydrolytic metalloenzyme active-site. **K. English**, C. Pizza, M. Harris, A. Lajmi
- CHED 582.** Elderberry extract modifies the proteostasis network and extends lifespan in *C. elegans*. **K. Manning**, **N. Botelho**, B.C. Nguyen Viet, S. Swope
- CHED 583.** Metabolism of different amino acids by cells lacking the tumor suppresser p27. **R. Kaur**, R.J. Sheaff
- CHED 584.** Extraction, characterization, and screening of plant extracts used in the traditional medicine of Zambia. **A. Cowart**, C. Mills
- CHED 585.** Exploring the ethanol inhibition of protein synthesis. **K.A. Pohl**, G.H. Purser, R.J. Sheaff
- CHED 586.** Terpene storage in *Nicotiana benthamiana* leaf lipid droplets. **W. Crum**, Y. Cai, K. Chapman, A. Stoeckman
- CHED 587.** Synthesis of a tri-functional, cysteine specific D and L-amino acid probe library to investigate the effects of probe chirality on protein selectivity in breast cancer cells. **K. Harrison**, **N. Suminski**, S. Couvertier, N.E. Lee, C. Saitow
- CHED 588.** Effect of hydrogen bonding on the conformation dynamics of an Ω -loop of iodothyronine deiodinase. **A. Tran-Thompson**, J. Garcia, E.S. Marsan, C.A. Bayse
- CHED 589.** Withdrawn
- CHED 590.** Interaction of diazabicyclooctane β -lactamase inhibitors with class C β -lactamases. S.T. Lefurgy, A. Fedorov, E. Fedorov, **H. Servius**, M.D. Barnes, K. Papp-Wallace, S. Almo, R.A. Bonomo
- CHED 591.** Recombinant expression of preptin analogs for alanine scanning mutagenesis of residues 21-24. **T. Anguilm**, **A. Scott**, J. Love, J.M. Meyers
- CHED 592.** Does hydrogen sulfide inhibit DNA double strand break repair? **A.K. Singh**, L. Harrison
- CHED 593.** Using marinobufagenin as a biomarker for the diagnosis of mild traumatic brain injuries. **M.M. Dent**, E. Csuhai
- CHED 594.** Using RNA interference for the identification of the acp3U enzyme in higher eukaryotes. **J. Burchett**, D. Ruwe, M. Thomas, R. Bales, J. Rabe, J.B. Mamaril, M. Guy



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- CHED 595.** Investigation of carnosic acid mitigation of amyloid beta (A β) effects in SH-SY5Y cybrid neuroblastoma cells. L.A. Wetmore, **Z. Hand**
- CHED 596.** Studies of the oxidative mechanism of the copper amine oxidases. **B.C. Taylor, R.A. Krevh**, S.A. Mills
- CHED 597.** Elucidation of the efficacy of the antitumor quinones, isobutyl-deoxyxyboquinone and beta-lapachone in a *BRCA1*-mutant breast cancer cell line expressing elevated NQO1 levels. **K. Brokaw**, L. Palmquist, M.C. Srougi
- CHED 598.** Effects of kavalactones on acetylcholinesterase (AChE) activity in *Caenorhabditis elegans*. **J. Chappel**, B. Kautu, O. Casanueva
- CHED 599.** Bacterial adherence of *Streptococcus sanguinis* to pulmonary heart valve replacement tissue. **K. McKenzie**, B. Norling, L. McKinley, A. Stoeckman, K.E. Rohly
- CHED 600.** Identification of affibody molecules that target crotalid snake venoms and targeted protein identification. C. Collom, **C.Z. Garcia**, E. Osborne, C.J. Noren, K.A. Noren
- CHED 601.** Exploring the effects of single point mutations of *Arabidopsis thaliana* cryptochrome 1 (*AtCry1*), a plant protein involved in blue light response. **E.R. Shockley**, L. Haerr, J. Kavanagh, J. Sternen, S.A. Mills, J.J. Link, D. Engle, M. Ahmad
- CHED 602.** Examination of the DNA binding affinity and specificity of *p*-bromo- and *p*-iodo salicylaldehyde aldimines. **A. Klingel**, L. Ndambuki, **K.R. Gallagher**
- CHED 603.** How tumors survive suffocation: The role of p27kip1 in adapting to hypoxia. **A. Saleh**, R.J. Sheaff
- CHED 604.** Characterization of G-protein coupled receptors for EET isomers. **C. McElrath**, W. Campbell, A. Herrreiter
- CHED 605.** Flotation biochemical markers in healthy and anxious participants. **S. Arledge**, R. Zhu, A. Alarbi, J. Feinstein, W. Potter
- CHED 606.** Novel RNA phosphoramidite monomers: Distinguishing 2'-OH from 3'-OH. **J. Davis**, V.K. Dunlap
- CHED 607.** Temporal dynamics of the extrinsic pathway of apoptosis. **C. Zwemer**, R. Reif
- CHED 608.** Comparison of propagation rates in the M13mp bacteriophage series. **R. Aldakhlallah, M. Salemi**, M.F. Hall
- CHED 609.** Alternate locations for the lacZ α insert in an M13-based cloning vector. **E. Botelho, D. Sheedy**, M.F. Hall
- CHED 610.** Genetic analysis of the M13mp bacteriophage series. **L. Gray**, M.F. Hall
- CHED 611.** Oxidation of lignin monomers. **Z. Taylor**, B.E. Sturgeon
- CHED 612.** Hyponitrite reactivity with heme proteins. **Q.C. Durfee**, B.N. Bradley, E. Tresch, C.R. Andrew
- CHED 613.** Aptamer selection assisted by graphene oxide. **M.D. Hoppe**, B.C. Peterson, B.G. Staebler-Siewell, A.G. Cavinato
- CHED 614.** Template-based engineering of stacked c-type hemes. **C. Sommerville**, J. Kleingardner



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- CHED 615.** Using MOE to investigate potential ligands for StarD6. **D. Borchart**, G. Papale
- CHED 616.** Effect of LIF on the integrity of the dendritic synapsis in neuronal cells after HIV-Nef protein treatment *in vitro*. **N. Guevara-Rivera**, J. Alves, Z. Reyes Bou, M. Cruz Rentas, B. Velázquez Pérez, E. Santiago, Z. Rios, R. Hunter Mellado, R. Noel
- CHED 617.** Analysis of antibacterial properties of *Phlox divaricata*. **A. O'Rourke**, M.A. Fisher
- CHED 618.** Enhancing the rate of ester hydrolysis with peptides. **R. Morris**, A.F. Kleman, S.H. Gellman
- CHED 619.** Inhibition of oxidative DNA damage by an aqueous extract of spinach. **D. Lezo**, **A. Ramirez**, A. Gallano, T. Nguyen, M. Martinez, P. Perez, E.D. Stemp
- CHED 620.** Comparing macromolecular crowding's effect on protein aggregation in globular proteins to intrinsically disordered proteins. **S. Whittaker**, M.A. Fisher
- CHED 621.** Protein prenylation and implications in Alzheimer's disease. **C. Brown**, M.D. Distefano
- CHED 622.** Characterization of the monomeric form of the Sigma-1 Receptor. **C.J. Koch**, M.R. Macbeth, W.C. Hong
- CHED 623.** Characterization of the effects of deprenyl on developmental rates in *C. elegans*. **H. Folse**, **W. McLean**, K. Weeks
- CHED 624.** Design and implementation of an undergraduate nanotechnology lab: Generation of double crossover DNA tile with gel electrophoresis characterization. **A. Abram**, R.C. Nangreave
- CHED 625.** Preliminary studies on the biosynthesis of the chemotherapeutic bleomycin by *Streptomyces verticillus*. **H. Befekadu**, C.T. Calderone
- CHED 626.** Investigating the active sites of the succinyltransferases DapD and TabB. **E. McGregor**, C.T. Calderone
- CHED 627.** Effects of elderberry extract on the Insulin/ IGF-1 (IIS) pathway of *Caenorhabditis elegans*. **C.L. Frignoca**, K. Manning, N. Botelho, S. Swope
- CHED 628.** Synthesis and evaluation of a series of carbazole derivatives with anti-virulence activity methicillin-resistant *Staphylococcus aureus* (MRSA). **R. Berndsen**, W.A. LeFever, A.J. Wommack, H.B. Miller, M.S. Blackledge
- CHED 629.** Structure-activity relationship analysis of MutY variants for OG:A recognition. **J. Zaleta**, C. Majumdar, S.S. David, A. Manlove
- CHED 630.** ATM signaling pathway mediates apoptosis in *SF3B1* mutant zebrafish. **E. Sharvit**, S. Nik, T.V. Bowman
- CHED 631.** Utilization of the NAH7 metabolic pathway in fracking waste remediation. **C. Fogg**, K. Drake
- CHED 632.** Withdrawn
- CHED 633.** Effect of concentration and mutation on the conformational dynamics of MTHFR. **R. Guo**, E.M. Marzluff, E.E. Trimmer, A. Glebov-McCloud



TECHNICAL PROGRAM

- CHED 634.** Investigating the catalytic potential of supramolecular nucleopeptide assemblies. **J. Dorsainvil**, J.E. Smith-Carpenter
- CHED 635.** Use of an inexpensive surface plasmon resonance instrument to determine the binding of α -lactalbumin to fragmented antibodies. **K.E. James**, D.A. Wing
- CHED 636.** Thermal stability and kinetic constants of a model enzyme to improve computational design. **H.L. Torres**, P. Huang, J.B. Siegel
- CHED 637.** Antifreeze proteins shape ice crystals to prevent freezing injury. **N. Dembitzer**, R. Drori
- CHED 638.** Profiling reactive cysteines in the endoplasmic reticulum. **C. Li**, M. Abo, T.J. Bechtel, E. Weerapana
- CHED 639.** Investigating the ability of a bleomycin analog to cleave RNA. **M. DeFeo**, A. Angelbello, M.D. Disney
- CHED 640.** Development of agonist, antagonist, and positive allosteric modulator functional assays for the 5-HT₃ ligand-gated ion channel. **B.A. Eley**, R.A. Kramer
- CHED 641.** Identification and evaluation of small molecules with antibiotic activity in *Mycobacterium*. **M. Seemann**, M.S. Blackledge
- CHED 642.** Cost-effective CoA dimer purification through various types of charcoals and solvents. **M. Cha**, H. Choe, J.D. Stewart
- CHED 643.** Antibiotic activity of N,N'-bis-substituted 1,2,4-triazolium salts with cyclic substituents. **T. Guthrie**, C. Rose, J.M. Meyers
- CHED 644.** Characterizing cytotoxic activity of carbon-60 (buckminsterfullerene). **E. Loe**, R.J. Sheaff
- CHED 645.** Withdrawn
- CHED 646.** Deducing the mechanism by which ebselen delays maturation and protects against oxidative stress in *C. elegans*. **M. Guell**, K. Weeks, M. Kay
- CHED 647.** Identifying small molecules that modulate the ability of huntingtin to bind membranes. **A. Stonebraker**, J.A. Legleiter
- CHED 648.** Inhibition of oxidative DNA-protein crosslinking via an aqueous extract of kale. **A. Gallano**, **T. Nguyen**, D. Lezo, A. Ramirez, P. Perez, M. Martinez, E.D. Stemp
- CHED 649.** Kinetic isotope effects and transition state analysis for *Escherichia coli* poly-N-acetylglucosamine synthase. **A. Liu**, M. Poulin
- CHED 650.** Synthesis of resveratrol & quercetin derivatives for targeting cancer cell line T3HA. **C. Hammes**, C. Kriley
- CHED 651.** Production and characterization of 2,5-diketopiperazines produced by the cyclodipeptide synthase SNC-109. **P.G. Borgman**, A. Lane
- CHED 652.** Genetic engineering of *Escherichia coli* to produce nocardiozine natural products. **K. Patterson**, A. Lane



TECHNICAL PROGRAM

- CHED 653.** Anthocyanin as a potent inhibitor and/or remodeling effector of β -amyloid aggregation. **B.C. Nguyen Viet**, S. Swope
- CHED 654.** Characterizing 2,5-diketopiperazines produced by a cyclodipeptide synthase enzyme from *Streptomyces*. **J. Phillipps**, A.L. Lane
- CHED 655.** Biosynthesis of (R)-phenyllactyl-CoA in *E. coli*. **M. Wang**, A. Zhang, M. Matson, S. Atsumi
- CHED 656.** Metalloenzyme mimic with esterase activity. **M. Gulsby**, L. Carroll, S. Peyer, T. Best, A. Lajmi
- CHED 657.** Developing fluorescence correlation spectroscopy (FCS) method for fluorescence quantum yield determination. **R.A. Romero**, K. Hamadani
- CHED 658.** Endothelial cell-associated sialic acid and sickle cell disease. **G.L. Becker**, Z. Kiser, J. Belcher, G. Vercellotti
- CHED 659.** Protein bioconjugation to soft microgel particles. **L. Oliver**, J. Weatherington, M. Gaines
- CHED 660.** Protein quantification analysis on surface-functionalized microgel particles. **D. Ingabire**, N. Anderson, M. Gaines
- CHED 661.** Determining a progression timeline of type 1 diabetes through decreasing insulin production. **A. Short**, W. Joesten, M.A. Kennedy
- CHED 662.** Fluorescence localization of the conjugation machinery of *Bacillus subtilis*. **H. Dame**, M.B. Berkmen
- CHED 663.** Fluorescent detection of reactive oxygen species in *Saccharomyces cerevisiae* applied to chronological lifespan. **K. Schultz**
- CHED 664.** Analysis of oligomerization and protein-protein interactions within the conjugation machinery of *Bacillus subtilis*. **A. Ragucci**, M.B. Berkmen, K. Swerdlow
- CHED 665.** Computational identification of protein scaffolds for the generation of artificial metalloenzymes. **P. Robbins**, E. Reynolds
- CHED 666.** Where, how and how much: Novel porphyrins for photodynamic therapy of triple negative breast cancer. **A. Podguzov**, J.E. Bradshaw, T.E. Hayes
- CHED 667.** Characterizing the structure of styrene-maleic acid copolymer-lipid nanoparticles (SMALPs) using RAFT polymerization for membrane protein spectroscopic studies. **B. Harding**, G. Dixit, K. Burrige, I. Sahu, C. Dabney-Smith, R. Edelman, D. Konkolewicz, G. Lorigan
- CHED 668.** Investigation to locate the binding site and mode of electron transfer between two proteins, KshA and KshB. **C.F. Santos**, S.R. Soltau
- CHED 669.** New evidence for the diversity of mechanisms and protonated Schiff bases formed in the non-enzymatic covalent protein modification (NECPM) of HbA by the hydrate and aldehydic forms of acetaldehyde and glyceraldehyde. **B. Smith**, J. Lewis, H. Oakes, R.W. Holman, K. Rodnick
- CHED 670.** Characterization and inhibition of the Zika viral protease. **P. Roche**, B. Hicks



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- CHED 671.** Evaluating the roles of active-site residues in catalysis and iron-binding in L-DOPA dioxygenase. K.L. Colabroy, **V.R. Basciano**, **B.A. Shimanski**, **K.M. Travitz**, T. Hoffmann, K. Mayer
- CHED 672.** Development of multimodal drugs targeting the inhibition of the methylerythritol phosphate (MEP) pathway. **P. Gross**, C. Grosdemange-Billiard, D. Lièvreumont, M. Rohmer
- CHED 673.** Investigating the effects of ionizing space radiation on potassium ion channels through immunocytochemistry and cell viability studies. **M. Neal**, A. Walker
- CHED 674.** Mixed enzyme systems for biomass delignification. **R. Hughes**, **A. Maalouf**, E.M. Woolridge
- CHED 675.** Identification of conserved motifs important for Trm732 function. **D.J. DiVita**, M. Guy
- CHED 676.** Screening potential inhibitors of the Sigma-28 transcription factor. **J. Pieslak**, S. Apel, J. Allen, S. Shechter, M. Gage
- CHED 677.** Studying the methods of extraction and purification of insulin for diabetic treatment. **K. Malone**, N. Beres
- CHED 678.** Analysis of effects on tRNA modification on hyphal growth by the elongator complex in *C. albicans*. **J. Rabe**, D.J. DiVita, R. Morgeson, J. Kappes, J. Carmen, M. Guy
- CHED 679.** Mechanism studies of thiosemicarbazone inhibition on human topoisomerase II α . **K.R. Lyons**, M.A. Toma, X. Jiang, E.C. Liscic
- CHED 680.** Optimization of the expression, growth, and purification of toxoflavin lyase. **A. Long**, W. Gunderson
- CHED 681.** Effect of growth factors on the metabolism of cells lacking the tumor suppressor p27kip1. **R. Khattab**, R.J. Sheaff
- CHED 682.** Investigation of vinculin from *Monosiga brevicollis* in respect to multicellularity. **L. Ibarra**, R.H. Singiser
- CHED 683.** Effect of retinoid receptor agonists on K562 cellular proliferation. **W. Higgins**, S. Freyaldenhoven, M.D. Kelley
- CHED 684.** Chiral biasing of enantiomeric helical peptides composed of alpha-aminoisobutyric acid residues. **S. DeLucia**, B. Elvir, M. Korst, M.A. Kubasik
- CHED 685.** Investigation and perturbation of PEP-19's conformational ensemble. **J.W. Johnson**, D. Ordonez, T. Dunlap
- CHED 686.** Epigenetic interactions between methyltransferase SWN and chromatin remodeler PKL. **J. Dean**, J. Long, J. Ogas
- CHED 687.** Second dissociation constant (pK₂) of the zwitterionic buffer compound TES from 5 to 45°C. **G. Altan**, J. Omair, T. Wehmeyer, Y. Kang, L. Berquier, L.N. Roy, R.N. Roy
- CHED 688.** Analyzing correlations between genetics and ecology of Big Bend bacteriophages. **H. Hillert**, G. Krukonis
- CHED 689.** Elucidating the enzymatic mechanism of toxoflavin lyase. **C. Nissen**, W. Gunderson



TECHNICAL PROGRAM

CHED 690. Locating, cloning, and characterizing the anticoagulant properties of *Helobdella modesta*. **A. Maddox**, M. Nelson, R.V. Valcarce, P.J. Iles, L.D. Giddings

CHED 691. Protein-ligand docking: Neuraminidase mutation resistance to antiviral drugs. **A. Ward**, J. Grinstead

CHED 692. Green tea regulation of sugar metabolism. **N. Hmeluk**, R.J. Sheaff

CHED 693. Using peptide mimics to disrupt the binding of transcription factor NF- κ B to κ BDNA. **K. Guevara**, A.L. Stewart

Section I

Orange County Convention Center
West Hall C

Undergraduate Research Posters

Biotechnology

Cosponsored by BIOT and SOCED
N. Di Fabio, J. Roberts, *Organizers*

12:00 - 2:00

CHED 694. Transport activity of RLIP76 (RalBP1) across the biome: Identification of genomic targets. **V.M. Appelgate**, J.L. Smith

CHED 695. Improving total and active expression yields for adenosine receptor chimeras. A.R. Jain, **S.H. Stradley**, A.S. Robinson

CHED 696. Synthesis of an albumin-doxorubicin prodrug conjugate via a traceless, reductively labile cobalt crosslinking strategy. **A. Patel**, A. McGhee, R.A. Petros

CHED 697. Quantification of rutin and chlorogenic acid in *Sambucus mexicana* extracts using HPLC and analysis of their anti-inflammatory properties in macrophage cells. **K. Carter**, P.M. Joyner

CHED 698. Withdrawn

CHED 699. Biochemical inactivation of glucosinolates in *Brassica carinata* using molecular cloning techniques. **K.M. Hall**, T. Nguyen, J.D. Stewart

CHED 700. Engineering AQUAMORENE, a fluorescent biosensor prototype to report real-time water dynamics in living tissues. **K. Lin**, T. Kleist, H. Cartwright, y. xu, D. Ehrhardt, L. Feng, W. Frommer

CHED 701. Investigation of antiferromagnetic properties of Co_3O_4 nanoparticles produced via bacterial medium. **R. Loughran**, S. Nellutla, J. Mendell

CHED 702. Biosynthesis and characterization of Cd nanoparticles from metal reducing bacterium *Shewanella oneidensis*. **R.M. Payne**, D. Painter, S. Forney, G. Martini, M. Temple, S. Lampa-Pastirk



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

CHED 703. Developing the HK97 virus-like particle as a nanomaterial platform. **M. King**, D. Patterson

CHED 704. Withdrawn

Section I

Orange County Convention Center
West Hall C

Undergraduate Research Posters

Chemical Education

Cosponsored by SOCED
N. Di Fabio, J. Roberts, *Organizers*

12:00 - 2:00

CHED 705. Extraction of natural products as an introduction to commonly used laboratory techniques, polymer materials, and fluorescence in the organic chemistry laboratory. **M. Phan**, A. Villalta-Cerdas

CHED 706. Analysis of particulate level understanding in an atoms first general chemistry course. B. Roach, **C. Suess**, D.K. Dillner, T.S. Ritchie, M.A. Teichert, M.J. Schroeder

CHED 707. MTeach: Pathway to a successful career in chemical education. **R. Marlin**, J.M. Iriarte-Gross

CHED 708. Analysis of general chemistry student samples for concentration of copper in a percent composition laboratory experiment. **E. Storck**, C.J. Ohrenberg

CHED 709. Synthesis of o-thiocarbamoyl substrates for application in nucleophilic aromatic substitution in the undergraduate organic chemistry laboratory. **A. Kelly**, D. Viernes

CHED 710. Developing assessments that integrate students' chemistry and biology knowledge. **B. Pardinias**, L. Santiago Caobi, K. Parent, R.L. Matz, S.M. Underwood

CHED 711. Investigating students' perception of their general chemistry and introductory biology courses.. **L. Santiago Caobi**, B. Pardinias, K.P. Kohn, A.T. Kararo, M. Cooper, S.M. Underwood

CHED 712. Withdrawn

CHED 713. Coupling Raman and infrared spectroscopy in organic chemistry. **M.P. Fares**, **K.P. Smith**, **S.R. Hange**, M.D. Sonntag, C. Hamann

CHED 714. Using resonance to teach novel enolate chemistry and polymerization reaction mechanisms: A capstone organic laboratory experiment. **D. Dukes**, **L.A. Bonner**

CHED 715. Diversifying STEM through community college social integration. **A. Peck**, E. Salazar, A. Wilt, A. Sanderlin, M. Hoyle



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- CHED 716.** Investigating the alignment between secondary inquiry chemistry activities and assessments. **V. Borland**, A.G. Schafer, E.J. Yeziarski
- CHED 717.** 3D printing: A tool for creating accurate chemical models. **T.H. Pham**, W.T. Grubbs
- CHED 718.** General chemistry students' conceptual understanding of thermochemistry in a biological context. **N. Garza**, J. Nyachwaya
- CHED 719.** Developing a poly(lactic acid) / nylon 6-6 polymer experiment. **C. Coleman**, S.A. Henrie
- CHED 720.** Exploring the effects of *Quality Talk* discussions on students' scientific argumentation in a high-school chemistry laboratory. **C. Camplese**, S. Baszczewski, A. Butler, P. Murphy
- CHED 721.** General chemistry students' perceptions of the particulate nature of matter in different physical states. **S. Berg**, J. Nyachwaya
- CHED 722.** Withdrawn
- CHED 723.** Evaluation of three possible pathways to synthesize an asymmetrical alcohol by a Grignard reaction. **J. Bachmann**, **S.B. Ward**, N. Hollabaugh, B. Quarles
- CHED 724.** Withdrawn
- CHED 725.** Alcohol analysis in the undergraduate laboratory: A comparison of analytical methods. **M.C. Bernard**, S. Ghosh, M. Sabo
- CHED 726.** Using screencast and simulations to help chemistry students understand equilibrium. L. Miling, S. Archiyan, **J.R. Vandenplas**, D.G. Herrington, R.D. Sweeder
- CHED 727.** Developing an undergraduate lab that informs how experimental data guide the development of reaction mechanisms. **K. Weaver**, J.A. Reeves, E.J. Yeziarski, S. Bretz, D. Konkolewicz
- CHED 728.** Analysis of analogies related to particulate nature of matter in chemistry textbooks commonly used in Nigeria. **S.A. Somadhi**, M.M. Sulaiman
- CHED 729.** Using eye-tracking data to determine what general chemistry students attend to when completing a three-dimensional modeling activity. **T. Gordon**, J. Calvert, X. Prat-Resina, C. Terrell, A. Randolph, K.J. Linenberger Cortes
- CHED 730.** Synthesis and spectroscopic/spectrometric analysis of the pharmaceutical phenytoin demonstrating the Pinacol rearrangement. **M. Roberts**, B. Stockman, K. Valcarce, M. Andersen, C. Webb, R.V. Valcarce, P.J. Iles, L.D. Giddings, M. Alvarez, R. Kochambilli, W. Sanders
- CHED 731.** Increasing the accessibility of the rainbow flame test by utilizing household chemicals. **A. Rossi**, A.J. Carroll
- CHED 732.** Mathematics/chemistry tutorials influence student performance in College Chemistry II. **E.C. Wilcox**, F.M. Yarberry
- CHED 733.** Using eye-tracking data to determine what organic chemistry students attend to when completing a three-dimensional modeling activity. **L. Bateganya**, A. Hampton-Ashford, J. Calvert, C. Terrell, A. Randolph, K.J. Linenberger Cortes



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- CHED 734.** Effect of laboratory videos on student performance in College Chemistry II. **H. Barnes, E. Hollinger, F.M. Yarberry**
- CHED 735.** Does it resonate? Exploring the continuum of understanding related to the chemical concept of resonance. **A. Bishop, K. Enneking, T.C. Coombs, N.P. Grove**
- CHED 736.** Administration of the flame test concept inventory with confidence scale to general chemistry students. **C. Spieser, Z. Allred, S. Bretz**
- CHED 737.** First annual chemistry night: An exploratory opportunity for high school students to learn college-level wet lab and instrumentation techniques. **L. Lenczycki, A.M. Nienow**
- CHED 738.** Investigation of imine hydrolysis. **C. Ancharki, D.P. Predecki, J. Kegerreis**
- CHED 739.** Form versus function: A comparison of Lewis structure drawing tools and the extraneous cognitive load they induce. **E. Paulson, K. Amir Hakim, K. Enneking, N.P. Grove**
- CHED 740.** Utilization of GC-MS for arson accelerant determination. **C. Slezak, C.V. Gauthier**
- CHED 741.** Assessing students' misconceptions using the acid-base, redox, and bonding concept inventory. **K.L. Yeziarski, T.N. Abell, G.H. Allen, S. Bretz**
- CHED 742.** Does a targeted intervention utilizing physical manipulatives help students better answer quiz and exam questions on often difficult organic chemistry concepts? **S. Connell, K.Y. Neiles**
- CHED 743.** Development of an assessment to measure students' understandings of solution concentration. **C.J. Dobbs, T.N. Abell, S. Bretz**
- CHED 744.** Using 3D printing technology to recreate historically accurate teaching models from the 1800s. **C.E. Caldwell, J.D. Mendez**
- CHED 745.** Kinetics and characterization of gold nanoparticles synthesized from polyphenols of *Vaccinium corymbosum*: A green approach. **D.J. Shell, C.K. Saner**
- CHED 746.** Inorganic chemistry teaching lab: A metal-organic framework inspired experiment. **T. Barker, J.J. Meyers**
- CHED 747.** Development of an inventory to measure students' understandings of elements and compounds using particulate representations. **L. Huff, Z. Allred, S. Bretz**
- CHED 748.** Information retention and chemical demonstrations. **C. Mortensen, T. Hislop, A.J. Noble, T.L. Sorey**
- CHED 749.** Microwave-assisted digestion of alloys coupled with spectroscopic analysis of manganese, nickel, and chromium: Modern sample preparation in the analytical chemistry laboratory. **B.J. Estes, D.B. Green**
- CHED 750.** Immediate benefits of incorporating an undergraduate maintenance team at a small military college. **Z. Webster, G. Dominguez, M.L. Agan**
- CHED 751.** Examining Chaverri's 1953 periodic table: A chemical and historical study. **J.J. Montero, S.E. Solano, M. Jimenez, N. Ulloa, L. Corea, J. Leiton, S. Sandi**



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- CHED 752.** Near-peer mentoring: Building leadership skills and communal relationships through an immersive living-learning STEM camp. F. Musko, **A. Lesko**
- CHED 753.** Engaging middle school students with chemistry demonstrations in an after-school program. **D. Moriarty**, A.J. Carroll
- CHED 754.** What is the periodic table to college chemistry students? **J.P. Artavia Solano**, J. Brenes, B. Ulate, C. Valenciano, S. Sandi-Urena, J. Leiton-Chacon
- CHED 755.** Terminal alkyne reactions in organic laboratory development: Microwave assisted hydration vs. hydroboration. **Q. Savage**, **F. Sink**, P.A. Shelton
- CHED 756.** Reduction of 9-fluorenone to 9-fluorenol as an undergraduate organic laboratories using FastWoRX-M. **M. Regotti**, D. Brownholland
- CHED 757.** Using the COPUS Analyzer to interpret results from the COPUS. **I. Lopez**, **J. Harshman**
- CHED 758.** New techniques for demonstrating renewable energies in a classroom setting. **E. D'Eredita**, S. Lampa-Pastirk
- CHED 759.** Alternative methods for the demetalation and metal insertion of iron-free cytochrome c for implementation in undergraduate laboratories. **R. Pedretti**, S. Lampa-Pastirk
- CHED 760.** Effect of repeated low-stakes assessments on students' test-anxiety, attitude, self-concept, and achievement in a non-science majors chemistry course. **M.M. Villegas**, J.Y. Chan
- CHED 761.** Identifying the knowledge and skills needed for chemistry: An exercise in precision of language. **N. Usher**, J. Harshman
- CHED 762.** Temperature controlled sample holder for reimagining the iodine absorption experiment. **M. Minich**, D. Albert
- CHED 763.** General chemistry students' reasoning about bonding: Translating between symbolic and space-filling representations of a combustion reaction. **K. Ferguson**, M. Popova, T.N. Abell, S. Bretz
- CHED 764.** Promoting chemistry through effective chemistry outreach. M.W. Fultz, **O. Gharib**
- CHED 765.** Withdrawn
- CHED 766.** Investigation of correlations between mental rotation ability, sex, and solid-state learning in general chemistry students. **R.M. Towne**, S.D. Wiediger
- CHED 767.** Modified S_N2 ether synthesis mechanism as safer alternatives in the undergraduate laboratory. **R. Dohoney**, S.M. Schelble
- CHED 768.** Development of a guided-inquiry based undergraduate laboratory module: The preparation & analysis of copper (II) sulfate crystal formations. **C.N. Miller**, C.E. MacGowan, R. Groom
- CHED 769.** An undergraduate teaching oriented approach to reaction investigation and optimization. **A. Spencer**, **J. Floreancig**, S. Lulhe
- CHED 770.** Development of an online organic chemistry course and the most faced challenges. **M. Cordero**, J. Figueroa



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

CHED 771. Integrating chemistry and biology: Student application of intermolecular forces in denaturation of DNA. **A. Farias**, K. Parent, R.L. Matz, S.M. Underwood

CHED 772. Improving analyses for general chemistry laboratory students: Comparison of methods for the determination of percentage copper in a solid sample. **M. Daniel**, C.J. Ohrenberg

CHED 773. Comparison of the performance of General Chemistry 2 students who have taken the Chemistry 1A/1B series and the accelerated General Chemistry 1 course. **A.I. Eugster**, J. Donnelly, N. Lapeyrouse, C. Yestrebsky

CHED 774. Analyzing the effectiveness of a pilot community service learning project in the undergraduate chemistry laboratory. **H.H. Grewal**, **J. Khalil**, C.C. Lovallo, K. Ho

Section I

Orange County Convention Center
West Hall C

Undergraduate Research Posters

Colloid & Surface Chemistry

Cosponsored by SOCED
N. Di Fabio, J. Roberts, *Organizers*

12:00 - 2:00

CHED 775. AFM characterization of alkanethiolate self-assembled monolayers on zinc selenide thin films. **B. Rhodes**, S. O'Boyle, A. Sredenschek, A.R. Noble, N. Hellgren

CHED 776. Development of robust hydrophilic self-assembled monolayer resists for putrescine oxidase immobilization on gold nanostructures. **T.M. Nguyen**, N.J. Kamathewatta, R.T. Lietz, D.O. Deay, S. Seibold, J. Meyer, B. Tomas, B.T. Karaca, T. Hughes, M.L. Richter, C. Tamerler, C.L. Berrie

CHED 777. Feasible synthesis of high surface area, porous and magnetic graphitic carbon spheres. **J.G. Jeskey**, M. Jaroniec, A.C. Dassanayake

CHED 778. Deformability analysis of ultra-soft microgel particle to adhesive surfaces. **G. Brim**, P. Kamuche, E. Westbrook, L. Williams, M. Gaines

CHED 779. Investigating physiochemical properties of nanoemulsions and effects on particle size. **A. Bigness**, V. Nouri, E. Perez, S. Franceschi

CHED 780. Morphological changes of semiconductor nanocrystals in ligand-saturated solutions. **I. Bergman**, D. Khon

CHED 781. Synthesis and deposition of silica and gold nanoparticles for sensing applications. **Y. Astter**, **S. Bingham**, **M. Regotti**, J.S. Kirk

CHED 782. NMR investigation of the effect of pH on counterion binding to amino acid-based surfactant micelles. **G. Mahant**, F.H. Billiot, E. Billiot, Y. Fang, K.F. Morris



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- CHED 783.** NMR investigation of micelle formation by phenylalanine-containing biosurfactants. **E. Pieroni**, F.H. Billiot, E. Billiot, Y. Fang, K.F. Morris
- CHED 784.** Functionalized materials for oxyanion capture. **E.E. Robinson**, M.H. O'Neil, K.M. Nell
- CHED 785.** Exploring the addressability of DNA decorated multifunctional gold nanoparticles with DNA origami template. **R. Nixon**, W. Liu, S. Yang, R. Wang
- CHED 786.** Graphene oxide-polyethylenimine lightweight solution processed rust barrier for aluminum copper alloys. **S. Medor**, C. Gerwitz, R.K. Larsen, T. Townsend
- CHED 787.** Modifying carbon electrodes with sulfur and gold nanoparticles to study the kinetics of redox reactions. **J.E. Kelm**, **E.M. Ness**, J.C. Lytle, J. Parker, D.R. Rolison, J.W. Long
- CHED 788.** Synthesis and functionalization of nitrogen-doped graphene with benzene chromium tricarbonyl. **K.N. Robinson**, K. Vinodgopal, A. Elias, M. Terrones, K. Fujisawa, H. Zhu
- CHED 789.** Patterning conjugated polymer growth by microcontact printing. **I.E. Postle**, P. Lundin, B. Augustine
- CHED 790.** Concentration-specific interfacial activity of polymer/surfactant complexes at the oil/water interface. **E. Hopkins**, B. Schabes, G. Richmond
- CHED 791.** Amino acid behavior studied at relevant conditions with EC-STM. **I. Baljak**, J.A. Phillips, K. Boyd, E.V. Iski
- CHED 792.** Thermal stability of silver halide nano-alloys on Au(111). **L.K. Harville**, J.A. Phillips, H. Morgan, G. LeBlanc, E.V. Iski
- CHED 793.** Effects of ligand electron structure on the molar absorptivity of InP QDs. **C. Henderson**, K. Schnitzenbaumer
- CHED 794.** Nanoprecipitation of functionalized resorcinarenes. **M.D. Lohr**, A. Benedict, B. Ramjee
- CHED 795.** Investigating the effects of amino acids on silver halide thin films on Au(111). **K. Boyd**, J.A. Phillips, I. Baljak, L.K. Harville, E.V. Iski
- CHED 796.** Chiral functionalization of resorcinarene cavitand nanocapsules. **M.E. Johnson**, S. Allmon, B. Ramjee
- CHED 797.** Electrodeposition of synthetic melanin on transparent electrodes. **M. Cole**, D.M. Wirth, G. LeBlanc
- CHED 798.** Electrochemical deposition of polyaniline onto flexible and transparent electrodes. G. LeBlanc, D.M. Wirth, **M.J. Petty**
- CHED 799.** Surface chemistry of crystal violet on titanium dioxide. **K. Boehnke**, S. Coon
- CHED 800.** Can physical properties of polymers be used to predict stability of gold nanoparticle films? **S.T. Nicolau**, L.B. Thompson
- CHED 801.** Semiconductor-Independent effect of pH on the growth of photodeposited silver nanoparticles. **T. Maxson**, M. Collins, T.S. Zubkov



TECHNICAL PROGRAM

- CHED 802.** Transfer of biomolecules from an aqueous to non-aqueous liquid phase. **M. Beckoff**, S.E. Maurer
- CHED 803.** Controlled gold nanoparticle (AuNP) aggregation: Aggregate toxicity in *D. Magna*. **C. Vandermeer**, S.E. Lohse
- CHED 804.** Phase partitioning of nucleic acids into non-polar solvents. **P. Thorpe**, S.E. Maurer
- CHED 805.** Transferring RNA into organics. **M. Dooling**, B. Burcar, L.D. Williams
- CHED 806.** Hybrid graphene oxide-gold nanomaterials for targeted cancer theranostics. **K. Bukovec**, A. Smith, Y. Jones
- CHED 807.** Multifunctional graphene composites for targeted detection and destruction of multiple myeloma cancer cells. **A. Smith**, K. Bukovec, Y. Jones
- CHED 808.** Investigation of nanomaterials for inhibition of amyloid plaque formation in multiple myeloma cancer. **R.B. Vance**, Y. Jones

Section I

Orange County Convention Center
West Hall C

Undergraduate Research Posters

Computational Chemistry

Cosponsored by COMP and SOCED
N. Di Fabio, J. Roberts, *Organizers*

12:00 - 2:00

- CHED 809.** Analysis of solvatomorphic transitions in acyclovir. **B.J. Lopes**
- CHED 810.** Protein-protein surface modeling of DSB repair complexes. **V. Acuna**, R. Hopper, R. Petreaca, R.J. Yoder
- CHED 811.** Stabilization calculations on the anion states of *cis*- and *trans*-1,3,5 hexatriene. A.J. Sutter, M.C. Fair, **M.F. Falcetta**
- CHED 812.** Paths to quitting: Substrate trajectories and energetics in and out of cytochrome P450 2A6. **A. Chandrasinghe**, K.E. Johnson
- CHED 813.** Crowding or accommodation: How a surfactants structure and orientation affect an organic-water interface. **S. Opfer**, K.E. Johnson
- CHED 814.** Prediction of a non-valence temporary anion shape resonance for a model (H₂O)₄ system. D.N. Maienshein, M.C. Fair, **M.F. Falcetta**
- CHED 815.** *Ab initio* structure prediction and homology modeling of recombinant tissue plasminogen activator. **H.L. Torres**, A. de Jesús, J.A. Santana



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- CHED 816.** Comparison of the stabilization and smooth exterior scaling methods in determination of the energy and lifetime of temporary anions using 1-D model potentials to model shape resonances. H.G. Tack, M.C. Fair, **M.F. Falcetta**
- CHED 817.** Automated and accessible computational chemistry benchmarking. **W. Adams**, R.S. Paton
- CHED 818.** Understanding the fate of products after reactivation of acetylcholinesterase with QM/MM simulations. **M. Haerle**, F. Célerse, E. Derat
- CHED 819.** Assigning trigger bonds in novel high energy density materials using DFT and Wiberg bond indices. **J. Garcia**, C.A. Bayse
- CHED 820.** Molecular dynamics simulation study of AG10 and tafamidis binding to the V122I mutant of transthyretin. **R. Geoghegan**, Y. Fang, M. George, W. Southerland, K.F. Morris
- CHED 821.** Electron correlation, cascading and collisional effects in the 3C/3D line ratio in Ne-like ions. **E. Pena**, M. Gu, P. Beiersdorfer, J.A. Santana
- CHED 822.** Relativistic MR-MP Energy Levels for the Li isoelectronic sequence. **E. Pabon Vazquez**, J.A. Santana
- CHED 823.** Modeling solid-fluid transitions of biological tissues. **J. Kang**, P. Sahu, G. Erdemci-Tandogan, L. Manning
- CHED 824.** Ensemble efficiencies in osmotic pressure simulations of concentrated aqueous salt solutions. **K. Beardslee**, B.L. Eggimann
- CHED 825.** Binding of rhenium(I) tricarbonyl-labeled cocaine-like compounds to the dopamine transporter protein. **A. Miller**, N.R. Lien, C. Jordan
- CHED 826.** Computational molecular dynamics study of heteroepitaxial growth patterns comparing Cu/Ni and Pt/Ni on Ni(100). **P. Weiss**, K. Haug
- CHED 827.** Regioselectivity of acid-catalyzed epoxide ring-opening reactions. **P.L. Broom**, D.A. Osborne, S.A. Smith, D.H. Magers
- CHED 828.** Computational investigation of the ring-opening polymerization of ϵ -Caprolactone and the low dispersity of the polycaprolactone. **D. Garcia**, B. Wilson
- CHED 829.** Computational modeling of the absorption spectrum of gold nanorods in explicit solvent. **A. Tran**, E.B. Guidez
- CHED 830.** Computational studies of gas-phase hydrogen-deuterium exchange of tetrapeptides containing lysine and its homologs. **S. Farmer**, J. Poutsma, J.C. Poutsma
- CHED 831.** DFT + thermodynamics analysis of cation release from complex metal oxides: LiCoPO₄ (001) surface transformation. **N. Cartagena**, A. Abbaspour Tamijani, J.W. Bennett, J.A. Santana, S.E. Mason
- CHED 832.** Computational chemistry study of acinetobactin and its structural derivatives. **I. Garfias**, S. Ambre, C. Miller, P.M. Todebush
- CHED 833.** Halogenated warfarin derivatives bound to blood serum albumin. **E. Mitchell**, L.C. Bishop, E. Munyaneza, B.B. Magers, E.J. Valente, K.M. Bishop, R. Bishop



TECHNICAL PROGRAM

- CHED 834.** Computation of host-guest free binding energies with a QM-MM mining minima algorithm. **H. Yasini**, E.B. Guidez, K. Montgomery, T. Sattasathuchana, P. Xu, M.S. Gordon, S.P. Webb
- CHED 835.** Identifying potential inhibitors of the enzyme ERK5 using virtual screening. **J. Williamson**, P.M. Joyner
- CHED 836.** Making virtual screening accessible to non-experts through automation of library generation, ligand screening, and binding pose scoring in a single workflow. **S.M. Parker**, P.M. Joyner
- CHED 837.** Exploring wine data through data mining and data visualization. **B. Patel**, E.A. Aleman, M. Martin
- CHED 838.** Using natural bond order to understand bond length variation in molecules. **A. Ahmad**, E.D. Glendening
- CHED 839.** Animations of electron rearrangement in pericyclic reactions. **L. Brown**, E.D. Glendening
- CHED 840.** Theoretical studies on the length dependence of molecular rectification. **I.F. Guzmán González**, J.L. Palma
- CHED 841.** 12- and 18-electron rules for first-row transition metal complexes. **J.J. Nysschen**, E.D. Glendening
- CHED 842.** Benchmark of density functional theory for the transition metals. **D. Dahlberg**
- CHED 843.** Theoretical adsorption of lactic acid through benchmark metal-organic frameworks: Applications in computational chemistry. **A. Varghese**, T. Pham
- CHED 844.** Density functional theory study of cooperative ligand-centered reactivity in triaminoborane-bridged diphosphine complexes. **C. Kirkvold**, K. Lee, S.R. Daly, D. Vlaisavljevich
- CHED 845.** Computational analysis of corrole tautomers in various solvents. **N. Kaur**, C. Reed, J.A. Garfield, E.A. Aleman
- CHED 846.** HSP90 inhibitor binding kinetics and thermodynamics predictions using the SEEKR software program. L. Votapka, **J.M. Mitchell**
- CHED 847.** Theoretical studies of coherent transport in pi-pi stacking systems. **R. Peña**, J.L. Palma
- CHED 848.** Molecular dynamics investigations into pyrophosphatase hydrolysis and its effect on phosphorus nuclear spin entanglement. L. Votapka, **A. Stokely**

Section I

Orange County Convention Center
West Hall C

Undergraduate Research Posters

Environmental Chemistry

Cosponsored by ENVR and SOCED
N. Di Fabio, J. Roberts, *Organizers*

12:00 - 2:00



TECHNICAL PROGRAM

- CHED 849.** Diurnal enrichment of an initially minor bioactive rearrangement product from the aqueous photolysis of dienogest. **K.C. Breuckman**, E.E. Meyer, N.C. Pflug, D.M. Cwiertny, K.H. Wammer
- CHED 850.** Role of the deep brine layer in trace element cycling in the great Salt Lake. **A. Piskadlo**, F. Black, W.P. Johnson, A. Roberts, S. Yang, R. Rowlands, C. Rumsey, A. Reynolds, G. Pandey, M. Trejo
- CHED 851.** Irrigating wheat with produced water: Impacts on soil and crop health. **H. Hare**, H.A. Miller, T. Borch
- CHED 852.** Assessing the movement of heavy metals through soil using electro kinetic remediation processes. **B. Copeland**, B. Adair
- CHED 853.** Experimental use of plant based polymers as effective removal agents of solid and ionic contaminants from water. R. Srinivasan, **M. Mudd**
- CHED 854.** Involvement of outer membrane vesicles in the S(0) metabolism in *Chlorobaculum tepidum*. **C.B. Dull**, T.E. Hanson, A.T. Levy
- CHED 855.** Comparison of strontium isotopic ratios to nutrient and sediment concentrations in Ohio rivers. **B. Barno**, A.R. Roerdink
- CHED 856.** Revisiting the laboratory simulation of open limestone channels. **K. Grasso**, M. Karpinsky, K. Troxell, J. Schulte, A. Vassalotti, E.P. Zovinka
- CHED 857.** Quantification and removal of phosphorus from algal derived biodiesel. **E. Timmel**, D.S. Heroux
- CHED 858.** PDMS Sponge for remediation of endocrine disruptors and pharmaceuticals in water samples from South Florida. **M. Brown**, B. Ng, N.S. Quinete, P.R. Gardinali
- CHED 859.** Evaluation of heavy metals stored in mussel and fish tissue from the Kiamichi river of Southeast Oklahoma. **P.V. Dearington**, K. Roberts
- CHED 860.** Comparison of photolysis rate constants and identification of products in aqueous atmospheric aerosol mimics. **J.R. Sharp**, D. Grace, M.M. Galloway
- CHED 861.** Using multiple probe molecules to elucidate factors affecting the photoreactivity of excited triplet state dissolved organic matter in natural waters. **Y. Podorova**, **J.J. Kelley**, J.D. Thoemke
- CHED 862.** Quantification of aqueous nitrate phytoremediation by *Justicia Americana*. **M.A. Martin**, B.S. Arbaugh, M.E. Railing, J.F. Fuller
- CHED 863.** Application of biochemical polymers in sorption of crude oils. R. Srinivasan, **M. Meadows**
- CHED 864.** Nitrogen uptake and release by *Justicia Americana* in a tributary of the Ohio River. **B.S. Arbaugh**, M.E. Railing, J.F. Fuller, B.M. Stout
- CHED 865.** Factors affecting hydraulic sweep 'pills' efficiency in highly inclined well bores. **S. Batra**, N.E. Takach, E.M. Ozbayoglu, F. Rodriguez
- CHED 866.** Pertechnetate reduction by reactive rhodochrosite, a common Mn(II) mineral. **A. Cadet**, **N. Tran**, **V. Anagnostopoulos**



TECHNICAL PROGRAM

- CHED 867.** Determining trace amounts of semi-volatile pharmaceuticals and personal care organic compounds in effluent wastewater. **K. LaiHing**, J.R. Wood, R. Williams
- CHED 868.** Chemicals of emerging concern in plants, sediment, and water in a constructed wetland in Oregon. **G.C. Diepenheim, C. Harb**, S. Gift, J. Layshock
- CHED 869.** Interactions of nucleosides with montmorillonite. **H. Kats**, R. Sanders
- CHED 870.** Investigation on silver nanoparticles effects on *Brassica rapa*. **B. Dean**, B. Fox
- CHED 871.** Hydrodechlorination of trichloroethylene using rhodium 5% wt on alumina catalyst. **K. Flores**, A.A. Peterson
- CHED 872.** Isotherm studies for the removal of textile dye methylene blue by chitosan for wastewater treatment. **J. Taylor, A.H. Pinto**
- CHED 873.** Correlating dissolved oxygen concentration with dissolved organic matter. **M. Karim, V.I. Jaramillo**
- CHED 874.** Photocatalytic degradation of ibuprofen, ketoprofen, and naproxen with BiOCl. **K. DeFries**, R.B. Arthur, H.H. Patterson, E.A. Stemmler
- CHED 875.** Withdrawn
- CHED 876.** Comparison of calibration methods for the graphite furnace atomic absorption spectroscopic analysis of lead in drinking water. **M. Schanandore**, R. Mauldin
- CHED 877.** Impact of VOC functional groups on secondary organic aerosol formation. **J. Hall**, C. Avila, A. Hallward-Driemeier, A.J. Carrasquillo
- CHED 878.** Determination of PAH levels in Lake Champlain sediment. **A.C. Flueckiger**, C. Chant
- CHED 879.** Methane emissions from Galveston Bay and the northwestern Gulf of Mexico. **D. Gonzales**, S. Yvon-Lewis, J. Dedrick
- CHED 880.** Intrinsic reactivity of ions derived from anionic uranyl complexes that contain a mix of carboxylate and halide ligands. **A. Iacovino**, M.J. Van Stipdonk
- CHED 881.** Effectiveness of oyster aquacultures. **P. Giannini, C. Farnan**, D. Rogers
- CHED 882.** Transverse rupture strength of CeO₂ as a surrogate nuclear fuel. **J. Foster**, A. Lupercio, B. Jaques
- CHED 883.** Photocatalytic degradation of furosemide with TiO₂ catalysis: Effect of bicarbonate. **K. Flynn**, J. Chovelon, E. Menjivar, C. Ferronato, L. Fine, M.A. Tarr, M. Brigante
- CHED 884.** Effects of soil redox conditions on riparian zone ecosystem services and disservices. **W. Chace**, A.J. Gold, K. Addy
- CHED 885.** Particle formation in an environmental chamber: Reactions of trimethylamine, reduced sulfur compounds, and hydroxyl radical. **C. Michael**, R. Drover, T. Cress, P. van Rooy, D. Cocker, P.J. Silva, A. Foote, K. Purvis-Roberts



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- CHED 886.** Methods to study the interactions of mercury species with biological membranes. **K. Malone**, A. Johs
- CHED 887.** Photocatalytic degradation of naphthalene in simulated fracking water. **J.P. Driver**, J.E. Boyd
- CHED 888.** Photocatalytic degradation of propranolol. **S.E. Taylor**, J.E. Boyd
- CHED 889.** Bioaccumulation of methylmercury: Investigation of contamination in *Pylodictis olivaris* and *Ictalurus punctatus*. **A. Austin**, A. Brustkern
- CHED 890.** Defluorination of fluoroarenes under mild conditions using Rh-MOFs. **J. Mitchell-Jones**, A.A. Peterson
- CHED 891.** Geochemical and redox interactions between technetium and manganese (II,III) mineral haussmanite. **N. Shawver**, **J. Chang**, V. Anagnostopoulos
- CHED 892.** Preliminary study of microplastics in marine animals from Cape Cod bay. **C.D. Enos**, D.K. Bertram, B.S. Phalen, C.D. King
- CHED 893.** Genotoxicity studies of nanoscale Lithium Cobalt oxide to model bacterium *B. subtilis*. **M. Gari**, T. Pho, E. Laudadio, R.J. Hamers, V. Feng
- CHED 894.** Evaluating the long-term environmental impacts of carbamic acid derivatives. **R. Piper**, **K. Bland**, **J.J. Wirick**, K. Shuman, M.J. D'Souza
- CHED 895.** Factors affecting eutrophication: The health of the Chicago River. **J. Ramos**, T. Lam, F. Calderon, R. Sepulveda, M. Musa, D. Espiritu
- CHED 896.** UV photolysis of the polycyclic musk AHTN: Biological activity of photoproducts. **E.A. Stickney**, J. Cho, T. Grieder, M. Yeboah, S. Shadle, D. Martinovic-Weigelt, K.H. Wammer
- CHED 897.** Water adsorption on polyhydroxylate microspheres as a function of relative humidity using an FTIR spectrometer equipped with a flow cell. **H.H. Dana**, C.D. Botner, R.L. Parham, K.E. Morris, H.H. Hayes, M.M. Cassingham, C.D. Hatch
- CHED 898.** Withdrawn
- CHED 899.** Determining baseline water quality in the Fox River in anticipation of Waukesha, Wisconsin's switch to a Lake Michigan drinking water supply. **K. Burmeister**, J. Piatt
- CHED 900.** Investigation of colored dissolved organic matter in natural waters from the Chesapeake Bay Watershed in Upstate New York. **L. Milano**, T. Thomas-Smith
- CHED 901.** Phytoremediation in *Helianthus annuus*: Seedling establishment inhibition and translocation of cadmium in a simulated bioswale system. **A. Barto**, R. Mauldin, K. Larson
- CHED 902.** Improved understanding of the importance of bimolecular reactions of alkoxy radicals in organic aerosol. **J. Heini**
- CHED 903.** Sulfur dioxide is to dye for. **A. Eckert**, P. Hymas, J. Rosentreter



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- CHED 904.** Photodegradation of organic molecules using microporous vanadosilicate AM-6 based on size and polarity. **S. Streimer**, J. Mastandrea, K. Kilduff, J. Mattheisen, E. Hishiya, R. Tekin, A. Sacco, J. Warzywoda, M.N. Ismail
- CHED 905.** DDT extraction and analysis: A comparison of methods. **J.S. Wright**, P. Benz, M. Hopko, J. Liebens
- CHED 906.** Withdrawn
- CHED 907.** Photochemical degradation of the herbicide dicamba on heterogeneous surfaces. K. Gruber, **A.M. Nienow**
- CHED 908.** Contaminant transformation in the St. Louis River: The role of indirect photolysis. **J.A. Herrli**, R. Winkels, Q.T. Whiting, S.M. Berg, C.K. Remucal, K.H. Wammer
- CHED 909.** Determining the metal pollutants from the Elizabeth Mine: An EPA superfund site in Vermont. **S. Vaal**, S.M. Lamos
- CHED 910.** Water adsorption on polyhydroxylate microspheres as a function of relative humidity using a quartz crystal microbalance. **H.H. Hayes**, R.L. Parham, K.E. Morris, H.H. Dana, C.D. Botner, M.M. Cassingham, C.D. Hatch
- CHED 911.** Southern Illinois well water quality analysis project. **H. Frerker**, **L. Dameris**, H.D. Iler
- CHED 912.** Analysis of additive migration from bio-based plastic during simulated food contact. **L. Smith**, J. Layshock
- CHED 913.** Analysis of PM_{2.5} organic fraction: Quantification of bis(2-ethylhexyl)phthalate. **M.M. Cassingham**, G.G. Featherston, M.R. Sipes, K.E. Morris, R.L. Parham, H.H. Dana, O. Eddings, C.D. Hatch
- CHED 914.** Wastewater-based epidemiology. K.J. Bisceglia, G. Kroening, **M. Lakuleswaran**, **O. White**
- CHED 915.** Catalytic reduction of oxyanions using bimetallic nanoparticle carbon microsphere composites. **M. Beall**, **S. Schultz**, P.E. Colavita, K.M. Metz
- CHED 916.** Sediment composition in the barrier reef system near San Pedro, Belize. **M. Cohn**
- CHED 917.** Analysis of pollutant removal from environmental water samples by carbon nanotubes. **K. Cusick**, C. Cummings, T. Brady, M. Bida, R.E. Rogers, T.E. Pagano
- CHED 918.** Micro-plastic identification in the Anacostia River using micro-Raman spectroscopy. **A. Siskey**, M. Robinson, J. Meiller, R.K. Larsen
- CHED 919.** Monitoring volatile organic compounds from decomposition of cooking oils. **A. Davis**, D. Albert
- CHED 920.** Determination of iron and copper concentrations from various fields on the Willis family farm. **S. Willis**, R. Fietkau
- CHED 921.** Quantitative comparison of microcystin abundance in water by LCMSMS, Abraxis strip-test, and Abraxis ELISA methods. **M. Munneke**, A. Xiong, T.R. Miller
- CHED 922.** Withdrawn



TECHNICAL PROGRAM

CHED 923. Functionalized electrospun polymer mats as sorbents for polyfluoroalkyl substances (PFAS) in aqueous solution. **B.L. Bresnahan**, M. Nagorzanski, J. Qian, A. Martinez, D.M. Cwiertny

CHED 924. Evaluation of metal concentrations in near-stream sediments, Tri-state Mining District, Miami, OK. **C. Dallimore**, **C. Dallimore**, Q. Zhang, M. Schulmeister

CHED 925. Bioaccumulation capacity and physiological characterization of *Chlorella vulgaris* exposed to elevated Mn concentrations. **N. Perry**, A. Smythers, D. Kolling

CHED 926. AFM imaging of calcite surfaces. **M. Karpinsky**, K. Grasso, J. Schulte, K. Troxell, A. Vassalotti, P. Youmbi, E.P. Zovinka

CHED 927. Measuring Total Dissolved Solids (TDS) levels of drinking water samples using gravimetric methods. **A.N. Bowen**, E.C. Sylvester

CHED 928. Determination of total dissolved solids (TDS) in local drinking water using a TDS meter. **A.N. Yoho**, E.C. Sylvester

CHED 929. Instability and complexity of polycyclic musk galaxolide. **A. Crawford**, D. Makey, D.C. Harnes, K.H. Wammer, D.R. Stoll

CHED 930. Investigation of microplastic contamination of Pacific sea salts. **T. Potts**, K.A. Woznack, G. Gould

CHED 931. Characterization of secondary metabolites of *Fallopia japonica* by GC-MS. **S. Renninger**, M.J. Price, M. Li

CHED 932. Mapping elemental mercury emissions from gold shops in Portovelo and Zaruma, Ecuador: 2014-2017. **K.H. Moody**, **K. Hasan**, A.M. Kiefer

Section I

Orange County Convention Center
West Hall C

Undergraduate Research Posters

Geochemistry

Cosponsored by GEOC and SOCED
N. Di Fabio, J. Roberts, *Organizers*

12:00 - 2:00

CHED 933. Fluctuation analysis of redox potential during the formation of a chemical garden. **A. Miller**, A. Enright

CHED 934. Adsorption of multiple metal cations by Mn oxides. **K. Lugo**, Y. Tang

CHED 935. Role of cation hydrophobicity in mineral-assisted membrane formation. **R.K. Larsen**, G.M. Bowers



TECHNICAL PROGRAM

CHED 936. Cloud condensation nuclei (CCN) measurements: Design and calibration of a CCN analysis system. **R.L. Parham, K.E. Morris**, H.H. Hayes, O. Eddings, M.M. Cassingham, C.D. Hatch

CHED 937. Radiocarbon dating to determine time and cause of death of corals in Laie Bay, Hawaii. **A. Morgan, M. Nguyen, Y. Chang**, M. Cannon

Section I

Orange County Convention Center
West Hall C

Undergraduate Research Posters

Green Chemistry & Sustainability

Cosponsored by CEI and SOCED
Financially supported by ACS Green Chemistry Institute; I&EC Green Chemistry Subdivision
N. Di Fabio, J. Roberts, *Organizers*

12:00 - 2:00

CHED 938. Texas Christian University Green Chemistry Cleanup: Revamp, reorganize and recycle. **L. Goehring**, H. Carey, T.I. Gray, N. Henderson, H. Conrad, J. Fry, K.N. Green

CHED 939. Benign alkyne deprotonation in the high speed ball mill. **E. Quinn**, L.N. Trankina, J. Mack

CHED 940. Partial oxidation of methane at high equivalence ratios. **N. Penaloza**, A. Tran, E.B. Ledesma

CHED 941. Development of bifunctional thiourea catalysts for direct amidation reactions. **A. Guzman**, L. Boisvert

CHED 942. Conversion of CO₂ and CH₄: A research partnership between industry and academia. **C. Luong**, A. Tjandra, A. Nguyen, E.B. Ledesma

CHED 943. Biosynthesis and characterization of silver nanoparticles using extracts of *Leucaena leucocephala* leaves. **W.M. Betances-Perez**, C. Torres-Soto, C. Osorio Cantillo, J.I. Ramirez Domenech

CHED 944. Development of sustainable rechargeable batteries for use in grassroots electrification initiatives. L.A. Wetmore, **S. Arthurs-Schoppe**

CHED 945. Bifluoride ionic liquids with ultra-high stability for metal-ion *batteries*. **T. Hmissa, A. Mirjafari**

CHED 946. Methimazolium-based ionic liquids as potential gene delivery vectors. **D.J. Siegel**, J.E. Muller, A. Mirjafari

CHED 947. Mercaptothiazolium-based ionic liquids: Synthesis and thermophysical characterizations. **J.E. Muller**, T. Hmissa, D.J. Siegel, A. Mirjafari

CHED 948. Improving an organic potassium-ion battery. **P. Walsh**, S.J. Gravelle



TECHNICAL PROGRAM

- CHED 949.** Synthesis and thermophysical characterization of novel bio-based chiral and achiral ionic liquids. **R.D. Burton**, A. Mirjafari
- CHED 950.** Isotherm studies of equilibrium sorption of Pb^{+2} , Zn^{+2} , Ni^{+2} , Cd^{+2} , Cu^{+2} , V^{+2} unto modified composition algae. **D. Vo**, **A. Castillo**, R. Razeghifard, J.S. Brown, **D.G. Giarikos**
- CHED 951.** Heavy metal biosorption ability of *Neochloris* algae. **N. Nagabandi**, **J. Gaffney**, **J.S. Brown**, D.G. Giarikos
- CHED 952.** Synthesis of secondary amines with epichlorohydrin for reaction with cellulose to improve hydrophobicity. **M.M. McCloskey**
- CHED 953.** Preliminary investigation of the qualitative and quantitative exposure of college students to Bisphenol A. **A. Berube**, E.J. Brush
- CHED 954.** Exploring green chemistry methodologies in an analytical teaching laboratory. **F. Milazzo**, C.R. Pulliam, A. Thomas, N.J. O'Neil
- CHED 955.** From nature to materials: Progress towards the synthesis of novel polymers via the photocycloaddition of Fumaric Acid. **I. Bertini**, N.E. Huddleston
- CHED 956.** Concise and green synthesis of imines using microwaves. **A. Cestrono**, A.B. Waghe
- CHED 957.** Water effects on room temperature ionic liquids during electrochemical reduction process of crystalline silicon from silicon dioxide. **L.O. Juarez**, J.D. Sharp, G. LeBlanc
- CHED 958.** Cyclic asymmetric aldol additions and dehydrations in hot pressurized water. **O.V. den Besten**, **J.K. Berch**
- CHED 959.** Withdrawn
- CHED 960.** Investigating the breakdown of cellulosic materials in environmentally benign conditions. **C.A. Feagin**, **M.K. Stading**, J.K. Berch
- CHED 961.** Green Chemistry enhancing our daily lives. **S.M. Pérez Lajara**, **P. Rivero Santiago**, **D. Rosso Gonzalez**, **D.I. Oyola Soto**, L.I. Santiago
- CHED 962.** Fuel property assessment of *Shorea robusta* seed and oil from physico-chemical properties and thermal analysis. **M. Hasan**, M. Islam, M. Ismail
- CHED 963.** Economical and environmentally sustainable alternative to propylene oxide production. **S. Schweickart**, S.P. Phivilay, T. Agbi, I. Hermans
- CHED 964.** Urea-catalyzed Biginelli reaction via microwave irradiation. **E. Chapman**, M.T. Wentzel

Section I

Orange County Convention Center
West Hall C

Undergraduate Research Posters



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

Inorganic Chemistry

Cosponsored by INOR and SOCED
N. Di Fabio, J. Roberts, *Organizers*

12:00 - 2:00

CHED 965. Synthesis and catalytic studies of molybdenum complexes bearing analogues of the trimethimazolylborate ligand for use as biomimetic models of the sulfite oxidase enzyme. **N. Fitzpatrick**, M. Youmans

CHED 966. Quest of synthesizing new polynuclear transition metal complexes with the use of 4,5-bis(hydroxymethyl)-2-methylpyridin-3-ol (PNH₂). **K. Moncur**, A. Saha

CHED 967. Zirconium complexes as photosensitizers for solar energy conversion. **R. Gantzer**, Y. Zhang, C. Milsman

CHED 968. Syntheses, single-crystal x-ray analyses, spectroscopic and magnetic characterizations of polynuclear transition metal complexes incorporating the anion of 4,5-bis(hydroxymethyl)-2-methylpyridin-3-ol. **N. Shumate**, A. Saha

CHED 969. Water-soluble CdSe quantum dots by ligand exchange. **R. Jaquez**, R. Levesque, S. Lampa-Pastirk

CHED 970. XPS characterization of alkanethiolate self-assembled monolayers in zinc selenide thin films. **S. O'Boyle**, A. Sredenschek, B. Rhodes, N. Hellgren, A.R. Noble

CHED 971. Asymmetrical Bimetallic Ruthenium (II) complexes' interactions with DNA. **K. Powylan-Petschauer**, M. Mongelli, D. Milan

CHED 972. Synthesis and characterization of manganese carbon monoxide-releasing molecules (CORMs) containing a triazine ligand. **H. Daniels**, F.A. Beckford

CHED 973. Electrocatalytic carbon dioxide reduction with rhenium complexes. **M. Edwin**, **A. Tubbs**, S. Prasad, E. Freeman, J.W. Seyler

CHED 974. Catalytic conversion of carbon dioxide into value-added chemical over Fe₂O₃ supported catalysts. **A. Rosario**, C. Zhang, S.D. Senanayake

CHED 975. Optimization of metal-organic polyhedra (MOPs) for drug delivery and other biomedical applications. **C. Metcalfe**, Z. Fralish, J.F. Eubank

CHED 976. Synthesis, structure and electrochemical properties of nickel(II) compounds bearing a chiral, amino-acid derived phosphine ligand. **D. Sabo**, M.A. Bezpalko, W.S. Kassel, W.G. Dougherty

CHED 977. Arsenic levels in protein powder. **L. Lomeli**, F. Crean

CHED 978. Synthesis of chloro-oxime ligands and their transition-metal complexes. C.M. Davis, **A.D. Moore**

CHED 979. Synthesis of a metallacryptand complex. **S. Ramstrom**, C.M. Zaleski

CHED 980. Analysis of the structural and energetic properties of pyridine-SiCl₄ complexes via computations and IR spectroscopy. **B. Zehner**, A. Ley, P. Treacy, J.A. Phillips



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- CHED 981.** Functionalized gold nanorods as contrast agents for optical coherence tomography imaging of molecular retinal biomarkers in age-related macular degeneration. **J. Wolff**, A.E. Radwan, M. Amiji
- CHED 982.** Using charged metal-organic frameworks (MOFs) for controlled drug delivery. **B.T. Keller**, A.B. Spore
- CHED 983.** Exploring the structural and energetic properties of $H_3N-GeX_3CH_3$ complexes via IR spectroscopic and computational methods. **P. Treacy**, B.C. Zehner, A. Ley, J.A. Phillips
- CHED 984.** NMR solution studies of a novel pincer ligand with lanthanum(III) ion. **M. Newby**, M. Guino-o
- CHED 985.** Comparison of Re and Co complexes in the electrocatalytic reduction of CO_2 . **A. Dhawan**, M. Edwin, C. Scales, A. Todd, J.W. Seyler
- CHED 986.** Utilizing cyclophosphazenes as a drug delivery system. **E.G. Thomae**, C.L. Turpin, L.L. Hepp, N.A. Johnson
- CHED 987.** Synthesis and characterization of zinc chloride histidine, nickel chloride histidine, and cobalt chloride histidine. **N. Wilson**, F. Jackson
- CHED 988.** NMR characterization of pyruvaldehyde thiosemicarbazones (TSC's) and their metal complexes. **A.C. Koch**, E.C. Lisic
- CHED 989.** Synthesis and NMR characterization of new tert-butyl thiosemicarbazone compounds and corresponding palladium complexes. **C.E. Methvin**, E.E. Rush, E.C. Lisic
- CHED 990.** Synthesis and characterization of new photoactive and solvatochromic retinoid/carotenoid-based complexes of rhenium(I) attached to CdSe quantum dots. **D. Kee**, J. Bond, M. Shim, L. Zieammermann, A.J. Cruz, D.P. Rillema
- CHED 991.** Synthesis and characterization of a novel Zn(II) porphyrin incorporating TAMRA for use as a PDT agent. **S. Harris**, J.E. Bradshaw
- CHED 992.** Photoelectric production of methanol. **S. Ninneman**, **H. Dean**, **S. Cave**, **A. Morris**, **E. Lucciola**, K.C. McGill
- CHED 993.** Magnetic circular dichroism characterization of 3-mercaptopropionate dioxygenase variants. **E.P. Craddock**, R. Fernandez, T.C. Brunold
- CHED 994.** Facile synthesis of Chevrel-phase molybdenum selenides with applications in energy conversion and storage. **S. Jones**, J. Perryman, J. Velázquez
- CHED 995.** Synthesis, characterization, and contrast of novel tricarbonyl rhenium (I) octahedral complexes for fluoroscopic esophagography. **A. Spear**, S. Binkley
- CHED 996.** Exploring the boundaries of the Mannich condensation for preparing ligands to bind transition metals. J.R. Farrell, **W.J. Crowley**, **A.X. LaMothe**, L. Masnyk, T.J. Boyle
- CHED 997.** Synthesis and characterization of biopolymer-capped mesoporous silica nanomaterials loaded with toluidine blue dye. **C. Kinane**, B.G. Trewyn
- CHED 998.** Synthesis of pyridyl compounds to mimic bioinorganic enzymes. **K. Sommers**, W.M. Ames



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- CHED 999.** Europium-doped cerium oxide nanomaterials for the photocatalytic degradation of malachite green. **K. Aldrich**, A. D'Achille, J.L. Coffey
- CHED 1000.** Nuclear magnetic resonance analysis of atrazine chlorohydrolase small molecule mimics. **C. Carbajal**, S.S. Rocks
- CHED 1001.** Synthesis of unsymmetrical bidentate ligands from secondary phosphine oxides for "chiral-at-metal" complexes. **E. Nordquist**, **M.J. Brink**, J.R. Pedroarena, D.R. Tyler, B.P. Nell
- CHED 1002.** Reaction of a copper(II) centered Schiff-base complex with strong acid: A kinetic investigation. **C.J. Hansen**, J.J. Stace
- CHED 1003.** Synthesis and characterization of novel Re^{III} and Re^V based metalintercalator complexes. **E. Schwartz**, S.C. Haefner
- CHED 1004.** Different coordination stoichiometries using a novel pincer ligand with Eu(III) and La(III) ions. **N. Battaglia**, M. Guino-o
- CHED 1005.** Inorganic chemistry discovery laboratory: Utilizing solventless techniques in the synthesis of coordination metal complexes. M. Wilk, R. Alkhalaf, C. Grizer, H. Kouadio, T. Kirk, A. Limones, M. Nelson, C. Nguyen, H. Quoc Hai Pham, **J. Siverand**, A. Yanez, M. Omary
- CHED 1006.** Synthesis of titanium oxofluorides under hydrothermal conditions. **E.P. Miller**, D.H. Johnston
- CHED 1007.** Combinatorial synthesis of polyoxometalate derivatives. **R. Bentz**, **C.P. Hodges**, **R. Phillips**, **J. Williamson**, J.D. Powell
- CHED 1008.** Synthesis and reactivity of the diosmium diamide carbonyl complexes Os₂(CO)₆(RCONH)₂ (R = CH₃, Ph). **S. Costa**, M. Pearsall
- CHED 1009.** Study of Schiff base metal complexes for biomedical research applications. **S.M. Patberg**, M. Jeitler, J.R. Jeitler
- CHED 1010.** Synthesis of ruthenium(II) complexes of di-(2-picolyl)amine. **G. Hansen**, D.N. Blauch
- CHED 1011.** Mn(III)-porphyrin as catalyst in carvacrol oxidation by iodosylarenes under an eco-friendly approach. **B. Moraes**, A.S. Guimarães, A.M. Meireles, A.A. Lage, D.C. Martins, G. DeFreitas-Silva
- CHED 1012.** Synthesis of bis(cyclopentadienone)dicarbonyl complexes of Mo and W via cyclocarbonylation of α,ω -diynes. **H.I. Barr**, A.L. Poptic, M. Hoffbauer, R.J. Shively
- CHED 1013.** Investigations into the bonding preferences of lanthanide ions. **A.A. Brown**, E.M. Fatila
- CHED 1014.** Methods to target mixed-metal metal-organic frameworks for catalytic applications. **E.A. Alonso**, J.F. Eubank
- CHED 1015.** Toward the synthesis of unprecedented transition-metal nitride molecules. **A.R. Sumner**, **A.M. Dew**, N. Yamamoto, K.D. Herring, G.X. Monasterio, S.C. Addy, M.P. Nguyen, L.G. Beauvais, M.V. Bennett
- CHED 1016.** Moving anion sensing towards the finish line. M.O. Odago, **Z.F. Peterson**



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- CHED 1017.** Synthesis and characterization of heterodinuclear lanthanide complexes (Eu-Tb) for the generation of color-tunable LEDs. **R.E. Cooper**, B.J. Cooper, A.A. Brown, L. Sylvain, E.M. Fatila
- CHED 1018.** Evaluation of crystal packing motifs observed in structures of 5-methyl-6-phenyl-4-methyl-1,3,4-oxadiazinane-2-thione. **K.P. Kuzelka**, S.R. Hitchcock, G. Ferrence
- CHED 1019.** Synthesis of substituted trispyrazolylborate ligand-metal complexes as atrazine chlorohydrolase mimics. **M.D. Rittmanic**, S.S. Rocks, C. Carbajal
- CHED 1020.** Discovery laboratory style for Inorganic chemistry course: Tuning the photophysical properties of copper coordination complexes by modifying the synthetic methods and molar ratio. M. Wilk, R. Alkhalalah, A. Akinniyi, **A.A. Christopher**, C.R. Fraire, A. Gaspar-Mendoza, J. Logan, C. Perez, J. Pham, G. Scott, E. Theard, M. Omary
- CHED 1021.** Evidence of biomimetic type reactivity for a model system of nickel acireductone dioxygenase (Ni-ARD). **D. Saldana**, G. Blade, S.A. Toledo
- CHED 1022.** DFT study of the structure and biomimetic reactivity of nickel acireductone dioxygenase model systems. **J.B. Lumpan**, **B. Westbrook**, R. Parveen, S.A. Toledo
- CHED 1023.** Withdrawn
- CHED 1024.** Characterization and investigation into the anticancer activity of palladium and platinum phosphinoferrrocene metal complexes. **K. Girtain**, S.H. Schreiner
- CHED 1025.** Probing the effects of the ligand environment on the biomimetic reactivity of a nickel acireductone dioxygenase model system. **J. Jaimes**, S.A. Toledo
- CHED 1026.** New cationic and neutral nickel and platinum complexes based on PNP, PNN and POP ligands. S.H. Schreiner, **B. Shaw**
- CHED 1027.** Biomimetic reactivity of the first resting state analogue of nickel acireductone dioxygenase. **W.G. Ilustre**, S.A. Toledo
- CHED 1028.** *In-situ* assessment of shell surface cation exchange capacity of heavy metals Cd²⁺, Pb²⁺, and Zn²⁺ by XRF. **D. Rackie**, S.K. O'Shea
- CHED 1029.** Tuning efficiency and product formation in the iron-Induced decomposition of the potent greenhouse gas SF₆ and its analogs SF₅Cl and SF₅CF₃. W.S. Taylor, **C.L. Foscoe**, C. Emmerling, A.L. Harris
- CHED 1030.** Synthesis and characterization of some novel samarium organic framework complexes. **I. Williams**, C. Kriley, A. Morse
- CHED 1031.** Metal complexes of a heteroscorpionate with unique symmetries, optical, and magnetic properties. **A. Abdulrahim**, J. Fortner, m. martin, P. Desrochers, M. Provorse Long, N. Gerasimchuk
- CHED 1032.** Synthesis and characterization of soft-donor transition metal complexes. **K.M. Carson**, M.M. Miller, J.L. Brown
- CHED 1033.** Synthesis and characterization of a new Anderson-Evans polyoxotungstate with Cu(II) in its central cavity. **M. Pina**, S. Nellutla



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- CHED 1034.** Structural and electronic insights on supported mixed metal oxide catalysts. **K.L. Lawrence**, N. Stephens, R.K. Thakur, J.A. Moncada, C. Carrero
- CHED 1035.** Modeling cytochrome c_{552} / Cu_A interfacial electron transfer at gold electrodes modified with functionalized SAMs. **C. Cullip**, S. Hunter, N. Muren, K. Yokoyama, M.G. Hill
- CHED 1036.** Synthesis and metalation of expanded porphyrins. **H. Zafar**, J.T. Brewster, J.L. Sessler
- CHED 1037.** Organoarsine oxide metal–organic framework with electrophilic arsenic sites available for post synthetic modification. R.E. Sikma, **J.W. Fryer**, S.M. Humphrey
- CHED 1038.** Synthesis of CaF_2 and LaF_3 nanocrystals for use in silicon patterning. **R.R. Mitton**, A.W. Keller, C.B. Murray
- CHED 1039.** Photoluminescent boron avobenzene complexes with *R*-mandelate. **A. Wilke**, D.E. Janzen
- CHED 1040.** Structural studies of N-benzylcinchonidinium bromide for use in triboluminescent complexes. **M.S. Butler**, D.E. Janzen
- CHED 1041.** Synthesis and characterization of 1T-MoS₂ electrodes for CO₂ conversion. **K.E. Rivera Cruz**, F.P. Hyler, J. Velázquez
- CHED 1042.** Molecular sieving through pore window partition. **A. Dinh**, X. Zhao, X. Bu
- CHED 1043.** Synthesis and reactions of hexafluorocyclotriphosphazene. **I. Pierce**, C. Chen, H.R. Allcock
- CHED 1044.** Synthesis of linear multi-dentate ligands incorporating long-chain aliphatic aldehydes. **A. Rogers**, C. Blackwell, M.A. Benvenuto
- CHED 1045.** Preparation of thiocarboxylate ligands and related metal-organic frameworks. **K.S. Malloy**, J.W. Jamboretz, M.K. Mangun, E.A. Morley, J.J. Pak
- CHED 1046.** New family of lanthanide squarate containing materials. **N. Brenner**, **M. Polinski**
- CHED 1047.** Understanding how dipole dilution in hybrid perovskites affects photovoltaic properties. **J. Trowbridge**, E. Mozur, J.R. Neilson
- CHED 1048.** Synthesis and characterization of multinuclear Cu(II) clusters supported by pyridylamide ligands. **J. Schneider**, L. Yang
- CHED 1049.** Synthesis and characterization of Si(BIP)₂ complexes: Novel material for organic electronic device applications. **L.M. Stevens**, M. Kocherga, T.A. Schmedake
- CHED 1050.** Synthesis and characterization of a square planar Pt(II) carbene. **A.P. Deziel**, V.M. Iluc
- CHED 1051.** Development of a new synthetic method for the synthesis of iron containing ionic POSS polymers. M.T. Hay, **K. Fogerty**
- CHED 1052.** Synthesis and characterization of manganese carbon monoxide releasing molecules bearing ferrocenyl thiosemicarbazone ligands. **M. Lawrence**, F.A. Beckford



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- CHED 1053.** Investigation of ruthenium supramolecular hexamers from a chemical and biochemical standpoint. **J. McCray**, M. Niece, F.A. Beckford
- CHED 1054.** Synthesis of heterometallic metallacrowns. **A. Lewis**, C.M. Zaleski
- CHED 1055.** Synthesis and luminescent studies of heterometallic metallacrowns and sandwich molecules. **A. Smihosky**, C.M. Zaleski
- CHED 1056.** Catalytic transesterification of esters with cobalt and nickel(PNP) catalysts. **N.P. Stafford**, T. Thananathanachon
- CHED 1057.** Trapping guest molecules in MOF-5 with bulky capping groups. **K. Fossum**, J. Cintron, R. Cameron, R.L. Grimm, J. MacDonald, S.C. Burdette
- CHED 1058.** Steric and electronic effects of varying the ortho position of Ni(II) α -diimine catalysts on the properties of poly(1-hexene). **A. Metzger**, D. O'Connor, C. Tower, T.W. Chapp
- CHED 1059.** Synthesis and reactivity of a dimethyl diphosphine diruthenium complex. **N. Jovic**, R.M. Chin
- CHED 1060.** Exploring the formation of ionic cocrystals with zinc(II) salt. **E. Tinapple**, D.H. Johnston
- CHED 1061.** Topological variations of tungsten complexes of N₄ Ligands. **B. Kessler**, J.M. Keane
- CHED 1062.** Synthesis and characterization of novel rhenium(I) complexes for PDT and PACT. **M. Keane**, C. Rezsnyak
- CHED 1063.** Synthesis and characterization of a chiral, C₂-symmetric, tetraamine ligand and molybdenum complexes. **P. Menon**, J.M. Keane
- CHED 1064.** Development of nanoprecipitated water-insoluble gallium complexes for treatment of infections caused by cystic fibrosis. **K.M. Greskovich**, S. Huang
- CHED 1065.** Dynamic chelation behavior in neutral hypercoordinate diorganosilicon complexes of 1-hydroxy-2-pyridinethione. **E.R. Tiede**, B.D. Wilson, W.W. Brennessel, B.M. Kraft
- CHED 1066.** Synthesis and characterization of cationic organosilicon complexes of 8-hydroxyquinoline N-oxide. **K.I. Lowry**, W.W. Brennessel, B.M. Kraft
- CHED 1067.** Synthesis of Ru(bpy)₃²⁺rubredoxin-iridium(CP)(bpy)Cl photocatalytic hydrogen evolution system. **A. Brown**, S.R. Soltau
- CHED 1068.** Pyridine and sulfonate substituted M-NHC complexes. **J. Luo**, J. Corcoran, R.J. Swails
- CHED 1069.** Electrochemical impedance spectroscopy analysis of DSSCs fabricated with novel ruthenium dye species. **H. Wakidi**, C.J. Timpson
- CHED 1070.** Structures of metal complexes featuring heterocyclic nitrogen ligands. **K. Mulosmani**, R.K. Upmacis
- CHED 1071.** Synthesis of ZnO-SiO₂ nanocomposite in elastomeric foam for the photodegradation of pharmaceutical compounds. **M. Karod**, A. Perlin, M.N. Ismail, M. Berger, J.L. Goldfarb



TECHNICAL PROGRAM

CHED 1072. Complexation of lanthanides with the rhodizonate anion. **C.A. Nodarse**, J.A. Silverman, K. Kavallieratos

CHED 1073. *o*-Phenylenediamine derived sulfonamides for lanthanide and actinide extraction from alkaline aqueous media. **A.A. Rains**, E.V. Govor, K. Kavallieratos

CHED 1074. Silylation of pyridine and pyridine derivatives with diruthenium complexes. **J. Prybil**, R.M. Chin

CHED 1075. Solution vs. mechanochemical syntheses of lanthanide coordination complexes. **B.J. Cooper**, R.E. Cooper, A.A. Brown, L. Sylvain, E.M. Fatila

CHED 1076. Synthesis and characterization of titanium tantalum metal oxides. **M.L. Emmons**, J.L. Hunting

CHED 1077. Investigation in to the fundamentals of metal-organic frameworks and their potential biomedical applications. **R.M. Marusko**, J.F. Eubank

CHED 1078. Synthesis and stability of bis(imino)pyridine iron methyl complexes. **G. Pombar**, P.J. Chirik

Section I

Orange County Convention Center
West Hall C

Undergraduate Research Posters

Medicinal Chemistry

Cosponsored by MEDI and SOCED
N. Di Fabio, J. Roberts, *Organizers*

12:00 - 2:00

CHED 1079. Apoptosis induction and the effect of novel naphthoquinone analogues on the JAK-STAT pathway. **R. DeWeerd**, M. Manpadi

CHED 1080. Synthetic building blocks for drug development. **A.M. Lopez**, **E.F. Jurado**, T. Tieu Ngo, K.J. Friedrich

CHED 1081. Investigations into pancreatic anticancer activity of DCM-MJ-I-21 isoprenylated coumarin. **P.A. Hauke**, E. Kusaka, A. Webb, D. Carrico-Moniz

CHED 1082. Synthesis and anti-proliferative activity of *N,N'*-bis-substituted-2,4-triazolium salts with lipophilic and hydrophilic substituents. **T. Ta**, Z. Lin, S.S. Johnson, J.D. Gorden, M. Frazier, J.M. Meyers, K.L. Shelton

CHED 1083. Synthesis and analysis of novel furanocoumarin derivatives. **S.T. McComis**, D. Mulhearn

CHED 1084. Optimization, characterization and encapsulation efficiency analysis of Eudragit L100 nanoparticles loaded with fenofibrate by nanoprecipitation method. **G. Torres**, N. Günday Türeli, A. Türeli

CHED 1085. Synthesis and characterization of pyruvic aldehyde-1-oxime thiosemicarbazones and their complex formation with Cu(II).. **S.B. Crum**, E.C. Lisic



TECHNICAL PROGRAM

- CHED 1086.** Cleavage of DNA by aryl sulfoxides. **S. Loney, A. Hurley Predecki**
- CHED 1087.** Isolation of allantoin and apigenin from *Plantago major*. **E.O. Wade, J.M. Jerrils**
- CHED 1088.** Natural products to combat leishmaniasis: Chalcone-based anti-parasitics. **K. Solley, G.R. Naumiec**
- CHED 1089.** Thermal- shift assay development for finding novel antibiotics targeting a Cystic Fibrosis pathogen. **K.F. Meyberg, T.C. Leeper**
- CHED 1090.** Synthesis and screening of trehalose derivatives for antitubercular activity. **J. Kreisel, D. Chakrabarti, Y. Yuan**
- CHED 1091.** Fractionation of Hierba Manayupa extractions via flash column chromatography and their effects on HeLa cells. **C. Castillo, S. Deprele, L. Nogaj**
- CHED 1092.** Experimental and calculated distribution coefficients for the catechol flavones.. **S. Tuck, J.D. Hernandez, M.J. Risher, M.H. Abraham, W.L. Whaley**
- CHED 1093.** Investigating the antimicrobial properties of Mahamarichyadi oil. P. Dhar, H. Ho, **D. Mariniello, J.B. Greenough, K. Lemus Mortaya, E. Perez-Cabrera**
- CHED 1094.** Drug repositioning and diversification strategy for discovery of compounds with anti-cancer activity. **M. Chapa, D. Gibson, D. Bateman**
- CHED 1095.** Evaluation of nitro analogs of *trans*-cinnamaldehyde as mechanism based inactivators of cytochrome P450 2A6. **A. Nguyen, V. Chau, T. Raheel, J.M. Chan, J. Harrelson**
- CHED 1096.** Characterization of erlotinib polymorphs by solid-state NMR. **A. Viggiano, R. Iulicci, R. Quinones**
- CHED 1097.** Green synthesis of cholic acid derivatives as novel antimicrobials.. **D. Bolding, D.C. Bromfield-Lee**
- CHED 1098.** Design and synthesis of liver X receptor ligands. **C. Eaton, F.L. Payton, C. Gettridge, N.H. Tran, D. Spadoni**
- CHED 1099.** Isolation, characterization, and efficacy of quercetin derivative SRH 1-17-21 on T3HA mouse cancer cells. **S. Henson, E. Conto, D. Boyle, C. Kriley**
- CHED 1100.** Comparison of antioxidant activity mechanisms. **S. Carty, T. Ho, S. Ghaoui**
- CHED 1101.** Design, synthesis, and biological evaluation of isoindoliny moieties. **L. Planinc, D.C. Bromfield-Lee**
- CHED 1102.** Biomarkers of sleep-loss vulnerability and total sleep deprivation by metabolomics. **D. Van, A. Weljie, A. Sengupta**
- CHED 1103.** Spectroscopic studies on metallo- β -lactamases and inhibitors. **C.G. Miller, M. Crowder**
- CHED 1104.** Effects of alpha-hemolysin inhibitors on intraosteoblastic *Staphylococcus aureus*. **J. Rockafellow, B. Harville**



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- CHED 1105.** Synthesis and biological evaluation of new flavonoid-containing ceramide analogs having self-fluorescence. **C. Do**, T. Perry, M. Hill-Odom, T. Ponnappakkam, T. Huckaba, N. Goyal, M. Foroozesh
- CHED 1106.** Analysis of the folding and misfolding of Shadoo by nuclear magnetic resonance (NMR). **E.Q. Williams**, C. Chant
- CHED 1107.** Characterization of the transmembrane region of a novel ceftazidime resistance gene. **R. McDonell**, J. Donato
- CHED 1108.** Promise of natural products from actinomycetes located in tropical marine environments for drug discovery efforts. **S. Bailey**, J. Korchak, E. Protasov, A. Lane
- CHED 1109.** Molecular modeling on anticonvulsant enamines inhibiting voltage-gated sodium channels. **J. Kirkland**, I. Amaye, P. Jackson-Ayotunde, Y. Fang
- CHED 1110.** Evaluation of *Heracleum maximum* extracts as acetylcholinesterase inhibitors. P. Dhar, **J.B. Greenough**, **D. Mariniello**, **E. Perez-Cabrera**, **K. Lemus Mortaya**
- CHED 1111.** Biophysical characterization of a G quadruplex structure within MBNL 1 mRNA. **A. Moses**, M. Mihailescu
- CHED 1112.** MTN knockout attenuates vitamin synthesis and global metabolism in *E. coli* O157:H7. **M. Szolomayer**, **E. Paz Munoz**, M. Boll, K. Cornell, J.H. Thurston, S. Pu
- CHED 1113.** Efficient synthesis of squaramides from dibutyl squarate: Toward a treatment for Chagas disease. **A. Arykbayeva**, G.R. Naumiec
- CHED 1114.** Prenatal stress model of GAD abundance in the prefrontal cortex. **A.M. Hedges**, S. Cassella
- CHED 1115.** Importance of microglial activation in sex differences and their neurological effects on stress response and viable controls. **A. Carter**, S. Cassella
- CHED 1116.** Synthesis of *N*-benzoyl-2-hydroxybenzamide analogues for the treatment of malaria. **A. Nguyen**, G.R. Naumiec
- CHED 1117.** Differences in microglia activation in the actuate nucleus of the hypothalamus between males and females. **L.G. Schroeder**, S. Cassella
- CHED 1118.** Synthesis of a 1,2,4-triazolidine-3-thione library to be used as narrow spectrum antibiotics against *Acinetobacter baumannii*. L.J. Perez, **K. Gray**, S.V. Philippi, W. Civatte, R. Tenuto, A. Butterick, F. Morency
- CHED 1119.** Synthesis of espintanol-based natural products for the treatment of leishmaniasis. **K. Vinh**, G.R. Naumiec
- CHED 1120.** Developing a new water-soluble porphyrin as a potential photodynamic cancer therapy agent. **C. Shirley**, J.E. Bradshaw
- CHED 1121.** Synthesis of a novel water-soluble porphyrin derivative for use as a potential phototherapeutic cancer treatment. **T. Hankins**, J.E. Bradshaw
- CHED 1122.** Toxicology studies of potential therapeutics for the resurrection of the aged form of acetylcholinesterase after exposure to organophosphorus chemical nerve agents. **R. Hopper**, C. McElroy, C.M. Hadad, R.J. Yoder



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- CHED 1123.** Synthesis and apoptosis testing of a novel tris-indolyl compound for anticancer properties. **A. Wallace**, A. McNamee, T. Tolentino, C.R. Whitlock
- CHED 1124.** Cell viability studies of novel tripodal indolyl amines. **A. McNamee**, A. Wallace, T. Tolentino, C.R. Whitlock
- CHED 1125.** Squaramide-based anti-parasitics: The search for a new treatment for Chagas disease. **H.G. Howard**, G.R. Naumiec
- CHED 1126.** Effects of buffer concentration and temperature on the hydrolysis of aqueous L-arginine ethyl ester. **P.A. Harville**, A. Beffa, M.D. Reavis, G.H. Purser
- CHED 1127.** Synthesis of novel auxiliary molecules for stereospecific peptide ligation. **E. Stevens**, L. Impicciatore, N. Capriglione, M.T. Peterson, B.H. Williamson
- CHED 1128.** Artemisinin and its derivatives, a computational study of solubility in water and olive oil compared to *in vivo* elimination half-lives. J.D. Alia, **T. Kelly**, L. Judd
- CHED 1129.** On-resin solid-phase peptide synthesis of optimized peptide therapeutics. **Z. Fralish**, D. Flood, P. Dawson
- CHED 1130.** Synthesis and evaluation of macrocyclic carfilzomib analogs as inhibitors of the human 20S proteasome. **R.M. Price**, **G. Produturi**, G. Merrill-Steskal, R. Dorn, K.M. Godwin, M. Groll, M.G. Gotz
- CHED 1131.** Synthesis of substituted quinazolines as PTP1B inhibitors. **V. Isley**, A.M. Reeve
- CHED 1132.** Ambiguous nucleosides that heighten the HIV error load: Using viral mutagenesis to develop antiviral agents. **R. King**, V.K. Dunlap
- CHED 1133.** Natural remedies and cancer: *Bromelia pinguin's* aerial root extract induces HeLa cell and HCT-116 apoptosis. **S. Luna**, **S. Deprele**, L. Nogaj
- CHED 1134.** Exploration of natural remedies: The fractionation of *Annona cherimola* seeds and its effects on mammalian cancer cells. **P. Cheng**, S. Deprele, L. Nogaj
- CHED 1135.** Microencapsulation of anthocyanins in alginate hydrogels for potential applications in anti- β amyloidosis therapies. **A.D. Santiago-Mercado**, C.M. Osorio-Cantillo
- CHED 1136.** Synthesis and antioxidant evaluation of thioether derivatives of carvacrol. A. Cocolas, **E. Parks**, A. Ressler, M. Havasi, **G.E. Henry**
- CHED 1137.** Synthesis of the anticancer ene-hydrazide geralcin B. **T. Chavez**, R. Tello-Aburto
- CHED 1138.** Assessing aggregation of quinazoline inhibitors of protein tyrosine phosphatase 1B through a nuclear magnetic resonance assay. **A. Martin**, J. Kleingardner, A.M. Reeve
- CHED 1139.** Synthesis and antioxidant evaluation of thioether derivatives of thymol. M. Havasi, A. Ressler, A. Cocolas, E. Parks, **G.E. Henry**
- CHED 1140.** Effects of rosmarinic acid, an antioxidant found in *Salvia officinalis*, on triple negative breast cancer cell viability. **C.M. Holden**, K.A. Daus, M. Odom, H. Howard, K. Shannon



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- CHED 1141.** Fractionation of Hierba Santa extracts via flash column chromatography and their effects on HeLa cells. **A. Aceves**, S. Deprele, L. Nogaj
- CHED 1142.** Synthesis and biological activity of N,N'-bis-substituted-triazolium salts as potential anti-viral and antimicrobial agents. **Z. Lin**, T. Ta, J. Wilson, S.S. Johnson, J.D. Gorden, L. King, J.M. Meyers, K.S. Taylor
- CHED 1143.** Synthesis and biological examination of antibacterial peptide derivatives. **M. Pietrusiak**, E.K. Leggans, Z. Spahr
- CHED 1144.** Development of novel inhibitors to modulate trained immunity. **A. Cipriano**, F. Janssen, A. Lacour
- CHED 1145.** Screening medicinal plant extracts for inhibitors of breast cancer cell migration. **R. Petit**, S. Gutierrez, A. Peterson, **M. DiSanti**, **G. Cotto-Gonzalez**, J.M. Brown, C. Planchart, M. Cruz-Polanco, V. Trokhymchuk, A. Valls, D. Maul, L.C. Fernandez, M. Pina, A. Tapanes-Castillo
- CHED 1146.** Synthesis of a library of IspF inhibitors containing new zinc binding groups. **M.J. Rouffet**, J. Frye
- CHED 1147.** Antibiotic and anticancer activity from bacteria collected at a Roman archeological site. **A. Schick**, A. Hoffman
- CHED 1148.** Ciliary neurotrophic factor promotes regeneration of cochlear synapse after noise-induced cochlear synaptopathy in mice. **E. Rivera-Rosario**, N. Hu, S. Green
- CHED 1149.** Singular value decomposition and global fitting of fluorescence and circular dichroism spectra in combination with differential scanning calorimetry reveals the complex thermal denaturation of serum albumins.. **I. Pittman**, L.C. Bishop, D. Gou, C. Williams, K.M. Bishop, R. Bishop
- CHED 1150.** Study of antibiotic compounds from soil actinomycetes. **A. Gutierrez**, A. Hoffman
- CHED 1151.** Acute toxicity evaluation of a novel ceramide analog. **K. Bongay-Williams**, M. Hill-Odom, T. Saulsberry, N. Goyal, T. Ponnappakkam, M. Foroozesh
- CHED 1152.** Separation, purification, and spectroscopic characterization of chiral kavalactones from kava kava. **L.C. Bishop**, R.S. Effland, M. Wier, S. Weber, H. McAlexander, E. Brandon, K.M. Bishop, G.R. Bishop
- CHED 1153.** Modification of mithramycin SA for improved cytotoxicity. **K. Jenkins**, E. Miller, D. Scott
- CHED 1154.** Drug screening for metabolic inhibitors in cells lacking the tumor suppressor p27kip1. **A. Kalantari**, D. Raval, R.J. Sheaff
- CHED 1155.** Efficacy and efficiency of five desensitization drugs for the optimization of HLA incompatible kidney transplantation *in vitro* using ELIspot. **Y. Lee**, E. Cornwell, Y. Bae, J. Kwun, J. Yoon, S. Knechtel
- CHED 1156.** Synthesis of resveratrol analogues for testing on triple-negative breast cancer (TNBC) cells. **H. Benmerabet**, D. Paull
- CHED 1157.** Strategies toward combatting antimicrobial resistance through small molecule efflux pump inhibitors. **M.A. Nguyen**, S. Gremillion, S. Zingales



TECHNICAL PROGRAM

CHED 1158. Progress towards the synthesis of novel flavonoid derivatives that incorporate rhodanine for the treatment of Alzheimer's Disease. **G.A. Layfield**

Section I

Orange County Convention Center
West Hall C

Undergraduate Research Posters

Nanochemistry

Cosponsored by SOCED
N. Di Fabio, J. Roberts, *Organizers*

12:00 - 2:00

CHED 1159. Sensitive, selective, and quantitative copper sensor using click-chemistry with gold nanoparticles. R. Cary, O. Hess, I. Monroe, **J. Holbrook**, S. Unser, L. Sagle

CHED 1160. Functionalized electrospun nanoscaffolds on 3D printed microelectrode arrays (MEAs). **M. Royse**, N. Azim, Y. Li Sip, L. Zhai, S. Rajaraman

CHED 1161. NIR-to-NIR upconversion nanoparticles for latent fingerprint development: Determination of optimal particle size. **M. Zachman**, G. Sigdel, A. Baride, P. May

CHED 1162. Modifying glassy carbon electrodes with graphene oxide derivatives to control conductivity. **A. Schmeltzer**, G.J. Mancini-Samuelson

CHED 1163. Determination of optimal mild organic solvents for synthesis of PdNPs for carbon-carbon coupling reactions. **T. Biswas**, B.B. Penland

CHED 1164. Singlet oxygen generation by gold nanoparticles: Detection and applications. **K. Fenner**, S.M. Basu

CHED 1165. Photovoltage and hydrogen evolution studies on doped BiVO₄ and SrTiO₃ photocatalytic nanoparticles. **L. Twight**, A. De Denko, R. Han, F.E. Osterloh

CHED 1166. Green synthesis of gold nanoparticles using spinach leaf extract. **A.M. Koehler**, B. Fox

CHED 1167. Catalytic activity of Au and Ni nanocatalysts in the reduction of 4-nitrophenol and nitroanilines with NaBH₄. **C. Reyes**, J. Mbindyo

CHED 1168. Cell viability of CHL-1 skin melanoma cells infused with gold nanoparticles due to photothermal laser treatment. **A. Tran**, T. Dominguez, A. Tjandra, L. Mullenix, M. Carter, X. Benavides, M.A. Steiger, B. Mellis

CHED 1169. Metal nanowire fabrication utilizing PDMS stamps modified with hydrophilic thin films. W.C. Sanders, **G. Johnson**, R.V. Valcarce, P.J. Iles, J.S. Smith, H. Fourt, K. Drystan, **D. Edwards**, J. Vernon, S. Ashworth, A. Barucija, Z. Curtis



TECHNICAL PROGRAM

- CHED 1170.** Coating and biofunctionalization of gold nanospheres and nanorods using polytannic acid and polypyrogallol. **S. Schroeder**, A. Wark
- CHED 1171.** Investigating the aqueous phase transfer of CuInS₂ nanocrystals and their potential toxicity using zebrafish embryos. **R.W. Stuart**, S. Hughes
- CHED 1172.** Mesoporous silica nanoparticles (MSN) as a delivery system of anti-cancer drugs: A comparative study of synthesis and drug loading. E. Ferrer Torres, **P. Garcia Gonzalez**, M. Maldonado
- CHED 1173.** Characterization of drug loading and release from gold nanoparticles. **C. Hilt**, D. Scott
- CHED 1174.** Nanomaterials for fingerprint analysis: Comparative study with traditional techniques. **C.L. Cabrera**, R. Perez, E. Ferrer Torres
- CHED 1175.** Impact of metal concentration on the optical properties of cadmium-free quantum dots. **B. Yanick**, W.H. Steel
- CHED 1176.** Specific binding interactions of cytochrome C and β -lactoglobulin with gold nanoparticles by protein footprinting. **J.J. Cerda**, E. Tollefson, E.E. Carlson
- CHED 1177.** Gold nanorod-protein composites as a novel material for viral therapeutics. **M.R. Blahove**, J.W. Stone
- CHED 1178.** Bulk alignment control of novel donor-acceptor columnar liquid crystals. **G. Pleitez Gomez**, J.J. Reczek
- CHED 1179.** Evaluation of coated gold nanorods on zebrafish embryos. **B.W. Stewart**, M.E. Braselton, J. Smith, M. Kilpatrick, V. Sittaramane, J.W. Stone
- CHED 1180.** Size dependent optical properties of InP quantum dots. **S. Ahmed**, K. Schnitzenbaumer
- CHED 1181.** Synthesis and characterization of InP/ZnS core/shell quantum dots. **J. Dunaway**, K. Schnitzenbaumer
- CHED 1182.** Synthesis, characterization and catalytic activity of modified mesoporous zirconia. **H. Poitras**, **A. Spink**, D.S. Heroux
- CHED 1183.** Synthesis and characterization of electrospun fibers doped with quantum dots. **J.L. Lewis**, **H.E. Bethune**, D.E. Riegner
- CHED 1184.** Nickel sulfide nanocrystal synthesis using substituted thiophenols. **J. Veglak**, J.M. Rhodes, J. Macdonald
- CHED 1185.** Analyzing synergistic interactions between silver nanoparticles and antibiotics: Implications for microbial growth. **N. Opoku**, G. Graham, E. Vanterpool, K. LaiHing, S.K. LaiHing
- CHED 1186.** Synthesis and photophysical characterization of push-pull thiazolothiazole compounds for sensing and molecular electronics. **S.M. Patberg**, J. Sailer, N. Sayresmith, M.G. Walter
- CHED 1187.** Catalytic effect of nickel nanoparticles in hydration of carbon dioxide. **N. KC**, P. Barnes, T.L. Guasco
- CHED 1188.** Synthesis of stable nitric oxide-releasing nanoparticles for the preservation of cultural heritage items. **H.E. Crawley**, R.A. Hunter



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- CHED 1189.** Repeated immersion of silver ion exchange glasses in a single molten bath. **C.M. Nichols**, R.M. Magruder, D.W. Ferrara
- CHED 1190.** Interaction of silver, gold and Au/Ag core-shell nanoparticles with cardiovascular drugs on *Daphnia magna*. **A.A. Roman Roubert**, P. Garcia, C.B. Pellicier Rodriguez, E. Ferrer Torres, T. Felix Massa
- CHED 1191.** Fullerene C₆₀ cycloalkane solutions. **S. Clark**, C. Torres, **E. Kane**, L.D. Bienski
- CHED 1192.** Biosynthesis of iron oxide nanoparticles by ammonia diffusion. **S.O. Ekiyor Katimi**, B.B. Penland
- CHED 1193.** Development of antimicrobial and fluorescent ZnS:Mn nanoparticles. **Z. Thwin**, A. Ozcan, M. Young, N. Modha, S. Santra
- CHED 1194.** Stability of commercial solutions of C₆₀ fullerene dissolved in vegetable oils. **S. Clark**, **E. Kane**, **C. Torres**, L.D. Bienski
- CHED 1195.** Synthesis of calcium oxide microparticles and nanoparticles: A comparative study of spontaneous adsorption for drug loading. **M. Maldonado**, P. Garcia, E. Ferrer Torres
- CHED 1196.** Influence of CdSe nanocrystal shape on optical and vibrational spectra. **B.R. Nelson**, **B. Nottleson**, E.A. Reasoner, M. Wilker
- CHED 1197.** Anti-doping method using nanoparticles for sport drugs detection. **L. Colon Ithier**, A.Z. Ruiz Ferrer, P. Garcia, E. Ferrer Torres
- CHED 1198.** Greener approach for the kinetic controlled-growth synthesis of cadmium selenide quantum dots. **J. Bond**, L. Zieammermann, M. Shim, D. Kee, A.J. Cruz
- CHED 1199.** Collection of rare earth metals utilizing silica coated magnetic nanoparticles. **M.M. Ulrich**, J. Smith

Section I

Orange County Convention Center
West Hall C

Undergraduate Research Posters

Organic Chemistry

Cosponsored by SOCED
N. Di Fabio, J. Roberts, *Organizers*

12:00 - 2:00

- CHED 1200.** Fluorination of molecules using electrochemical methods. **K. Flynn**, T. Durgham, W. Liu
- CHED 1201.** S_N1 alkylation of heterocycles in aqueous reaction mixtures. **F.H. Lundy**, C. Ballard



TECHNICAL PROGRAM

- CHED 1202.** Synthesis of 1,2-bis(3,5-dimethyl-4-pyridyl)acetylene-N,N'-dioxide as a donor for the preparation of donor/acceptor cocrystals. **K. Wayne**, T.D. Selby
- CHED 1203.** Conversion of 2-hydroxy-benzeneacetic acid to ortho-fluoroethyl phenol. **M.M. Dent**, R.E. Rosenberg
- CHED 1204.** Benzothiazole-curcumin derivatives as photosensitizers. **T. Uehara**, R. Ciochina
- CHED 1205.** Fluorination and reduction of 1-indanone as a method to study carbon-fluorine hydrogen bonding. **S. Gooding**, R.E. Rosenberg
- CHED 1206.** Organic synthesis of aluminum ligands. **H. Aliff**, **J.P. Rickett**, D. Stone, M.W. Fultz
- CHED 1207.** Synthesis of conjugated macrocyclic polypyridinylethynylarenes. **N. Selim**, T.D. Selby
- CHED 1208.** Synthesis of 1-pentyl-3-(1-naphthoyl)indole analogues for use in cannabinoid and serotonin receptor studies. **N. Fitzpatrick**, A. Bradley
- CHED 1209.** Synthesis of macrocyclic polyphenylbuta-1,3-diynylarenes. **M.A. Martin**, T.D. Selby
- CHED 1210.** Utilizing cyclopropanones in strain-releasing methodologies. **B.M. Klootwyk**, **J.E. Muir**, G.R. Boyce
- CHED 1211.** Total synthesis of γ -curcumene. **D.R. Quiroz**, **J.R. Foster**, G.R. Boyce
- CHED 1212.** Synthesis of a resorcin[4]arene based benzal-quinoxaline heterocapsule. **J.M. Ruiz**, L.M. Tunstad
- CHED 1213.** Effects of light on the structure of select organic compounds commonly found in latent fingerprints. **E.L. Bray**, T.R. Hayden
- CHED 1214.** Design and synthesis of new ceramide analogs with different aromatic substituents on the side chain. **T. Perry**, C. Do, N. Goyal, M. Foroozesh
- CHED 1215.** Optimization of the synthesis of an octavalent dendrimer core. **K. Zeman**, J. Cerney, K.D. McReynolds
- CHED 1216.** Diquinoxaline, dimethylene-bridged resorcin[4]arene cavitand synthesis and purification. **D. Moreno**, **J. Woojuh**, **G.L. Walker**, L.M. Tunstad
- CHED 1217.** Efforts towards cycloadditions with pyridoxal via an *ortho*-pyridinone methide intermediate. **M.X. Bozor**, G.R. Boyce
- CHED 1218.** Acetone and ethanol as alternatives: Extraction of juglone from black walnut hulls. **M.A. Borst**, R.M. Paris, C. Rogers, G.T. Majors, I. Crouch, O.A. Cojocar, T.W. Majors
- CHED 1219.** Utilization of green chemistry for the synthesis of resveratrol analogues to target cancer cells. **C.L. Knudstrup**, H. Benmerabet, D. Paull
- CHED 1220.** Green synthesis of novel resveratrol analogues for cancer research. **M. Tase**, I. Baxter, D. Paull
- CHED 1221.** Selective chiral recognition by modular supramolecular cucurbit[8]uril complexes. **J. Zeng**, J.J. Reczek



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- CHED 1222.** Electrolytic oxidative coupling of alcohols with aldehydes to form esters. **D. Smeyne, K. Verboom**, M.A. Lnu
- CHED 1223.** Investigation of marine bacterial compounds that inhibit biofilm production in mycobacteria. **T. Tran**, J.A. Trischman, D. Mellor, A. Diamond
- CHED 1224.** Analysis of the binding relationship between curcumin derivatives and human serum albumin by steady-state fluorescence spectroscopy. **S. Rolland, H. Nyiera**, O. Michels
- CHED 1225.** Synthesis of phosphorus-based surfactant using a two-solvent method. **V. Lee**, S. Deprele
- CHED 1226.** Mechanistic challenges in transesterification during the synthesis of hypophosphite esters. **E.N. Shokoya**, V. Lee, A. Gonzalez, S. Deprele
- CHED 1227.** Quantitative measurement of the relative acidities of alcohols in water. **C.T. Nealon**, C.J. Smart, Z. Donhauser
- CHED 1228.** Building a library of simplified analogs for phomoxanthone A. **E.B. Vaughan**, R. Ali, A.E. Mattson
- CHED 1229.** Synthesis of linked chalcones as nematocides. **M. Kim**, A. Calderón-Urrea, C. Arpin
- CHED 1230.** Propargylic isoxazoline antimicrobial agents. **A. Schull**, J.L. Duffy-Matzner
- CHED 1231.** Alkoxy aryl side chain effects on poly(phenylvinylene) derivatives for use in organic light-emitting diode (OLED) devices. **G. Benito, Y. Tran, J. Nguyen**, E. Magionos, C.A. Young
- CHED 1232.** F-19 NMR determination of relative rate constants for hydrogen abstraction by *p*-fluorophenyl radicals from fatty acid methyl esters. **B. Murray**, R. Dorn, T.W. Nalli
- CHED 1233.** Development of chiral bisphosphorylimides as organocatalysts for asymmetric Friedel–Crafts reactions. **O. Apolinar**, L. Ahlberg, R.G. Iafe
- CHED 1234.** Synthesis of a new chiral *N*-heterocyclic ligand for enantioselective synthesis. **W. Gilmore**, P.J. Lombardi
- CHED 1235.** Efforts towards the application of flow chemistry in the synthesis of crown ethers. **J.A. Shea**, Z. Matesich
- CHED 1236.** Synthesis of a family of antimalarial lead molecules. **E. Williford**, M.J. Campbell
- CHED 1237.** Dynamic kinetic resolution of aldehydes for C–C bond formation. **H.M. Nguyen**, Z. Chen, V.M. Dong
- CHED 1238.** Synthesis, biological evaluation and computer modeling of heteroaryl ketones as aromatase inhibitors. **S. Ramirez**, Q. Nguyen, A. Rosen, M. Neiser, A. Roy, L. Ma
- CHED 1239.** Convergent synthesis of photoactive naphthalimide compounds for localized drug delivery. **H. Lovstad**, J.E. Elbert, K. Parrott
- CHED 1240.** Gold-catalyzed arylation of benzylic alcohols to afford bioactive 1,2,3-benzotriazole derivatives. **J. Perez, M. Shabo, K. Fernandez**, M. Nguyen, V. Franco Bolanos, L. Ahlberg, R.G. Iafe



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- CHED 1241.** Application of factorial analysis to optimize microwave assisted organic synthesis. **H. Jia, B. Kalach, E. Alkhatib, L. Farber**
- CHED 1242.** Investigating the use of flow chemistry for the synthesis of ¹⁵N labeled amino acids from simple starting materials.. **T. Pinto, W. Carroll**
- CHED 1243.** Construction of peptide-based molecular building blocks for the controlled assembly of nanomaterials. **G. Bertles, S. Fraley, S.C. Butler**
- CHED 1244.** Absorption spectra of juglone in its anionic and neutral form in aqueous solutions of basic pH. **I. Crouch, T. Majors, O.A. Cojocar**
- CHED 1245.** Modelling for polymer chemistry: Using ¹⁹F NMR to determine furan-maleimide reaction properties. **N. Price, G. Hollis, P.A. Deck**
- CHED 1246.** Double salt ionic liquids based on phenothiazine cations and various anions. **E. Etheridge, L.G. Pipkin, O.A. Cojocar**
- CHED 1247.** Synthesis of bromo-alcohols from cyclic ethers. **P. Dhar, J.B. Greenough, D. Mariniello, E. Perez-Cabrera, K. Lemus Mortaya**
- CHED 1248.** Diastereoselective synthesis of *syn*- β -hydroxy- α -substituted phenyl carboxylates *via* boron-mediated aldol reaction of substituted phenylacetates. **A.Y. Thomas, T.L. Walls III, P.B. Chanda**
- CHED 1249.** Comparison of acid catalysts in process-scale Fischer esterification reactions. **J. Maurer, N. Zink, K.M. Halligan**
- CHED 1250.** Investigating endo/exo predictability in the intramolecular Diels-Alder reaction of E,E and E,Z diene appended quinones. **K.V. Waynant, K. Rigg**
- CHED 1251.** Immersive layer-by-layer (LbL) assembly on siloxy amino functionalized generation 1 and 3 silicone hydrogel contact lenses. **E. Wanous, J.L. Duffy-Matzner**
- CHED 1252.** Synthesis of new donor molecules for organic photovoltaics. **S. Shokooh, J. Madrigal, D. Everson**
- CHED 1253.** Development of an enantioselective allenolate Claisen rearrangement. **B. Smith, T. Gallagher, A. Dahi, A.G. Wenzel**
- CHED 1254.** Synthesis and characterization of BODIPY derivatives for early cancer detection. **J. Merchant, S. Carbajal, E. Dang, J. Hollingsworth**
- CHED 1255.** Progress toward the synthesis of expanded oxophlorins. **R. Haller, S.H. Leung**
- CHED 1256.** Synthesis and modification of epoxyisoindolines. **D. Scanlan, S. Luesse**
- CHED 1257.** Solubility studies of dual active ionic liquids with potential to eliminate drug-induced hepatotoxicity. **S. Visneski, O.A. Cojocar**
- CHED 1258.** Synthesis of phenyl pyridine analogs via Suzuki coupling to inhibit uridine nucleoside ribohydrolase. **A. Gil, M. Emilcar, J. Persaad, B.J. Stockman, M.A. Vanalstine-Parris**



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- CHED 1259.** Synthesis of an extended matrix metalloproteinase inhibitor. **J. Hungerford**, D.A. Fish
- CHED 1260.** Synthesis of enantiomerically pure carbazole analogs with quaternary carbons via a Birch-Heck reaction. **M. Haider**, W.P. Malachowski
- CHED 1261.** Synthesis of conformationally restricted kappa-opioid receptor agonists. **L. Bontreger**, B. Martin, B. Wunsch
- CHED 1262.** Synthesis of isoxazoles and isoxazolines as lavendamycin analogues. **G.S. Taylor**, R.E. Sammelson, H.D. Beall
- CHED 1263.** S_N1 alkylation of 1,3-dicarbonyl compounds in aqueous reaction mixtures. **T. Galili**, C. Ballard
- CHED 1264.** Preparation of isomerically pure substrates designed to explore the scope and limitations of an acid-initiated vinylogous aldol reaction. **Y. Awwad**, **Y. Ma**, J. Cooper, G. Found, J.E. Hofferberth
- CHED 1265.** Synthesis and characterization of carbazoles for photoredox catalysis. **M. Keller**, T.D. Weinhold, A. Longstreet
- CHED 1266.** Application of flow chemistry in the dehydration of 4-methylcyclohexanol. **A. Schroeder**, Z. Matesich
- CHED 1267.** Diarylimidazolium halogen bond donor catalysts for Lewis acid catalyzed transformations. **C. Millard**, E. Hall
- CHED 1268.** Approaches to synthesis of 4-nitrophenyl 4-thio-*N*-acetyl- β -D-muramic acid. **J. Bomhof**, J.E. Hanson
- CHED 1269.** Determination of phytosterols in mycorrhizal “burn” morel mushrooms by GC-MS. **C. Chu**, A. Overgard, N.Y. Walker, S. Quint, T.W. Nalli
- CHED 1270.** Progress toward quinone and heterocycle synthesis using continuous flow. **N. McKnight**, **S. Williams**, K. Volpe, E.E. Podlesny
- CHED 1271.** Computational and experimental studies of new cucurbit[n]uril containing building blocks. **S. Ellis**, U. Khadka
- CHED 1272.** Antioxidant properties of thymol and eugenol derivatives. **C. Sarring**, D.A. Fish
- CHED 1273.** Study of heavy-atom curcumin derivatives for use in photodynamic therapy. **S.E. Bonar**, R. Ciochina
- CHED 1274.** Preparation of naphthalene derivatives for coupling reactions. **I. Perry**, S.L. Carter, Y. Lysandrou, J. Rawson, S. Doyle, L. Buzzard, J. Markiewicz
- CHED 1275.** Establishing a general method for the copper-catalyzed asymmetric reduction of 2*H*-azirines. **M.K. Greenler**, J. Unger
- CHED 1276.** Toward the synthesis of stachybotrin D: A potential anti-HIV drug. **N. Glatz**, D.C. Bromfield-Lee
- CHED 1277.** Enantioselective construction of tricyclic ring systems with quaternary carbon stereocenters. **S. Tran**, W.P. Malachowski
- CHED 1278.** Synthesis of substituted carbaporphyrins from carbatripyrrins. **J.J. Woods**, T.D. Lash



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- CHED 1279.** Determination of the water adsorption capabilities of a variety of Nafion membranes saturated with ammonium chloride. **M.E. Kennedy**, D. Rogers, A.V. Carr, B.C. DeMier, C.E. Keating, J.C. Graf, A. Lamar
- CHED 1280.** Investigating the synthesis of LMA-P2. **S. Little, S. Bradley**, B.G. Vanness
- CHED 1281.** Application of an acid-initiated vinylogous aldol reaction for the formation of all carbon quaternary stereocenters. **H. Wendlandt**, M. Frischling, E. McCann-Smith, S. Reisberg, A. Lian, M. Powers, B. Clegg, J.E. Hofferberth
- CHED 1282.** Hydrogenations with frustrated Lewis pairs under microwave irradiation. **L.A. Robertson**, S.M. Basu, E.M. Valentin
- CHED 1283.** Design of methylene blue analogs as contrasting dyes for sentinel node biopsy. **N. Steadman, D. Thompson**, V.K. Dunlap
- CHED 1284.** Investigating acid-catalyzed enolization of acetophenones. **H. Tarbox**, N.M. Wachter
- CHED 1285.** Preliminary mechanistic studies on the halogenation of vanillin using bleach and sodium halide salts. **S.A. Winspear**, S.K. Goforth
- CHED 1286.** Reduction of isoxazole derivatives via catalytic hydrogenation compared to reduction using iron powder catalyst. **W.R. Morris**, A.M. Schoffstall
- CHED 1287.** Trityl catalyzed synthesis of bisindolylmethanes from imines. **V. Jones**, C. Brindle
- CHED 1288.** Synthesis of 1,4-disubstituted triazolopyridine carboxylates. **J. Bendesky**, A.M. Schoffstall
- CHED 1289.** Progress towards the synthesis of iron-based hydrogenation catalysts using hydroxypyridine bidentate and tetradentate ligands. **S. Rockow**, L. Boisvert
- CHED 1290.** Synthesis of ortho-sulfonamide analogues of the COX-2 inhibitor celecoxib. **J.S. Brister**, K.K. Hall, D.J. Lewis, J.D. Knight
- CHED 1291.** Understanding HIV protease inhibitor activity through computational modeling: An experiment for use in undergraduate organic chemistry laboratory. **A. Pathiranage, M. Pan, M. Osborne, A. Maczko**
- CHED 1292.** Synthesis and analysis of *meta*-substituted diboronic acids for carbohydrate sensing. **A. Skoromnaya, J. Willmore**, D.B. Cordes
- CHED 1293.** Tandem oxidation and dehydrogenative-coupling for the rapid synthesis of 1,3-diones. **E.R. Wearing**, M.T. Haynes
- CHED 1294.** Emissive pyridinium salts constructed through restriction of the intramolecular rotation of tetraphenylethylene. **S. Khalife**, G. Yin, A. Kellman, X. Li
- CHED 1295.** Alpha-sulfamidation of aliphatic aldehydes: Designing new catalysts and screening new conditions to overcome old problems. **J.R. Stroud, M. LaGanke**, T.C. Coombs
- CHED 1296.** *Trans/cis* photoisomerization and kinetics of a calixarene-capped azobenzene. **C.A. Litts, J.A. Shea**, P.A. Bonvallet



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- CHED 1297.** Investigation of *Rhamnus crocea* leaf extract effect on Hermes copper butterfly. **J. Dang**, L. Malter, J.A. Trischman
- CHED 1298.** Synthesis of benzyl sulfamide derivatives using microwave chemistry. **A. Madison**, L. Winfield, F.L. Payton
- CHED 1299.** 4-*tert*-Butylcyclohexanone as a candidate to study and confirm existence of carbon-fluorine hydrogen bonding. **D.P. Cooper**, R.E. Rosenberg
- CHED 1300.** Synthesis and characterization of *N,N*-bis-substituted benzimidazolium fluorescent hybrid salts. **A. Yue**, **L. Martz**, S.S. Johnson, J.D. Gorden, M. Frazier, K.S. Taylor, D.W. Holley
- CHED 1301.** Multistep synthesis of metal- pyrrole derived complexes and detection of pollutant ion. **H. Theriault**, L.L. Rossi
- CHED 1302.** Synthesis of organic dimer ligands for radical host-guest chemistry. **S. Youngs**, J.J. Reczek
- CHED 1303.** Structural modification of a natural angiotensin converting enzyme inhibitor and the effect on activity. **A. Swanson**, C. Kalberg
- CHED 1304.** Micelle-facilitated ring-closing metathesis, in flow. **M. Jones**, **D. Brownholland**
- CHED 1305.** Structure–function studies on phosphorus- and nitrogen-containing heterocycles. **J. Odulio**, J. Bard, C. Deng, L.N. Zakharov, D.W. Johnson, M.M. Haley
- CHED 1306.** Micelle-facilitated peptide coupling reactions, in continuous-flow conditions. **G. Goetz**, **M.L. Mullan**, D. Brownholland
- CHED 1307.** Identification of enamel based paint components which give false positives with Luminol, 5-amino-2,3-dihydro-1,4,phthalazinedione. **A.N. McMullen**, D.K. Jean
- CHED 1308.** Microwave synthesis of FAC-tricarbonyl (pentylcarbonato)(α - diimine) rhenium complexes. **A. Culmer-Gilbert**, A.J. Winstead, S. Mandal
- CHED 1309.** Synthesis of a small molecule mimic of the human D2 dopamine receptor site toward investigation into the binding strength of cyclobutane-1,1-dicarboxylic acid. **L.J. Trowbridge**, D.K. Jean
- CHED 1310.** Carbazole derivatives as photocatalysts for the dehalogenation of substituted benzenes. **T.D. Weinhold**, M. Keller, A. Longstreet
- CHED 1311.** Exploring the properties of cystine-based kidney stones. D.J. Schauer, **J. Campbell**, **J. Clark**
- CHED 1312.** Solubility of albuterol-NSAIDs ionic salts. **J. Scantland**, O.A. Cojocar
- CHED 1313.** Synthesis of novel linked viologen and Py₂TTz dimers to enhance radical stability in cucurbit[8]uril. **B. Cousineau**, J.J. Reczek
- CHED 1314.** Catalytic enantioselective synthesis of tricyclic ring systems with a remote quaternary carbon center using a Birch-Heck reaction sequence. **M.K. Hogan**, W.P. Malachowski



TECHNICAL PROGRAM

- CHED 1315.** Alloxan ethylthiosemicarbazone and alloxan tertbutylthiosemicarbazone ligands: reaction with copper (II). **M.C. Gray**, E.C. Lisic
- CHED 1316.** Investigating novel nanocrystals as catalysts for heterogeneous cross-coupling reactions. **K. Storo**, H. Li, S. Geyer, P. Lundin
- CHED 1317.** Synthesis and characterization of four new fluorine-labelled thiosemicarbazones. **L.M. Underwood**, E.E. Rush, E.C. Lisic
- CHED 1318.** Comparing efficiencies of organometallic coupling reactions to create 2,2'-bipyridine adducts. **S. Vazquez**, **K. Wilkinson**, B. Aukszi
- CHED 1319.** Extracting antifungal juglone from black walnut hulls using hand sanitizer. **G.T. Majors**, R.M. Paris, C. Rogers, M.A. Borst, I.L. Crouch, O.A. Cojocar, T.W. Majors
- CHED 1320.** To chill or not to chill: The effect of long term refrigeration of black walnuts on juglone extraction in comparison to fresh hulls. **C. Rogers**, R.M. Paris, M.A. Borst, G.T. Majors, I.L. Crouch, O.A. Cojocar, T.W. Majors
- CHED 1321.** Toward linear and soluble dioxaines for use in organic electronic materials. **W. Quigley**, D.G. Patel, S. Yoo, E. Gomez
- CHED 1322.** Comparative UV-Vis analysis of juglone extracted from frozen versus fresh black walnut hulls. **R. Paris**, C. Rogers, M.A. Borst, G.T. Majors, I.L. Crouch, O.A. Cojocar, T.W. Majors
- CHED 1323.** Synthesis and clinical use of LS-2616, a drug used to treat ocular cancer. **M. Snider**, K. Augustine, C. Fry, S. Blake, J. Bailey, B. Hargittai
- CHED 1324.** Synthesis and evaluation of ROS-activatable prodrugs. **J.E. Palmer**, B.M. Brietske, T.C. Bate, C.B. Cooley
- CHED 1325.** Exploring the potential of doublet state emission from a stable, luminescent, radical, organic molecule. **M. Patel**, G. Sazama
- CHED 1326.** Withdrawn
- CHED 1327.** Design principles of stable organic radicals with luminescent properties. **L. Reeves**, G. Sazama, S. Debbert
- CHED 1328.** Effect of component variation on Passerini-Smiles couplings. **C. Perry**, S. Luesse
- CHED 1329.** Determining the effects of reaction media on electronically mismatched Diels-Alder Reactions. **J. Lake**, Z. Wang, S.R. Hussaini
- CHED 1330.** Neutralization and isolation of *p*-xylene-bis-(4-aminopyridine). **B. Pauley**, C.L. Weeks
- CHED 1331.** Exploration of conjugated aldehydes in the Ugi-Smiles reaction. **J. Worms**, S. Luesse
- CHED 1332.** Fluorogenic polymerization in aqueous media as a detection strategy. **M.P. Hopps**, C.B. Cooley
- CHED 1333.** Solubility studies of dual functional phenothiazine ionic liquids. **L.G. Pipkin**, E. Etheridge, O.A. Cojocar



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- CHED 1334.** Development and synthesis of a switchable atropisomeric probe molecule for determining the shape of flexible molecules using Dipolar Couplings. **J.M. Ralston**, W. Carroll
- CHED 1335.** Efforts toward the synthesis of Fischer carbenes for intramolecular decarboxylative allylation. **P. Thai**, M.C. Slade
- CHED 1336.** Hydroamination of unactivated alkenes using organocatalysts. **R.B. Ferdowsian**, L. Liu, S. Ravikumar, A. Wenzel
- CHED 1337.** Substituent effect on aromatic imine basicity. **N. Javalý**, N. Capra, J. Bennett
- CHED 1338.** Understanding the charge transfer between the donor and acceptor components of organic polymers. **S. Lee**
- CHED 1339.** NMR study of phenylsemicarbazones. **S. Pokrzywa**, **R. Finster**, J. Bennett
- CHED 1340.** Copper-catalyzed, intermolecular, anti-Markovnikov hydroamination of olefins. **Y. Gao**, **M.Y. Chen**, A.G. Wenzel
- CHED 1341.** Synthesis of a tetrahydroxylated indolizidine from D-allose. **K. Bucking**, L.J. Liotta
- CHED 1342.** Enantioselective phosphorylation of diols. **A. Bucknam**, **E. Lynch**, B.R. Sculimbrene
- CHED 1343.** Trifluoroethoxide assisted formation of electron-withdrawing substituted bicylobutanes. **B.J. Purisky**, L.J. Tilley
- CHED 1344.** Electrophilic catalysis with heterobimetallic complexes. **C.A. Jensen**
- CHED 1345.** Improved synthesis of *N*-fluorenylmethoxycarbonyl-*N*-benzyloxycarbonyl-L-homoglutamine. **B. Belcher**, K. Harris
- CHED 1346.** Three step synthesis of a 4,4' methylenedianiline derivative. **S.J. Powells**, J.L. Luhman, D.E. Janzen, J. Wollack
- CHED 1347.** Synthesis of electron withdrawing oxoammonium salts. **V. Rapela**, L.J. Tilley
- CHED 1348.** Coordination of phosphate Diester Lligands to bismuth(III). **E. McKnight**, Z. Ali, G. Bailey, N. Kretekos, C. Milander-Mashlan, J. Stromberg, R. LaLonde
- CHED 1349.** Development of a method for the synthesis of nitrogen-nitrogen bonds. **J. McCrery**, A.J. Angellotti, M.R. Prinsell
- CHED 1350.** Synthesis and electrochemical dimerization of ionic liquids to be used as potential electrolytes in lithium ion batteries. **K. Luong**, R.N. Manchanayakage
- CHED 1351.** Structural elucidation of pyrrolizidine alkaloids from *Heliotropium procumbens* and *H. glabrisculum*. **P.E. Plucker**, **F.L. Hamerlynck**, **R.B. Kelley**
- CHED 1352.** Synthesis and evaluation of NSAID active pharmaceutical ingredient ionic liquids. **J. Pelton**, K. Callahan, R.N. Manchanayakage



TECHNICAL PROGRAM

- CHED 1353.** Synthesis and characterization of a series of 1,2-naphthoquinones. **K. Trejos Cuadra**, G. Lamoureux, K. Chaves, A.L. Perez
- CHED 1354.** Nickel-catalyzed borylation of aryl sulfamates. **A. Bulger**, M. Merriman, A. Judy, A.L. Silberstein
- CHED 1355.** Investigation of microwave and ultrasonic energy in the synthesis of imidazoles. **S. Myers**, R. Paris, E.A. Nalley
- CHED 1356.** Application of (cyclopentadienone)iron catalysts to the lactonization of diols. **Y. Tang**, R. Meador, T.W. Funk
- CHED 1357.** Synthesis and stereoselective reduction of novel P-38 α inhibitors. **H.K. Maben**, A.T. McGrath, A.M. Schoffstall
- CHED 1358.** Investigation of the scope of substituted benzaldehyde substrates for use in a non-traditional method of *N*-sulfonyl imine formation. **Z.C. Brandeburg**, A.J. Hanson, M.D. Hopkins, A. Lamar
- CHED 1359.** Exploring the mechanical properties of organic photochemical materials. **J. Delgado**, M. Nichol, J. Read De Alaniz
- CHED 1360.** Enhancing long-range salt bridges using intermediate aromatic and nonpolar amino acids. **W. Billings**, M. Smith, K. Stern, J.L. Price
- CHED 1361.** Progress toward copper catalyzed silylation of styrene and alkyne derivatives. **J.M. Posz**, S.R. Harruff, B.K. Mikesell, R. Van Hovel
- CHED 1362.** Catalytic enantioselective Birch-Heck reaction sequence for the efficient generation of potentially therapeutic molecules. **A. Matei**, W.P. Malachowski
- CHED 1363.** Organic dye-catalyzed chlorination of arenes and heteroarenes in the absence of light. **A.K. Pitzel**, D. Rogers, M.D. Hopkins, A. Lamar
- CHED 1364.** Visible-light photoredox chlorination of aromatic compounds using *N*-chlorosuccinimide and an organic dye photocatalyst. **J.M. Gallegos**, M.D. Hopkins, A. Lamar
- CHED 1365.** Light-mediated DNA cleavage by alkylcobalamins. **L.N. Gendron**, A.C. McCue, **D.C. Zites**, J.R. Shell, **T.A. Shell**
- CHED 1366.** Synthesis, kinetic, and electronic studies of (3,4-diarylcyclopentadienone)iron tricarbonyl compounds. **E. Bertonazzi**, X. Hou, T.W. Funk
- CHED 1367.** Electronic effects of (cyclopentadienone)iron tricarbonyl bifunctional catalysts on transfer hydrogenation and dehydrogenation reactions. **X. Hou**, E. Bertonazzi, T.W. Funk
- CHED 1368.** Synthesis of a deuterated isotopically labeled 2,2' MDI derivative. **A.M. Wiedmeier**, A.C. Hoffer, J. Wollack
- CHED 1369.** Ru-catalyzed pyridine-promoted oxidation of silyl ethers to silyl esters. **A.M. Weinhofer**, H.D. Cole, B.A. Mitchell, A.J. Ritz, J.E. Rabinovitch, B.C. Goess, S.K. Goforth
- CHED 1370.** Synthesis of a triazacyclic amine metalloenzyme mimic building block. A. Lajmi, **C. Pizza**, A. Condoroteanu-Orovean, M. Harris, P. Sandoval-Sanchez, A. Porter



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- CHED 1371.** Investigation of microwave and ultrasonic energy in the synthesis of heterocycles related to medicinal chemistry. **R. Paris**, S. Myers, E.A. Nalley
- CHED 1372.** Conjugate addition reactions of organocuprates to doubly activated alkenes. **M. Whalen**, F. Weng, M. Manpadi
- CHED 1373.** Asymmetric synthesis of novel ligands for the preparation of optically active α -amino acids. K. Williams, **T.K. Ellis**
- CHED 1374.** Design and synthesis of novel ligands for the dynamic resolution of racemic α -amino acids. E. Hicks, **T.K. Ellis**
- CHED 1375.** Comparative analysis of pyrrolizidine alkaloids in the genus *Cryptantha* and allied genera. **B.L. Stavaas-Jamack**, F.R. Nickerson, **R.B. Kelley**
- CHED 1376.** Preparation and reactivity comparison of a series of Ni(II) complexed nucleophilic glycine equivalents by competitive reaction rate experiments. M.L. Howe, **T.K. Ellis**
- CHED 1377.** Optimization of TMSLi conjugate addition using TPPO as a safer alternative to HMPA. **H. Mackay**, L.J. Tilley
- CHED 1378.** Synthesis of triazolopolyfluoropyridine derivatives. **L.J. Taylor**, A.M. Schoffstall
- CHED 1379.** Synthesis of cinnamaldehyde phenylsemicarbazones and exploration of their photochromicity. **E.J. Hose**, E. Treadwell
- CHED 1380.** Quinazolin-4(3*H*)-ones and 5,6-dihydropyrimidin-4(3*H*)-ones from β -aminoamides and orthoesters. **J.T. Gavin**, R.A. Bunce
- CHED 1381.** Synthesis of symmetric and asymmetric hydroxyfulvenes. **T. Sullivan**, **C. Johnson**, M.T. Blankenbuehler
- CHED 1382.** Systematic comparison of the one-pot dialkylation of imines and dimethylhydrazones to prepare disubstituted cycloalkanones and their equilibrium ratios. **J.B. White**, M. Krueel, A. Authement
- CHED 1383.** Synthesis and reactivity of charge-enhanced chiral thiourea catalysts. **K. Luu**, C. Payne, S.R. Kass
- CHED 1384.** Improved synthesis of “neoprofen”, a rigidified analogue of ibuprofen. **M. Vidaca**, A. Martin, G.B. Dudley
- CHED 1385.** Withdrawn
- CHED 1386.** Michael reactions of tricarbonyl(tropone)iron towards a synthesis of diverse bridged azapolycycles. **Z. Phelan**, **Z. Huang**, D. Griffith
- CHED 1387.** Synthesis and structure of a calix[4]arene incorporating a single oxazole unit via a 2-(hydroxyimino)calix[4]arene. **J.A. Hoffner**, D.H. Johnston, J.L. Fantini
- CHED 1388.** Synthesis of a 2,4-methylenedianiline (MDA) derivative. **M.J. Graham**, D.E. Janzen, J. Wollack
- CHED 1389.** Stereochemical analysis of saturated pyrrolizidine alkaloid diastereomers. **L.K. Johnson**, **R.A. Davis**, **H.J. Hawkes**, **J.N. Woodford**, **R.B. Kelley**



TECHNICAL PROGRAM

- CHED 1390.** Upsetting the cart of known amino acid quasiracemic crystalline phases. **K.D. Sahlstrom**, K.A. Wheeler
- CHED 1391.** Investigations directed towards the synthesis of phenaliporphyrin. **M.A. Mathius**, T.D. Lash
- CHED 1392.** Efficient access to hexahydrothieno[3,2-*b*]thiophene heterocycles. **D. Wong**, F. Robertson
- CHED 1393.** Synthesis of fused aromatic heterocycles by palladium-catalyzed C-H activation chemistry. **D. Yook**, T.A. Knoerzer
- CHED 1394.** Synthesis of covalently-linked fluorescent dye derivatives. **L. Pferdmenges**, N. Grinalds, K. Griffith, K. Fogarty, P. Lundin
- CHED 1395.** Copper-catalyzed silylations of aldehydes using a disilane as the silicon source. **J.R. Wilkinson**, **C.E. Nuyen**, B. McCarty, W.L. Kirkman, R. Van Hoveln
- CHED 1396.** Rapid synthesis of *N,N*-di-(2-methoxybenzyl)-*N*-methylamine. **A. Hamm**, L.I. Bobyleva, M.M. Bobylev
- CHED 1397.** Synthesis of 1-(1-*tert*-butylperoxy)-3,3-dichloropropylbenzenes. **M. Rosado**, R. Neff, Y. Su, M. Doyle
- CHED 1398.** Mechanochemistry leading to a series of diarylporphyrins. **M. Reyes**, A. Henderson, J.V. Ruppel, T.D. Hamilton
- CHED 1399.** Palladium-catalyzed direct α -C(sp³) heteroarylation of ketones under microwave irradiation. **A. Rosen**, M. Neiser, Q. Nguyen, L. Ma, T. Atesin
- CHED 1400.** Rapid synthesis of *N,N*-di-(3-methoxybenzyl)-*N*-methylamine. **E.M. Winterton**, L.I. Bobyleva, M.M. Bobylev
- CHED 1401.** Synthesis of new chiral N-heterocyclic carbene ligand for catalysis. **J. Payne**, P.J. Lombardi
- CHED 1402.** Synthesis of new N-heterocyclic carbenes. **A. Larsen**, D.J. Nelson
- CHED 1403.** Continuous preparation of alkylidene malonates. **E. Stryker**, C. Kong, F. Gupton
- CHED 1404.** Exploration of new laser writable donor-acceptor columnar liquid crystal materials. **J. Sheppard**, J.J. Reczek
- CHED 1405.** Synthesis of quinoxalinyltriazoles. **C.M. Clements**, A.M. Schoffstall
- CHED 1406.** Expanding the scope and utility of pentaerythritol acetal formation. **S.N. Simon**, S.M. Kennedy
- CHED 1407.** Synthesis of indoles through catalytic reduction of 2-nitrostyrene-derived epoxides and an examination of the Bartoli indole synthesis. **A. Mosebarger**, B. Soderberg
- CHED 1408.** Heteroaryl isocoumarins as potential aromatase inhibitors: Substrate scope investigation and mechanism study using ¹⁸O-acetophenone. **Q. Nguyen**, W. Renzenbrink, A. Quillen, E. Osifalujo, L. Ma
- CHED 1409.** Investigations into the synthesis of novel carbaporphyrinoids using a '3 + 1' approach. **S.J. Kempel**, T.D. Lash



TECHNICAL PROGRAM

- CHED 1410.** Construction of a drug candidate library using the copper(I)-catalyzed azide-alkyne cycloaddition and a fluorinated terminal alkyne. **K.A. Stewart**, A.M. Schoffstall
- CHED 1411.** Withdrawn
- CHED 1412.** Aryltriazolopolyfluoropyridine reactions with amines. **A.D. Outlaw**, A.M. Schoffstall
- CHED 1413.** Withdrawn
- CHED 1414.** Viability of peptide coupling reactions in water facilitated by detergents. **K.G. Fosnacht**, G.L. Milligan
- CHED 1415.** Determination of chiral analytes through bound metal complexes by circular dichroism. **J. O'Connor**, B.T. Herrera, E.V. Anslyn
- CHED 1416.** Mechanistic insights into deboronofluorination of alkyl-Bpin substrates with selectfluor and silver catalyst. **T. Taylor**, T.M. Perrone, B.V. Popp
- CHED 1417.** Rapid synthesis of *N*-(4-isobutylbenzyl)-*N*-methylformamide. **A. Hamman**, L.I. Bobyleva, M.M. Bobylev
- CHED 1418.** Rapid synthesis of *N*-(4-cyanobenzyl)-*N*-methylformamide. **B.S. Wilson**, L.I. Bobyleva, M.M. Bobylev
- CHED 1419.** Conformational and configurational analysis of a thiourea chiral hydrogen-bond donor organocatalyst. **E. Latawiec**, M. Recznik, J.D. Evanseck
- CHED 1420.** Synthesis of symmetrical trisubstituted 1*H*-1,2,3-triazolopyridines. **C.J. Hull-Crew**, A.M. Schoffstall
- CHED 1421.** Extraction of betulin and synthesis of a betulin analogue. **E.N. Wandling**, C. Atkins, A.L. Yousef
- CHED 1422.** Substitution of fluorinated 1*H*-1,2,3-triazolopyridines by secondary amines. **M.N. Trujillo**, A.M. Schoffstall
- CHED 1423.** Rapid synthesis of *N*-ethyl-*N*-(4-isopropylbenzyl)formamide. **S.E. Sundhagen**, M.M. Bobylev, L.I. Bobyleva
- CHED 1424.** Synthesis of indolyl/indazolyl (*N*1 substituted) quinolones (C6 and C8 substituted) for study as possible anticancer/antibiotic/antimicrobial agents: *N*-allylated and *N*-benzylated analogues. J.M. Duda, B. Fossum, A.J. Knoll, M.L. Lenertz, **T.M. Trygstad**
- CHED 1425.** Modification of porphyrinoid chromophores by the introduction of fused tropone units. **E.K. Cramer**, T.D. Lash
- CHED 1426.** Microwave synthesis of novel esters using sulfuric acid and imidazole as catalysts. **T. Hinkle**, E.A. Nalley
- CHED 1427.** Reactions leading to pentacyclo[4.3.0.0^{2,4}.0^{3,8}.0^{5,7}]non-4-ene. **C. DeAngelo**, E. Brutschea, M.A. Forman
- CHED 1428.** Rapid synthesis of *N*-(4-methoxybenzyl)-*N*-methylformamide. **K. Heick**, M.M. Bobylev, L.I. Bobyleva
- CHED 1429.** Development of anthranilic acid derived thiourea catalysts. **A. Witkowski**, **E. Arnold**, A. Fuchs, A. Peddle, K.J. Graham, M. Cloninger, T.N. Jones



TECHNICAL PROGRAM

- CHED 1430.** Solvatochromic compounds containing dimethylaniline-quinoxaline donor-acceptor chromophores. R.T. Lillis, B.M. Lucht, **M.C. Rosko**, J.M. Nadeau
- CHED 1431.** Synthesis of ligands for platinum drugs. **T.L. Head**, **A.E. Fraeyman**, O. Jang, C.S. Chow, K.J. Friedrich
- CHED 1432.** Novel copper catalyzed approach to nitrogen containing bicycles. **B. Carvalho**, A.K. Isaacs
- CHED 1433.** Synthesis of the TAN-1057 D antibiotic candidate and development of biologically relevant analogs. **R. Cantrell**, M. Nelli, R. Looper
- CHED 1434.** Microwave assisted Duff formylation reactions. **A.M. Markovich**, V.P. McCaffrey
- CHED 1435.** Transition-metal catalyzed meta-arylation of aryl carbamates. **N. Taylor**, L. Schluter, O. Ndayishimiye, A.L. Silberstein
- CHED 1436.** Tunable removal of carbonyl compounds through rapid bisulfite extraction: Method optimization and selective carbonyl compound removal. **M. Furigay**, C. Brindle
- CHED 1437.** Copper catalyzed approach to beta carboline alkaloids. **G. Gildersleeve**, C. Hennessey, A.K. Isaacs
- CHED 1438.** Synthesis of a fluorophore for the diagnosis of neglected tropical diseases. **E.H. Trinh**, C.D. Andrews, G.R. Naumiec
- CHED 1439.** Synthesis of 1,2-dihydroisoquinolines. **A. Palaia**, A.K. Isaacs
- CHED 1440.** Stereochemical control via a 1,3-dithiane moiety: Access to well-defined (1-hydroxy-2-methylbutyl) fragments. **M. Kincanon**, M. Mannchen, N. Morgan, M. Slade
- CHED 1441.** Physical organic study of ring strain on yellow dye containing couplers. **F.O. Fernandez**, S.M. Bonser
- CHED 1442.** Building the basis for novel syntheses of pi-extended porphyrins. **W. Rackers**, C. Stewart, **R. Perera**, H. Wang
- CHED 1443.** Synthesis and characterization of functionalized polysilalkylene modified siloxane monomers by hydrosilylation reaction. R.P. D'Amelia, W.F. Nirode, **S. Singh**
- CHED 1444.** Deprotonative zincation for the α functionalization of phosphonates. **H. Pauley**, K. Bitting
- CHED 1445.** Synthesis of uracils and fluorouracils. **D. Brady**, D. Shellhamer
- CHED 1446.** Development of a colorimetric displacement assay for the evaluation of peptide aldol catalysts. **M. Mays**, L. Witus
- CHED 1447.** Green synthesis and analysis of diaryl imine metal complexes. **A.L. Gaynor**, J. Bennett
- CHED 1448.** Synthesis of hydrolysable organic linkers and derivatives for localized drug delivery. **W. Rouse**, T. Divis, J.E. Elbert
- CHED 1449.** Efficiency of reductive amination in a variety of solvents. **J.J. Marcantonio**, J. Bennett



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- CHED 1450.** Deactivating group substitution impacts on reaction rates. **K. Lankford**, M.J. D'Souza
- CHED 1451.** Development of low-cost automated organic chemistry lab techniques using the arduino microprocessor and a 3D printer. **D. Flood**, C.E. Stilts
- CHED 1452.** Enantioselective synthesis of biaryl pyridines and quinolines via cinchona alkaloid-catalyzed nucleophilic aromatic substitution. M.M. Cardenas, **A. Sanchez**, C.J. Robinson, J.L. Gustafson
- CHED 1453.** Click-style Sonogashira deprotection and coupling reactions involving silyl-protected alkynes at room temperature. **M.J. Mio**, H.I. Ali, L.F. Baltaji, R. Benjamin, P. Bhagat, N.R. Boynton, S.M. Brikho, M.T. Dickow, M.E. Girardi, T. Mahjoub, M.M. Payne, B.M. Ross, C.N. Sayah
- CHED 1454.** Synthesis of an acyl-acyl carrier protein synthetase inhibitor to study fatty acid recycling. **M. Currie**, K.L. Jaremko
- CHED 1455.** Synthesis of 2-(2-furylmethylidene)cyclopentanone via isolation of the alcohol from aldol addition. **B. Gamelin**, J.C. Easdon
- CHED 1456.** Design of protein mimetics by dynamic combinatorial chemistry on folded peptidic scaffolds. **G. Webb**, B. Zagiel, T. Peker, R. Mourné
- CHED 1457.** Dancing crystals. **J.R. Brown**, D.J. Shields, A.D. Gudmundsdottir
- CHED 1458.** Electrochemical oxidation of sodium glucoheptonate to its dicarboxylic acid salt. **H.M. Barnette**, M.E. Hayes
- CHED 1459.** Synthetic approaches to benzofuran- and dihydrobenzofuran-containing calixarenes by intramolecular reaction at the lower-rim and methylene-bridge groups. **H. Tran**, H.R. Glick, D.H. Johnston, J.L. Fantini
- CHED 1460.** Studies of the imine inverse electron demand Diels-Alder. S.M. Kennedy, **G. Good**, **R.R. Laughlin**
- CHED 1461.** Room temperature hydrosilylation of imines catalyzed by an air stable rhenium(V)-oxo complex. **M. Clothier**, A. Ison
- CHED 1462.** Developing methods for the synthesis of bacteriochlorin-glycoconjugates. **M.E. Lech**, **J.E. Cuadra**, D.G. Dennis, M.B. Burch, G. Mukosera, M. Parris, N.L. Snyder, J.V. Ruppel
- CHED 1463.** Synthesis of substituted 2-benzylidenecalixarenes via Heck reaction of 2-methylene-*p-tert*-butyltetrahydroxycalix[4]arene. **A.A. Ferguson**, J.L. Fantini
- CHED 1464.** Synthesis of structurally complex aryl phosphonates. **M. Petersen**, **N. Jiter**, **S. Winchell**, A. Haugen, M. Schmid, J. Scanlon, P. Willoughby
- CHED 1465.** Squaramide-based anti-parasitic drugs toward the discovery of novel treatments for American trypanosomiasis. **E.N. Tran**, G.R. Naumiec
- CHED 1466.** Coupling reaction of ethyl diazoacetate with a tertiary thioamide. **N. Rajagopal**, A. Pal, S.R. Hussaini
- CHED 1467.** Solid-state studies of halogenated benzonitrile oxides and their dimers: Crystal structure of *bis*(2-fluorophenyl)furoxan. **M. Stodolka**, W.H. Ojala



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- CHED 1468.** Photo-active naphthalimide-drug compound synthesis and characterization. **T. Divis**, J.E. Elbert, W. Rouse
- CHED 1469.** Synthesis of C-glycosides modeled after type II diabetes treatments. **K. Krol, N. Graves**, J. Chaytor
- CHED 1470.** Toward isomorphous “bridge-flipped” isomers: Investigations of 3-pyridyl and hydrazine-based systems and the crystal structure of a hydrazine-based diimine. **M. Howk**, W.H. Ojala
- CHED 1471.** Synthesis and characterization of drug derivatives and drug derivative-naphthalimide compounds for localized drug delivery. **K. Parrott**, H. Lovstad, J.E. Elbert
- CHED 1472.** Toward isomorphous “bridge-flipped” isomers: Investigations of 4-pyridyl and glyoxal-based systems and the crystal structure of a pyridyl benzylideneaniline derivative. **E. Morone**, W.H. Ojala
- CHED 1473.** Solid-state studies of derivatives formed by reaction of nitrogenous bases with aldoses: Crystal structure of the 2-fluorophenylhydrazone of D-mannose. **A. Smith**, W.H. Ojala
- CHED 1474.** Investigation of oxy-Michael Ugi-smiles couplings. **J. Jones**, S. Luesse
- CHED 1475.** Quinoxaline-based donor-acceptor dyes: Synthesis, photophysical, and electrochemical properties. **B.M. Lucht, R.J. Monsky**, M.C. Rosko, J.M. Nadeau
- CHED 1476.** Unexpected failures in quasiracemic crystallizations. **M. Vanderwall, A. Brandt**, L. Cantrell, D. Boyle, A. Gillingham, M. Parks, J. Spaniol, K.A. Wheeler
- CHED 1477.** Copper mediated trifluoromethylation of benzylic Csp³-H bonds. **W.P. Carson**, M. Paeth, W. Liu
- CHED 1478.** Synthesis, characterization and biological activity of ferrocenyl curcumin analogs. **J.R. Hernandez**, S. Delgado-Rivera, A. Baerga-Ortiz, D.M. Pinero Cruz, I. Montes-Gonzalez
- CHED 1479.** Selection of the optimal counterion of ferrocenyl chalcone salt derivatives to enhance their biological activity. **D.Y. Díaz-Rohena**, S. Delgado-Rivera, A. Baerga-Ortiz, D.M. Pinero Cruz, I. Montes-Gonzalez
- CHED 1480.** Synthesis, characterization and biological properties of mono and disubstituted ferrocenyl chalcones. **S.A. Henriquez Lopez**, S.M. Delgado-Rivera, G.E. Pérez-Ortiz, A. Baerga-Ortiz, D.M. Pinero Cruz, I. Montes-Gonzalez

Section I

Orange County Convention Center
West Hall C

Undergraduate Research Posters

Physical Chemistry

Cosponsored by SOCED
N. Di Fabio, J. Roberts, *Organizers*

12:00 - 2:00



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- CHED 1481.** Influence of compositional variations on properties of misfit layer calcium cobalt oxide compounds. **S.L. Luty, R.A. Davis, D.G. Hauner, C. Heideman**
- CHED 1482.** Project alchemy: EPR spectroscopic investigation of the Bologna stone. **C. Fabiano, A. Angerhofer**
- CHED 1483.** Electronic structure of TaH in the visible region. **S.P. Gleason, P.P. Reischmann, T.D. Varberg**
- CHED 1484.** Temperature and methanol co-solvent effects on the critical micelle concentration, enthalpy of micelle formation, and micelle particle size for CTAB and DTAB in water. **H. Jackson, L.C. O'Brien**
- CHED 1485.** Design and fabrication of a homebuilt T-jump for kinetic characterization of chemotherapy drugs. **S. Glazier, D. Bain**
- CHED 1486.** High throughput crystal detection: An application of nonlinear processes. **J.R. Wagner, C.J. Smith, S.R. Griffin, G.J. Simpson**
- CHED 1487.** Spectroscopically probing the light-initiated reaction between lumazine and dAMP: Investigating the mechanism of cell death in photodynamic cancer therapy. **S. Bobadilla-Regalado, S. Strothers, L.M. Mier**
- CHED 1488.** Spectroscopic analysis of the interaction between DNA and the excited state of lumazine. **S. Strothers, S. Bobadilla-Regalado, L.M. Mier**
- CHED 1489.** Thermodynamics of fluoride binding in heme proteins in the presence of CaCl₂ and PbCl₂. **A. Frankenfield, D. Deysher, J. Cerda**
- CHED 1490.** Investigation of ¹O₂ quantum yield by the photodynamic cancer therapy agent lumazine. **W. Saumier, T. Valliere, L.M. Mier**
- CHED 1491.** ¹O₂ quantum yield dependence on varying concentrations of lumazine, oxygen, and pH. **T. Valliere, W. Saumier, L.M. Mier**
- CHED 1492.** A novel application of focused ultrasound for the treatment of port wine stain birthmarks. **K. Doucette, J. O'Malley, P.J. White**
- CHED 1493.** Determining the kinetic order of the degradation of L-ascorbic acid. **N. Syed, D. Gustitus, M. Garrett**
- CHED 1494.** Building and optimizing a nitrogen gas laser. **A. Wyatt, W.E. Schatzberg**
- CHED 1495.** Computational modeling of gas phase hydrogen deuterium exchange of peptides containing multiple arginines. **C. Zhang, E.M. Marzluff**
- CHED 1496.** Tracking structural changes in nanoparticle-bound proteins using 2D infrared spectroscopy. **K.D. Segner, K.R. Webb, L. Buchanan**
- CHED 1497.** Development of a modified Michaelis-Menten Langmuir kinetic model for supported lipid bilayer formation. **K. Baker, R. Kiss, J. Bridges, P.J. Kett**
- CHED 1498.** Selective CO production in CH₄ oxidation on TiO₂ through photoelectrochemical approach. **T. Gao, W. Li, D. He, G. Hu, X. Li, G. Banerjee, J. Li, S. Lee, Q. Dong, G.W. Brudvig, M. Waegle, D. Jiang, D. Wang**



TECHNICAL PROGRAM

- CHED 1499.** Understanding non-toxic oil dispersants at the oil and water droplet interface. **A. Mapile**, A. Carpenter, G. Richmond
- CHED 1500.** Investigating the role of a critical vesicle concentration in the formation of supported lipid bilayers. **J. Bridges**, K. Baker, R. Kiss, P.J. Kett
- CHED 1501.** Kinetic investigations of the gas phase reaction between the CH radical and cyclopentadiene. **Z. Donnellan**, K. Caster, T. Selby, F. Goulay
- CHED 1502.** Investigation of the adsorption behavior of desferrioxamine-B with the hematite/water interface using nonlinear spectroscopy. **J. Van Ardenne**, A.L. Mifflin, J. Brennan
- CHED 1503.** Exploring the chemistry of mordantage, a historic photographic process. **C. Fudala**, R.M. Jones
- CHED 1504.** Studying singlet fission in a tetracene derivative with femtosecond stimulated Raman spectroscopy. **B.R. Nebgen**, A.A. Cassabaum, L.J. Purvis, C.J. Douglas, R.R. Frontiera
- CHED 1505.** Generating a TDDFT model for electrochromic materials. A.L. Tomlinson, **A.V. Diodati**
- CHED 1506.** Role of carbon monoxide in atmospheric haze formation at cryogenic temperatures. **N. Bishop**, J. Sebree, J. Kaur Rishi
- CHED 1507.** Water-soluble porphyrins that show specificity towards G-quadruplex DNA: microwave synthesis, characterization and spectroscopic study. **K. Pytko**, E.M. Valentin, S.M. Basu
- CHED 1508.** Understanding the role of flow rate and lipid concentration in the kinetics of supported lipid bilayer formation. **R. Kiss**, K. Baker, P.J. Kett
- CHED 1509.** Photovoltaic systems using organic dyes and quasi-solid state electrolytes. **A. Paul-Orecchio**, S.M. Brothers
- CHED 1510.** Spectroscopic and relative rate studies of the oxidation of fluoromethane initiated by atomic chlorine. **J.A. Velasquez**, G. Rawling, R. Sapkota, P. Marshall
- CHED 1511.** Effect of pH on the aqueous oxidation of brilliant green dye. **C.J. Hlavacek**, A.M. Bunnag-Stoner, G.H. Purser
- CHED 1512.** Proposed mechanism and rate law for the non-enzymatic hydrolysis of l-arginine ethyl ester. **M.D. Reavis**, A. Beffa, P.A. Harville, G.H. Purser
- CHED 1513.** FRET's impact on solar cells: A study on how FRET dyes impact efficiency. **M. Petrey**, J.M. Wiester
- CHED 1514.** Technology applications of self-assembling DACLCs: Information storage and encryption techniques. **H. Wallace**, J.J. Reczek
- CHED 1515.** Using an auto-correlator to produce second harmonic generation and study the effects of dispersion on femtosecond pulses. **M. Sullivan**, C.S. Schnitzer, G. Gu
- CHED 1516.** BiNbO₄: A photocatalyst for hydrogen evolution. **C. Kovac**, S.J. Gravelle



TECHNICAL PROGRAM

- CHED 1517.** Will the spins align? Theoretical investigations into the magnetism of oxo-centered tri-metallic clusters decorated with nitroxide groups. **E. Hess**, S. Nellutla, S.C. Haefner
- CHED 1518.** Ammonia-SiX₃R complexes: Exploring properties via computational modeling and low-temperature IR spectroscopy. **A. Ley**, P. Treacy, B. Zehner, J.A. Phillips
- CHED 1519.** Role of the spectator ion in the "reverse chemical garden" reaction. **C. Cowley**, M.A. Horn
- CHED 1520.** External CapPack™ devices. **B. Gamelin**, J.C. Easdon, M. Huang, E. Wideman, K.H. Woelk, J. Huang, R. Gerald
- CHED 1521.** Computational modeling of lithiated carbon phosphonitride electrolyte materials. **M. Lanetti**, M. Dorko
- CHED 1522.** Comparison of ionic association indicators: Lithium triflate in polyamine and polyether systems. **H. Lee**, M. Vogt, K. Elder, R.N. Mason
- CHED 1523.** Revisiting the properties of fluoro-pyridine-SiF₄ complexes: Condensed-phase structural changes. **R. Mooney**, P. Treacy, A. Ley, B. Zehner, J.A. Phillips
- CHED 1524.** Measuring molecular diffusion in ammonium-based ionic liquids using fluorescence correlation spectroscopy. **N.G. Puskar**, A.M. Fleshman, S.M. Mahurin
- CHED 1525.** Activation parameters for fragmentation of three tetrapeptides at penultimate proline in ethanol. **K.R. Molloy**, C.S. Zhang, M.W. Perkins, D.A. Hales, D. Fuller, T.J. El-Baba, D.E. Clemmer
- CHED 1526.** Plasticizing effect of water on highly viscous sucrose films. **T.S. Qin-Terrill**, A. Edwards
- CHED 1527.** Activation parameters for fragmentation of a series of Arg-Xaa-Gly-Gly tetrapeptides. **M.W. Perkins**, K.R. Molloy, D.A. Hales, D.E. Clemmer
- CHED 1528.** Understanding the photophysical properties and self-assembly of *meso*-tetrakis(4-sulfonatophenyl)porphyrin in aqueous solution. **H. Schmidt**, **O. Makinde**, J. Hollingsworth
- CHED 1529.** Gas-phase fragmentation pathways of bradykinin ions and comparison to solution-phase results. **C.S. Zhang**, K.R. Molloy, D.A. Hales, D. Fuller, D.E. Clemmer
- CHED 1530.** Usage of localized surface plasmon resonance to study interfacial effects on environmental electron transfer mediators. **N. Nguyen**, N. Slenning, P. Hall, A. Pavitt, P.G. Tratnyek
- CHED 1531.** Effect of electron-donating and withdrawing groups in the photophysical, electrochemical, and spectroelectrochemical properties of corrole tautomers. **A. Leon**, K. Webb, R. Raker, S.K. Mendez, E.A. Aleman
- CHED 1532.** Noble metal nanoparticles as targeted drug delivery vehicles. **A. Alfaro**, B.D. Gilbert
- CHED 1533.** Photophysical, electrochemical, and spectroelectrochemical characterization and solvent effect on the tautomerism of free-base corrole. **K. Webb**, **V.E. Hernandez**, C. Reed, E.A. Aleman
- CHED 1534.** Observation of photobleaching lifetimes of Cy3-alkyne and Cy5-alkyne fluorescence. **I.A. Orantes-Orellana**, M.A. Garcia, D. Cooper



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- CHED 1535.** Taming polypyrrole oligomer synthesis with mass spectrometry. **J.L. Stair**, D. Moore
- CHED 1536.** Characterization of the vibrational properties of copper difluoride anion and neutral ground states via direct and indirect photodetachment spectroscopy. **J. Hamilton**, J. Lyle, S. Chandramoulee, B. Traylor, T.L. Guasco, T. Jagau, R. Mabbs
- CHED 1537.** Kinetics and thermodynamics of heavy metal removal from water using starch polyacrylonitrile composite polymer. **B.M. Smith**, A. Chaparadza
- CHED 1538.** Electronic nature of 2-butyne-1-yl and 1-butyne-3-yl radicals. **G. Brown**, M. Ellis, T. Martin, L.R. McCunn
- CHED 1539.** Spectroscopic study of tiglic aldehyde. **M. Ellis**, G. Brown, T. Martin, L.R. McCunn
- CHED 1540.** Lipid membrane permeability of imidazolium chloride ionic liquids: Combined studies on model vesicles and biological cells. **A. Swinton**, **K. Tarnawsky**, K. Cook, D. Yang, G.A. Caputo, B. Carone, T.D. Vaden
- CHED 1541.** Isothermal compressibility of liquid binary mixtures. **B.C. Wada**, O. Baldwin, G.R. Van Hecke
- CHED 1542.** Predicting NMR chemical shift anisotropy of cimetidine with dispersion corrected plane-wave DFT. **O. Engl**, S.T. Holmes, J. Harper, R. Iulucci
- CHED 1543.** Photophysical characterization of novel rhodamine B dimers. **N. Grinalds**, L. Pferdenges, B. Hunter, K. Fogarty, P. Lundin
- CHED 1544.** TATP: An exploration of practical applications for highly sensitive explosives. A. Nance, **L. Brock**, M.B. Jacobs
- CHED 1545.** Organic materials for thermal energy storage: Binary mixtures of consecutive straight-chain carboxylic acids form low-melting solid solutions. **D.S. Guo**, C. Adams, G.R. Van Hecke
- CHED 1546.** Time-dependent Raman spectroscopy of acidic Crystal Violet on TiO₂ nanoparticles. **H.I. Shah**, S. Coon
- CHED 1547.** Standardization of sucrose films as a model for water diffusion in brown carbon mimics. **W. Ackermann**, A. Edwards
- CHED 1548.** Identifying and solving problems in integrity of tissue samples after cryopreservation. **A.S. Torres Yabar**, **A.N. Howell-Munson**
- CHED 1549.** Isothermal titration calorimetry study of the ligand exchange of oleate-CdSe quantum dots with pyridine. **L. Hicks**, J.D. Keene
- CHED 1550.** Catalytic effect of CO₂ environment on OH + CH₂O → H₂O + CHO reaction rate. **E.E. Wait**, A. Masunov, S. Vasu
- CHED 1551.** Towards carbon-based nanotechnology: A spontaneously self-assembled, supramolecular dipolar electric motor, from a betaine rotator and a hydrogen-bonded, host-guest, {bicyclo[2.2.2]octan-1-aminium 18-crown-6} dyad stator. **M. Costa**, A. Pineda-Knauseder, S. Munoz
- CHED 1552.** Towards carbon-based nanotechnology: A spontaneously self-assembled supramolecular rotor from a 4,4'-diethynyl-p-terphenyl rotator and [10]cycloparaphenylene-C₆₀ dyad stator. **M. Martin**, S. Munoz



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

CHED 1553. Towards carbon-based nanotechnology: Conformational energy profile of a spontaneously self-assembled supramolecular rotor from a 1,4-bis(butadiynylbenzene) rotator on a hydrogen bonded, host-guest, {bicyclo[2.2.2]octan-1-aminium 18-crown-6} dyad stator. **A. Pineda-Knauseder**, S. Munoz

CHED 1554. Towards carbon-based nanotechnology: A spontaneously self-assembled supramolecular rotor from a 1,4-bis(butadiynyl)benzene rotator and [10]cycloparaphenylene-C₆₀ dyad stator. **C. Luque**, S. Munoz

CHED 1555. Towards carbon-based nanotechnology: A spontaneously self-assembled supramolecular rotor from a 4,4"-diethynyl-p-terphenyl rotator and {bicyclo[2.2.2]octan-1-aminium 18-crown-6} dyad stator. **K. De Villiers**, S. Munoz

Section I

Orange County Convention Center
West Hall C

Undergraduate Research Posters

Polymer Chemistry

Cosponsored by PMSE, POLY and SOCED
N. Di Fabio, J. Roberts, *Organizers*

12:00 - 2:00

CHED 1556. Synthesis and application of crosslinkable ionic liquid monomers. B. McFarland, **J. Sandoz**

CHED 1557. Toward an understanding of dielectric breakdown through incorporating defects into polyetherimides. **J. Lockwood**

CHED 1558. Effects of crosslinking on polyurea-shell microcapsules containing a free-radical initiator core. B. McFarland, **S.P. Anderson**

CHED 1559. Heavy metal detection via the reactive dye method and natural fiber welding. **A.S. Tanner**, M.W. Reichert, K.J. Wallace

CHED 1560. Obtaining large-size single crystals of linear anthracene polymer through light-triggered topochemical polymerization. **Q. Yu**, M. Li, Y. Chen, Z. Zhang, P. Cheng

CHED 1561. Synthesis of heterotelechelic polymers via RAFT polymerization for tagging red blood cells as drug carriers. **Y. Huang**, J. Niu

CHED 1562. Characterization of mechanical properties of hydrogel nanofibers for wound healing application. **F. Hernandez Luna**, A. Diaz, Y. Li Sip, H. Kang, L. Zhai

CHED 1563. Effects of hydrogen bond organization on the dielectric relaxation and electrical conductivity behavior of bis-MPA based hyperbranched polymers. **R. Ditzler**, B. Chen, S.M. Grayson, S. Nazarenko

CHED 1564. Determining methods for inducing crystalline β -phase PVDF and PVDF-HFP copolymers in thin films without post-annealing. **M.J. Demmings**, A. Dale, A. Mosey, R. Cheng



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- CHED 1565.** Synthesis of horseradish peroxidase (HRP)-polymer bioconjugates by grafting-from HRP-initiated RAFT polymerization. **C. Kozuszek**, K. Burrige, R.C. Page, D. Konkolewicz
- CHED 1566.** Kinetics of the organophosphoric acid catalyzed ring opening polymerization of methyl caprolactones. **M.S. Meyersohn**, D. Batiste, A. Watts, M.A. Hillmyer
- CHED 1567.** Silicone microspheres: Synthesis, characterization, and application. **S. Metheny**, L. Rahm, J. Overcash, J. Esbenshade
- CHED 1568.** Anilinium salts in polymer networks: Computational modeling of dynamic polymer kinetics. **L. Kuhn**, P. Chakma, Z. Digby, M.P. Shulman, J. Sparks, D. Konkolewicz
- CHED 1569.** Regenerative Diels-Alder step-growth polymer. **T. Eliason**, N.E. Huddleston
- CHED 1570.** Heavy metal water filtration by chitin with varying degrees of acetylation. **S. Baumgartner**, J.D. Mendez
- CHED 1571.** Synthesis of highly emissive covalent organic frameworks for optoelectronic properties. **A.Q. Syed**, **G.H. Pearson**, **K. Allen**
- CHED 1572.** Stereolithographic 3D printing of photocurable resins for tissue engineering. **T. Colpitts**, J.A. Morrill
- CHED 1573.** Synthesis of polymeric microspheres using ultrasonic spray photopolymerization. **M.E. Short**, L. Rahm, J. Overcash, J. Esbenshade
- CHED 1574.** Synthesis of multifunctional, well-defined polyacrylates as precursors to superior hemoglobin-based oxygen carriers. **N.Z. Singleton**, O. Alomainy, A. Diaz-Avella, H.J. Schanz
- CHED 1575.** Hydroamination as polyaddition methodology to access multifunctional polymers. **E.R. Anderson**, S. Schrickel, A.J. Caroland, H.J. Schanz
- CHED 1576.** Synthesis and characterization of perfluorocyclohexenyl aryl ether homopolymer. **J. Hankemeyer**, G. Narayanan, D.W. Smith
- CHED 1577.** Photo-degradation of polylactic acid and polyethylene terephthalate in different gas environments. **E. Lankford**
- CHED 1578.** Separation chemistry and crystallographic investigation of orthogonal catalysis of a conjugated polymer by an enzyme. **H. Spivey**
- CHED 1579.** Progress towards the synthesis of a novel catalyst for controlled synthesis of conjugated polymers. **G. McLeod**, R.M. Meier, N.E. Huddleston
- CHED 1580.** Antimicrobial VBT:TMQ:DMHDQ (1-(4-vinylbenzyl) thymine, vinylbenzyl trimethyl QUAT, and vinylbenzyl dimethylhexadecyl QUAT) terpolymer permanence and performance on hospital scrubs. **E. Baulsir**, M. Yandian, A. Jaber, R. Laemmle, R.W. Gurney
- CHED 1581.** Effects of microgravity on the self-assembly of PEGMA and drug delivery systems. **D. Schneider**, **C. Tallone**, **C. Uka**, P.G. Cohn



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- CHED 1582.** Encapsulation and controlled release of G-quadruplex DNA through PMAA/PVPON microcapsules. **J. Gearhart**, A. Alford, N. Gupta, E.P. Kharlampieva
- CHED 1583.** Segmented phosphonium ionenes as solid polymer electrolytes for all-solid-state lithium ion batteries. **K. Strong**, A. Abdulahad
- CHED 1584.** Solid polymer electrolytes for all-solid-state lithium ion batteries based on phosphonium ionenes. **L. Gist-Reed**, A. Abdulahad
- CHED 1585.** Synthesis of spherical metallo nanoparticles. **M.J. Fox**, W.M. Ames
- CHED 1586.** Structure-property relationships of dynamic biomaterial hydrogels based on hyaluronic acid and nucleobase-containing polymers. **A. Stephens**, A. Abdulahad
- CHED 1587.** Sustained drug release of doxorubicin from biocompatible hydrogels based on complementary hydrogen bonding. **A. Abanu**, A. Abdulahad
- CHED 1588.** Synthesis, characterization, and self-assembly of adenine- and thymine-containing polymers for biomedical applications. **S. Muhammad**, **J. Pratt**, A. Abdulahad
- CHED 1589.** Synthesis of polymers from plant derivatives: Progress towards green materials. **A. Morrenzin**
- CHED 1590.** Synthesis and characterization of novel polypeptide nanoparticles. **S. Carstens**, **L. Renfro**, D.W. Holley
- CHED 1591.** DOSY NMR for high dispersity polymers. **C. Cattafi**, P.G. Cohn
- CHED 1592.** Degradation of consumer plastics under simulated environmental weathering and biological conditions. **G. Chan**, N.A. Swartz
- CHED 1593.** Thiophene-based covalent organic frameworks. **L. Schroeder**
- CHED 1594.** Synthesis of novel hexavalent glycodendrimers. **J.F. Gonzalez**, D. Dimas, K.D. McReynolds
- CHED 1595.** Chemical Repellents in polymers undergo environmental strains. **B. Halliwell**, D.A. Fish
- CHED 1596.** Investigating the effect of diene core and cross-linking frequency in Diels–Alder self-healing polymer networks. **A. Sartori**, T. Smith, P. Tandler
- CHED 1597.** Imidazolium-based ionic liquid polyesters. **R. Weldon**, M.J. Campbell
- CHED 1598.** Polymers and composites from pine rosin. **K.A. Monroe**

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Sponsored by PROF, Cosponsored by AGFD, ANYL, BIOL, BIOT, CARB, CELL, CHED, CMA, COLL, COMP, ENVR, GEOC, I&EC, MEDI, MPPG, NUCL, ORGN, PHYS, PMSE, POLY, PRES, WCC and YCC



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

MONDAY EVENING

Section A

Orange County Convention Center
Room W315A

Revamping Practical Chemistry Teaching for the New Frontier

Cosponsored by PMSE, POLY and RUBB
S. C. Rukes, *Organizer, Presiding*

4:00 Introductory Remarks.

4:05 CHED 1599. Deepen your students' STEM experience by adding various inquiry/engineering design challenges with several Make-n-Take items. **S.C. Rukes**

5:05 Intermission.

5:10 CHED 1600. Through the eyes of a baby. **R.A. Wesolowski**, S.C. Rukes

6:00 CHED 1601. Withdrawn

6:45 CHED 1602. New frontier: Car chemistry moving from Carbon (How it was, to how it is, to where it is going). **A. Nydam**, S.C. Rukes

7:30 Concluding Remarks.

Section A

Orange County Convention Center
West Hall C

Sci-Mix

D. C. Bromfield-Lee, A. S. Cannon, I. J. Levy, *Organizers*

8:00 - 10:00

45, 49, 127-132, 137-138, 142, 151, 158, 176, 180, 277, 283. See previous listings.

1736, 1739, 1766, 1772, 1789, 1843, 1847-1848, 1851, 1856-1857, 1860, 1917, 1920, 1961, 1970, 1974. See subsequent listings.

Section B

Orange County Convention Center
West Hall C



TECHNICAL PROGRAM

Successful Student Chapters

Cosponsored by SOCED
N. Di Fabio, J. Roberts, *Organizers*

8:00 - 10:00

CHED 1603. Falcon chemistry club: Promoting chemistry in West Texas ACS student chapter at the University of Texas of the Permian Basin- Odessa, TX. **S. Ko**, K. Driver, A. Aranda

CHED 1604. Using chemistry for community engagement and professional development. **C. Eastmond**, R. Balarezo, B. Bokor, P. Nilchian, C. Mederos, S. Nodal, L. Quesada, M. Bellon, A. Torres, B. Lopez, G. Rasch, S. Kim, U. Swamy

CHED 1605. Building a chemistry community at Stony Brook University. **B. Herrnkind**, J.E. Zambito, J. Zheng, M. Johnson, T. Singh, P. Lotlikar, C.J. Johnson

CHED 1606. Student chapter events and activities at Tennessee Technological University. **T. Pinto**, M. Dunn, S. Jones, L. Pipkin, J. Scantland, A. Rossi, J. Ralston, D. Cassidy, A.J. Carroll

CHED 1607. Bringing chemistry to alkynes of people. **A.C. Hartley**, **P.A. Skerratt**, **A.L. Coker**, E.L. Bray, E.R. Bishop, T.R. Hayden, J.E. Boyd

CHED 1608. Advancement of minorities and females in science. **M. Kaimenyi**, M. Gaines

CHED 1609. Building an outstanding international ACS student chapter. **J.J. Montero**, **A. Fernández**

CHED 1610. Bonding with Bithlo: Enhancing the quality of K-12 science education in an underprivileged community. **J. Kreisel**, S.M. Kuebler, **A. Zuleta-Visser**, **J.W. Chang**

CHED 1611. Chemistry is central at UCO: Successful student chapter activities. K. Bennett, K. Berger, K. Brogden, E. Cline, F. Matthews, C. Murphy, R. Wood, **C.B. Frech**, D. Rundle

CHED 1612. Advancing chemistry undergraduate career through annual professional development activities. **B.C. Nguyen Viet**, **C. Frignoca**, **A. Cestrone**, M. Crowell

CHED 1613. Fostering professional development and inter-chapter relations through the annual Florida chemistry conclave. **A. Preston**, **A. Ferguson**, **J. Kreisel**, S.M. Kuebler, N. Takenaka

CHED 1614. Fantasizing ethereal chemistry in Delaware. **O. Uyebi**, M.J. D'Souza

CHED 1615. Building a successful ACS student affiliate through professional development, community outreach, undergraduate research & community service. **N. Elmore**, **G. Johnson**, B. Kohler, A. Maddox, L.C. Huynh, S. Grosser, J. Maurer, D. Edwards, J. Al-Haddad, R.V. Valcarce, P.J. Iles, L.D. Giddings, W. Sanders, M. Alvarez, N.R. Bastian

CHED 1616. American Chemical Society student chapter at the University of Texas at Tyler. **J.M. King**, T. Rashid, L. Johnson, L.E. Boyd

CHED 1617. Truman State University student affiliate chapter. **D.S. Mattock**, **C. Wolf**, **P.T. Sullivan**, T.A. Humphry



TECHNICAL PROGRAM

- CHED 1618.** Activities and contributions of a newly established student chapter in a developing country. **M. Hasan**, M. Islam, M. Hossain, R. Ahamed, M. Hossain
- CHED 1619.** Successful workshops of an international chapter. **D. Carvajal Mora**, **J. Godínez Bolaños**
- CHED 1620.** Suffolk University: Expanding knowledge to all. **K. Jenkins**, M. Curcio, B. Gemechu, N. Grimaud, L. Riffert, E.J. Enyedy
- CHED 1621.** Morehead State University chemistry club. A. Anwar, **T. Sullivan**, **M.T. Blankenbuehler**
- CHED 1622.** Spreading the word: Chemistry is fun at Tecnológico de Monterrey. **N. Baeza**, P. Uribe Jimenez, G. Torres, M. Medina, J. Gómez, M. Medina, A. Medrano, J. Arriaga, I. Palestino, A. Murrieta
- CHED 1623.** Celebrating NCW 2018 at University of Puerto Rico Humacao. J.L. Cruz, L.M. Rosario, A. Guzman, A. Figueroa-Perez, N. Garcia, **J. Suarez**
- CHED 1624.** Ethics symposium: How to be a "good" chemist. **M. Ash**, F. Bruno, K.P. Kuzelka, C. Weitzel, J. Kim
- CHED 1625.** Lock Haven University chemistry club. **K. Elliott**, S. Hogan, H. Ostrander, K. Root
- CHED 1626.** Pulling a hat trick: Continuing a tradition of excellence. **J. White**, Y. Wang
- CHED 1627.** Involvement! Involvement! Involvement. **E.N. Tran**, **J. Schneider**, **A. Abdulrahim**, **W. Higgins**, **J. Dodson**, G.R. Naumiec, F.M. Yarberr
- CHED 1628.** SIUE chemistry club: Spreading chemistry knowledge on campus and in the community. **N. Schmidt**, S. Olendorff, T. Farmer, C. Arcelona, G. Hansen, M.J. Hankins
- CHED 1629.** Ball State University student affiliates of the ACS: Advocating for science. **B. Watson**, D. Dooley, S. Lemmon, J. Platt, S. Vogel, R. Jeske
- CHED 1630.** Northeastern University student chapter: Building a chemistry community. **P. Donnelly**, K. Coghlan, K.R. Mathiowetz
- CHED 1631.** Otterbein University student chapter: Getting involved! **E. Tinapple**, N. Forney, M.C. Marshall, J.M. Esson
- CHED 1632.** ACS student chapter at Millersville University 2018-2019. **F.O. Fernandez**, **G. Good**, C.J. Reyes, L. Schroeder, J.M. Sharrow, F.K. Wenrich, L.H. Rickard, D. Albert
- CHED 1633.** Green chemistry with the Cru: Serving the community and environment. **A. Nguyen**, L. Gao, B. Bishop
- CHED 1634.** Santa Monica College chemistry club: A student chapter with an emphasis on professional development, outreach, and green chemistry. **A. Kepper**, **J. Tan**, **S. Chung**, **M. Sharp**, J.M. Hsieh, T. Pecorelli
- CHED 1635.** Leading a successful ACS student chapter. **A.J. Sanders**, S. Richey, L. Jarka, K. Troyer, A. Main
- CHED 1636.** Student chapter activities at Angelo State University. **H. Hillert**, E. Osborne
- CHED 1637.** Green chemistry activities at Angelo State University. **B. Krug**, E. Osborne



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- CHED 1638.** Berry College division of ACS: Extending chemistry beyond the classroom. **K.J. Nichols**, M. Moeller, D. McGaha
- CHED 1639.** Carroll University chemistry club. **A. Larsen, C. McElrath, S. Frisque, K. Burmeister, S. Spence**, D. Patel, T. Katzman
- CHED 1640.** Awesome chemistry demonstrations by student members at Belmont University for the community. **A.S. Daniels**, C.J. Hansen, A. Parker
- CHED 1641.** In our element: ACS at Ouachita Baptist University. **J. Cook, C. Shirley**, J.E. Bradshaw, S.K. Hamilton, S.E. Hubbard
- CHED 1642.** Inspiring today's youth through science & geochemistry. **J.P. Stetzler**, M.E. Olsson
- CHED 1643.** Activities of the College of Mount Saint Vincent science club 2018-2019. **N. DeSouza, D. Quaranto**, P.K. Kerrigan
- CHED 1644.** Chapter growth as a result of student engagement and chemistry outreach. **Z.A. Webster, D.C. Zites, G. Dominguez, M.L. Agan**, T.A. Shell
- CHED 1645.** Aromatic resonance: A key component in the stability of the mayagüez chapter. **M.M. Rodriguez Quinones**, M. Barreto, A. Nuñez, P. Soler, Y. Merced, N. Betancourt, A. Robles, F. Velázquez, J. González, C. Hernández, N. Irizarry, N. Peña
- CHED 1646.** Enhancing scientific literacy in our community. **H. Wakidi, S. Hunt**, C. Murphy, S.K. O'Shea
- CHED 1647.** American Chemical Society student chapter at the University of St. Thomas, Houston, TX. **C. Luong, Y. Tran**, N. Nguyen, N. Penaloza, N. Senawong, S. Carty, A. Akhtar, **K. Vedan**, J. Hollingsworth, C.A. Young
- CHED 1648.** From club member to teaching labs: A path to leadership development. **F. Frech**, K. Lugo, J. Daye, E. Lorquet, M. Delgado
- CHED 1649.** Sparking scientific curiosity in the Toledo community. **M. Klingberg, E. Diemler, C.M. Schreidah, J. Koffman, N.L. Mai, E. Kenney, J.M. Maxwell, V. Sohasky, J. Schreur**, E.P. Kippenhan
- CHED 1650.** Increasing student chapter engagement within the Penn State Chemistry Department. **L.C. Velazquez Bello, E.S. Gogarnoiu**, L.R. Stepan, J. Houck
- CHED 1651.** Minot State University student chapter of the American Chemical Society. **T.A. Skinner**, M.M. Bobylev
- CHED 1652.** Year in review: University of Tennessee at Martin student member chapter. **S.E. Max**, M. Kerbersky, A. Orr, K. Kaul, A.H. Shelton
- CHED 1653.** Food chemistry division of ACS Inter ponce student chapter. **N.N. Peralta Pacheco, P.B. Reyes Santiago**, P. Garcia Gonzalez, T. Felix Massa, E. Ferrer Torres
- CHED 1654.** ChEmory: Emory University's undergraduate chapter of the American Chemical Society. **S.S. Hwang, A. Diaz**, A. Kim, J. Li, A. Zachmann, A. Yang, D.R. Mulford



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- CHED 1655.** Colorado State University chemistry club: Learning through community engagement and interdisciplinary relationships.. **J. Neuwirth**, V. Bachtell, J.T. Brookhart, H. Hare, C. Henderson, J. Trowbridge, M. Wellman, L. Zocchi, B.P. Reynolds
- CHED 1656.** Catalyzing a community in chemistry with UCSD American Chemical Society-Student Affiliates. **J.A. Chiong**, R. Ananth, R. Hesel, A. Tao, S. Bhakta, H. Busse, R. Chaar, M. Filipovic, C. Tan, N. Tu, S. Brydges, T.J. Bussey
- CHED 1657.** ACS Inter Ponce student chapter: Exploring new strategies to increase go green vision. **K. Salcedo, M.O. Santiago Pena, D.J. Sanchez Rodriguez**, T. Felix Massa, E. Ferrer Torres
- CHED 1658.** ACS Club at St. Thomas University: A new chapter serving south Florida. **J.M. Brown, K. Rivera, M. DiSanti, G. Cotto-Gonzalez, T. Wilson**, L.C. Fernandez
- CHED 1659.** ACS medicinal chemistry division: Promoting a healthy society through chemistry. **J.A. Rodriguez Santiago, M. Cruz Zambrana**, T. Felix Massa, E. Ferrer Torres
- CHED 1660.** Student members of the American Chemical Society University of Tampa chapter. **L. Truesdale**, J.A. Struss, L. Henchey
- CHED 1661.** TAMIU ACS: Advancing chemistry on the border. **E. Vazquez**, F.P. Ramirez, B. Nunez, V.M. Morales, K. Murillo, K. Ortiz, N. Valdez, M. De Leon, K.R. Jorgensen
- CHED 1662.** Chemistry is the science of matter, and it definitely matters @ St. Xavier University, Chicago. **L. Lomeli**, B. Alapat
- CHED 1663.** ACS student chapter at the University of Utah. **H. Ponce, C. Coplan**, R.P. Baskin, A. Thomas, M. Pham, A. Reifsnnyder, D. Drapeau, A. Borodai, H. Cummins, K. Loveridge, R. Pence, H.L. Sebahar, T.G. Richmond
- CHED 1664.** Inspiring excellence in chemistry through departmental and outreach events aligned with the core values of ACS and TCNJ. **A. Smith, B.A. Bogin**, A.R. O'Connor, B.C. Chan
- CHED 1665.** Ain't no party like a Chem club party cause a Chem club party don't stop. **M.J. Mio**, D.N. Maxwell, C.M. Johns, R. Benjamin, F.E. Volpe, T. Tieu Ngo, M.Y. Farraj, Z. Smith
- CHED 1666.** How we did it: Creating a named lecture series. **M.J. Mio**, D.N. Maxwell, F.E. Volpe, T. Tieu Ngo, M.Y. Farraj, Z. Smith, C.M. Johns, R. Benjamin
- CHED 1667.** Crowding the funds into your organization. **M.J. Mio**, D.N. Maxwell, F.E. Volpe, T. Tieu Ngo, M.Y. Farraj, Z. Smith, C.M. Johns, R. Benjamin
- CHED 1668.** Demonstration a week keeps the hazards away. **M.J. Mio**, D.N. Maxwell, F.E. Volpe, M.Y. Farraj, T. Tieu Ngo, Z. Smith, C.M. Johns, R. Benjamin
- CHED 1669.** Start your journey here: Georgia Gwinnett College chemistry outreach. **G.E. Rudd, R.K. Kalman, K. Coscia, E. Lopez, R.S. Varner, E. Sheffield, R. Sumling**
- CHED 1670.** Olivet College Gruen Chemistry Society: Student affiliate activities. **B. Sturgeon, J. Kiess, I. York, S. Verlinde**, S.M. Lewis



TECHNICAL PROGRAM

- CHED 1671.** San Germán chapter: Chemical resilience in action. **G. Martinez-Bracero**, A.N. Quintana-Martínez, F. Lopez-Pecunia, E.N. García-Acosta, A.M. Gonzalez-Mederos
- CHED 1672.** Developing an engaging ACS chapter at a private, liberal arts institution. C.A. Azaldegui, **J. Jaimes**, A. Roth-Rodriguez, **D. Saldana**, **B. Westbrook**, M. Kopecki Fjetland
- CHED 1673.** Students' involvement in community service: CIMATEC Avogadro Chem Club. **M. Morales**, I. Montes, J.A. Ramirez
- CHED 1674.** Park University chemistry club activities for 2018-19. **A.N. McMullen**, **L.J. Trowbridge**, **B. Trout**, **M. Klein**, **K. Branstetter**, D.K. Jean, G.D. Claycomb
- CHED 1675.** Western Washington University student chapter of the American Chemical Society. **A. Nadeem**, **J. Lo**, S.R. Emory, E. Raymond
- CHED 1676.** Union University SMACS chapter survey of outreach activities. **C. Coleman**, J.R. Williams, R.F. Johnston
- CHED 1677.** Sustaining community interest in chemistry. **K. Cline**, D.L. Whitman, A. Hudson, C.M. Smith, C.K. Saner
- CHED 1678.** Hofstra University student members of the American Chemical Society. M. Saleem, **M. Currie**, **H. Tarbox**, G. Kroening, S. Buttan, M. Basir
- CHED 1679.** Student affiliates of the American Chemical Society at the University of Northern Iowa. **N. Bishop**, **J. Prybil**, **N. Jovic**, M. Roach, **K. Parrott**, C. Snyder, J. Tibbs
- CHED 1680.** Chemistry outreach at Heidelberg University. **K.M. Iwanek**, K. Scrudders, C. Ihrig, K. Malone, M. Cohn, C. Morrison, N. Beres
- CHED 1681.** Elements of chapter diversity at the University of Michigan-Flint. **L. Harris**, C. Morse, K. Crowley, A. Ringle, D. Sanchez, M. Stubbert, J. Wilhelm, M.R. Wilhelm, J.L. Tischler
- CHED 1682.** Lobo chemistry club: American Chemical Society student chapter at University of New Mexico. **C. Hunter**, **N.A. Abeyta**, F. Delacruz, **G. Carrion-Gonzales**, L. Perez
- CHED 1683.** Blazing a path across National Chemistry Week. **L. Buchan**, **R. Andersen**
- CHED 1684.** Building leaders through the power of chemistry. I. Montes, **J.J. Maldonado Mendez**, **Y. Rosario**, **C.A. Maysonet Navarro**, **R.J. Garcia Del Valle**, **D.Y. Díaz Rohena**, **E. Pagán Colón**, **L.I. Penabad Peña**, **J. Rosa Rosado**, **G. Colon**, **A.E. Soto**, **H.L. Pabón Colón**
- CHED 1685.** Saint Vincent College chemistry club. **M. McGuier**, D. Fish
- CHED 1686.** Barry University chemistry club: Cultivating scientific zeal through service and community engagement. E. Schabot, L. Mesa, J. Baquier, G. Munoz, A. Amaya, T. Hamilton, **G.H. Fisher**
- CHED 1687.** Using chemistry as a platform to serve: An overview of Waynesburg University ACS student chapter activities. **J. Gearhart**, C. Gething, K. Cleer, A. Freiberger, B.F. Sumey, K. Taylor, E.A. Baldauff
- CHED 1688.** Thinking outside the typical ACS student chapter: Creating a chemical community at Eckerd College. **M. Cooper**, D. Dukes, E. Eggers, B. Trimmer, H. Hamontree, A. Sosa-Parada, H. Plummer, S. Bradley, L.A. Bonner



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- CHED 1689.** SMSU chemistry club: Striking a balance. **E.J. Popma, S.M. Erickson**, N.J. Beyer
- CHED 1690.** Sacred Heart University chemistry: It's a small world, with big outreach. **R.M. Russo, R.B. Yozzo, B. Kalach, B.E. Yesko, H. Jia, N.D. Fusco, G. Perkins, D.S. Yeboah**, L. Farber
- CHED 1691.** Xavier University of Louisiana's ACS student chapter: Enhancing local partnerships. **A. Stephens, L. Clark, E. Stevens, A. Walker, S. King, A. Madison, S. Barrett, J. Lupoe**, M.R. Adams, C.M. Lawrence
- CHED 1692.** Temple University Chemical Society. **L. Popilock, T. Tran**, S.A. Fleming
- CHED 1693.** Eastern Oregon University ACS student member chapter: Promoting community outreach and professional networking. **B.L. Stavaas-Jamack, Q.C. Durfee, R.A. Davis, J. Carter, E. Tresch, A.G. Cavinato**
- CHED 1694.** Aquinas Chemistry Society: Making big differences in little ways. **M.P. Mata, A. Gaspar**, J. Murphy-Gast, G. Brandonisio, J. Atherton, N. McKeown, T.L. Phillips, **E.A. Jensen**
- CHED 1695.** National Chemistry Week annual themes demonstrations at Plaza del Caribe. **D. Soler**, L. Santos
- CHED 1696.** Colorado Mesa University chemistry club: Re-establishing a student chapter in rural Colorado. S.E. Lohse, **C.I. Vandermeer**, T. Catlett, N. Paerschke-O'Brien
- CHED 1697.** Trash talk: Waste collection and disposal. **I. Pittman**, S. Durr, C. Johnson, P.J. Carlson
- CHED 1698.** ACS Alexandria University: Activities, events and community outreach. **S.M. Elntawy, A. Elshamy**
- CHED 1699.** ACS UPRB: Impacting diverse community sectors with chemical knowledge. **D.M. Rivera**, C.D. Golderos, E.E. Rivera Santiago, L.I. Santiago
- CHED 1700.** ACS inter ponce: A growing chapter transforming our community. **A. Febus Ramirez**, L. Colon Ithier, T. Felix Massa, E. Ferrer Torres
- CHED 1701.** Southwestern Oklahoma State University chemistry club activities for 2018: Developing a demo road show. E. Hicks, J. Nimsey, D. Tresp, D.E. Widick, J. Henrikson, **T.K. Ellis**
- CHED 1702.** Ramping it up. **N. Androes, K. Diodosio, K. Wyatt**, S. Lira, B. Mullen, K. Sheehan, M. Suzuki, D. Trujillo, B. Williams, D.L. Dillon
- CHED 1703.** Pasadena City College (PCC) chemistry club: Every student can contribute. **B. Clairday, R. Fukuda**, A. Martinez, E. Albert-Minckler, **V.I. Jaramillo**
- CHED 1704.** Continuing our journey: Our chapter's year of service and outreach. **Q. Dougherty, L. Atlas, V. Ganss**, A.H. Kjellson, H. Gordon, D. McGibbon, I.J. Levy
- CHED 1705.** Forensic Chemistry Division of ACS inter ponce. **C.L. Cabrera, G.I. Santiago Torres, D. Cruz Leon**, T. Felix Massa, E. Ferrer Torres
- CHED 1706.** ACS student chapter at Mississippi College. **M.A. Martin, K. Wayne**, N. Selim, P.L. Broom, T.D. Selby
- CHED 1707.** Tiffin University: Finding the formula to success. **B. Utley**, A. Frantz, H. Copley, M.C. Bernard, M. Sabo



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- CHED 1708.** Cypress Bay ACS Chem Club: In our element! M. Ballester, **A. Tracey**
- CHED 1709.** Academia Ponce Interamericana: Innovating! **A. Albertorio-Rosado, A.A. Roman Roubert, C.B. Pellicier Rodriguez, E. Ferrer Torres**
- CHED 1710.** Centenary College chemistry club: Continuing our traditions. **A.F. Moody, J. Faul, A.K. Singh, G. Doucet, T.M. Ticich**
- CHED 1711.** Connecting chemistry in DFW. N. Schmitt, M.M. Barnett, C. Keller, J. Snowden, H. Carey, K. Goytia, L. Goehring, A. Thompson, C. Parsons, G. Griffin, A. Laidman, H. Conrad, J. Fry, **K.N. Green**
- CHED 1712.** Westminster College and its tangled web of partnerships. S.C. Biehn, T.P. Palmer, **R.M. Hyde**
- CHED 1713.** Saint Francis University chemistry club: Becoming best buddies. P. Kasunic, **M. Snider, K. Patterson, M. Hogue, K. Grasso, E.P. Zovinka**
- CHED 1714.** Passion that drives frontiers. **Y. Hernandez-Perez, S. Valle-Cortes, R. Estremera-Andujar, B.J. Ramos-Santana**
- CHED 1715.** ACS student member events, activities, and accomplishments at Duquesne University. K. McDougal, A. Miskalis, E. Allego, E. Leung, H. Gering, J. Roth, P. Cannanbilla, **A. Iacovino, E. Latawiec, J. Miller, A. Moses, D. Dryzal, B. Roman, M. Then, P.G. Johnson, E.S. Gawalt, J. Evanseck**
- CHED 1716.** Applying green chemistry principles to interactive university and community-based activities with the Wilkes University ACS student chapter. **N. Fitzpatrick, D.L. DeFazio, D. Marcincavage, M. Shi, H. Kessler, C. Pelchar**
- CHED 1717.** ACS Inter Metro developing scientific leaders through chemistry. K.A. Parga Rivera, **S. Flores-García, L. Raucci-García, J. Torres-Díaz, P.E. Peña-González**
- CHED 1718.** Florida Southern College: ACS student chapter growth 2018-2019. **S. Brewer, T.B. Tyson, I. Mauzy, C. Metcalfe, J. Marshall, J.F. Eubank**
- CHED 1719.** Loras College American Chemical Society student chapter. A. Carter, **Z. Ney, S. Bahls, L. Horst, K. Lipetzky, S. Krieger, K. Mommsen, G. Smith, D.J. Oostendorp, A.T. Moser**
- CHED 1720.** Marvelous science outreach in South Texas. **C. Ventura, Y. Sanchez, K. Moreno, L. Avila**
- CHED 1721.** KU chemistry club: Catalyzing public outreach and undergraduate enrichment at the newest science building in Kansas. **E.G. Stewart-Jones, K. Kao, T.M. Nguyen, K. Barr, P. Radadiya, M. Duncan, K. Vander Laan, J. Stiel, B. Gougeon, R.S. Black**
- CHED 1722.** Dash of science at an early age can shape the scientist of the future. **D. Ciuro, K. Villa Del Valle, A. Torres, T. Escalera, N.F. Morales-Pennington, A. Rios**
- CHED 1723.** SMACS is out of this world. **C.E. Crawford, B.N. Norris**
- CHED 1724.** Investigating important water quality parameters in different bodies of water around Florida International University-Biscayne Bay campus. **S. Siddique, S. Thanawala, J. Hernandez, C. Lee, L. Valientes, M. Delgado**



TECHNICAL PROGRAM

- CHED 1725.** IVCC in their element. **S.M. Boehm**, M.E. Johll, P.K. Young, D. Breyne, K.V. Rudolph, M. Anderson, A. Anthony, T. Molln, M. Stoens, J. Theesfield
- CHED 1726.** Providing opportunities for student and community engagement in science. **L. Kim**, E.M. Ness, C. Fisher, K. Johnson, A.M. Klussmann, J. Freeman
- CHED 1727.** American Chemical Society Student Chapter of Idaho State University. M. Mangun, E.A. Morley, L.J. Maxton, **K.S. Malloy**, J.J. Pak, C.M. Evilia, B.K. Chabuka, C.C. Norby, **B. Smith**
- CHED 1728.** Growing and sustaining outreach practices for a Student Affiliates chapter. **S. Kempf**, E. Michael McLaughlin
- CHED 1729.** ChemClub Outreach Day: St. Alban's Boys and Girls Club. **H. Aliff**, **J.P. Ricket**, **E.U. Lopez-Torres**, **O.E. Gharib**
- CHED 1730.** Stanislaus State Warriors Chemistry Club: Breaking community barriers with chemistry. **J.L. Godinez**, P.R. Ayson, A. Leon, L. Hillberg, L. Brown, M. Cox, A.S. Manchanda, G. Schara
- CHED 1731.** ACS-UPRB promoting the Chemical Education and impacting the community. **D. Avellanet Ramos**, **A.M. Varela Martínez**, L.I. Santiago
- CHED 1732.** Student involvement the heart of UA Little Rock ACS. **J. Desai**, C. Kornelsen, E. Anderson, T. Lee
- CHED 1733.** Chapter activities for the Henderson State Univeristy Student Affiliate Chapter in 2018. J. Mosely, **S. Loarca**, **N. Steadman**, **C. Stephens**, C. Clem, B.A. Rowland

TUESDAY MORNING

Section A

Orange County Convention Center
Room W315A

ACS-CEI Award for Incorporation of Sustainability into Chemistry Education

Cosponsored by CEI and PROF
C. H. Middlecamp, S. O. Obare, *Organizers, Presiding*

8:30 Introductory Remarks.

8:40 CHED 1734. Keynote Address: Incorporating Sustainability into Chemistry Education. **D.J. Constable**

9:20 CHED 1735. Embedding sustainable nanotechnology into chemistry education and outreach. **S.C. Larsen**

9:45 CHED 1736. Climate Literacy Academy: Educational tools to fight for the planet. **R. Foy**, G.P. Foy

10:10 Intermission.



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

10:20 CHED 1737. Teaching environmental sustainability using real-world problems in project-oriented chemistry laboratories. **J. Zhang**

10:45 CHED 1738. Incorporation of environmental chemistry and sustainability into the graduate and undergraduate curriculum. **E. Roberts-Kirchhoff**

11:10 CHED 1739. Innovative approaches to educate students environmental remediation strategies. **M.A. Benvenuto**

11:35 Concluding Remarks.

Section B

Orange County Convention Center
Room W312A

ACS Award for Achievement in Research for the Teaching & Learning of Chemistry

Cosponsored by PROF
D. M. Bunce, *Organizer*
C. H. Atwood, *Organizer, Presiding*

8:30 Introductory Remarks.

8:40 CHED 1740. Method to significantly improve bottom quartile performance in large general chemistry classes. **C.H. Atwood**

9:00 CHED 1741. Benefitting unambiguously: Notable collaborations in education. **J. Moore**, E.A. Moore

9:20 CHED 1742. Using results from the performance of students on lecture and laboratory practical examinations and on laboratory notebooks to assess the effectiveness of the Science Writing Heuristic. **T.J. Greenbowe**

9:40 CHED 1743. Inclusive and collaborative chemistry education research with chemistry teachers in schools. **H. Sevian**, S.A. Murray, R.D. Lewis, G. Banks

10:00 CHED 1744. POGIL Project: A case study for diffusion of innovation. **R.S. Moog**

10:20 Intermission.

10:30 CHED 1745. Using symbolic forms and graphical forms to characterize student mathematical reasoning in a chemistry context. **M.H. Towns**, J.G. Rodriguez, K. Bain

10:50 CHED 1746. The relationship of mathematics fluency and success in general chemistry: How collaborations lead to better research. **V.M. Williamson**

11:10 CHED 1747. Beyond content knowledge: Measuring transferrable skills connected to experience as a peer-leader in a PLTL program. A. Chase, G. Kline, A. Rao, **P. Varma-Nelson**

11:30 CHED 1748. Answering questions about teaching and learning in chemistry. **R.S. Cole**



TECHNICAL PROGRAM

11:50 Concluding Remarks.

Section C

Orange County Convention Center
Room W312B

GSSPC: Artificial Molecular Machines & the Next Generation of Molecular Control

Cosponsored by COLL, I&EC, ORGN[‡], PHYS, POLY and PRES
C. Kei, J. A. Lutz, T. Myers, C. Sumner, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 CHED 1749. Thajjectory based thermodynamics and kinetics of molecular machines. **R.D. Astumian**

9:15 CHED 1750. Hydrazone-based switches and functional materials. **I. Aprahamian**

9:55 CHED 1751. Molecular nanomachines. **J.M. Tour**

10:35 Intermission.

10:45 CHED 1752. Current-driven dynamics in molecular-scale electronics. **T. Seideman**, R. Jorn

11:25 CHED 1753. Mesoscale architectures for amphidynamic crystals and molecular machiness. **M.A. Garcia-Garibay**

Section D

Orange County Convention Center
Room W311A

Research in Chemistry Education

New & Noteworthy

B. L. Gonzalez, J. P. Walker, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 CHED 1754. Improving general chemistry performance through a growth mindset intervention: Selective effects on underrepresented minorities. **R. Frey**, A. Fink, M.J. Cahill, M.A. McDaniel

9:15 CHED 1755. Writing in STEM: Faculty conceptions of writing and its role in the undergraduate classroom. **G.V. Szymczak Shultz**, A. Moon

9:55 Intermission.



TECHNICAL PROGRAM

10:10 CHED 1756. Modern qualitative studies: A novel qualitative method that improves access, elicitation, and sample diversification for enhanced transferability applied to studying chemistry outreach. **J.M. Pratt, E.J. Yeziarski**

10:50 CHED 1757. Goal orientations of general chemistry students via the achievement goal framework. **S.E. Lewis**

11:30 Concluding Remarks.

Section E

Orange County Convention Center
Room W311B

Advancing Undergraduate Research in Chemistry: Best Practices for New Frontiers

R. M. Jones, *Organizer*

B. L. Gourley, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 CHED 1758. Successes and challenges in incorporating research activities in laboratory courses. **A.G. Cavinato**

8:55 CHED 1759. Course-based undergraduate research experiences for non-majors as part of the transition to college. **R.E. Bachman**

9:15 CHED 1760. Partnering with art museums as a model for course-based undergraduate research. **K. Frederick**

9:35 CHED 1761. Collaborative course-based undergraduate research project for introductory chemistry laboratories. **K.L. Stone, D.M. Rubush**

9:55 CHED 1762. General chemistry assignment analyzing environmental contamination for the DePue, IL, National Superfund Site. **F. Geiger**

10:15 CHED 1763. Design and implementation of medicinal plants research project in organic chemistry laboratory. **A.A. Waghe, A.B. Waghe**

10:35 Intermission.

10:45 CHED 1764. Implementing a research based Organic Chemistry II Laboratory for chemistry majors. **T.K. Ellis**

11:05 CHED 1765. Old tricks for new solvents: Studying deep eutectic solvents in a physical chemistry laboratory. **T. Hopkins**

11:25 CHED 1766. Incorporating undergraduate mini research project exercises in advanced forensic science curriculum as a course-based research experience. **S. Coticone**

11:45 CHED 1767. Flipped-classroom and writing-intensive pedagogies enhance a course-based undergraduate research experience for the biochemistry laboratory. **K.L. Colabroy**



TECHNICAL PROGRAM

12:05 CHED 1768. Standard operating procedures as a means for preparing undergraduate students for careers in chemical research. **G.D. Claycomb**

12:25 Concluding Remarks.

Section F

Orange County Convention Center
Room W311C

Nanotechnology in Undergraduate Education & Research

D. S. Heroux, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 CHED 1769. Electrodeposition of metal nanowires in the capillaries of PDMS stamps modified with hydrophilic polymers: A laboratory exercise for introductory nanotechnology students. **W.C. Sanders**, G. Johnson, R.V. Valcarce, P.J. Iles, J.S. Smith, H. Fourt, K. Drystan, D. Edwards, J. Vernon, S. Ashworth, A. Barucija, Z. Curtis

8:55 CHED 1770. Simple experiment that teaches the concept of nanophytotoxicity: The effects of solutions of nanoparticles on the growth of mung beans. S. Ross, M.J. Owen, M. Haidari, N. Le, A. Phu, K. Johnson, G. Liu, **W.J. Miller**

9:15 CHED 1771. Nanotechnology course introduced to new liberal arts general education curriculum for non-science majors. **E. Park**

9:35 Intermission.

9:50 CHED 1772. Studying quantum dot optical properties at a small, liberal arts institution. **K. Schnitzenbaumer**

10:10 CHED 1773. Integrating physical chemistry of nanocrystals into an upper-level capstone chemistry laboratory course for undergraduates. **J.D. Keene**, A.M. Kiefer

10:30 CHED 1774. Nanotechnology experiment for beginning and advanced undergraduate students. **D.S. Heroux**

Section G

Orange County Convention Center
Room W311D

Transforming the Undergraduate Chemistry Laboratory to Teach Transferable Skills & Develop Young Scientists

Cosponsored by ANYL
R. Georgiadis, *Organizer*
B. Abrams, *Organizer, Presiding*

8:30 Introductory Remarks.



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

8:50 CHED 1775. Designing a laboratory experience that promotes mastery and retention of fundamental skills through purposeful and contextual training. **E.A. Baldauff**

9:10 CHED 1776. Finally! Eliminating the lab rotation schedule *and* enhancing transferable skills in the laboratory. **R. Georgiadis**

9:30 CHED 1777. How authentic research in the Biochemistry II teaching lab helped students gain biotech skills and discover colorful proteins. **B.J. McFarland**

9:50 CHED 1778. Investigating the determinants of substrate binding through a semester-long, project-oriented biochemistry laboratory course. **C.A. Sarisky, T.W. Johann**

10:10 Intermission.

10:30 CHED 1779. Implementation of research on drug target cloning and characterization in biochemistry laboratory. **C. Wu**

10:50 CHED 1780. Analytical chemistry project: Isolation of biologically active compounds from mangrove sediments. **K. Solntsev, S. Schramm, S. Kremb, K. Gunsalus, S.A. Amin**

11:10 CHED 1781. Self-efficacy, and incorporating collaborative research in the Organic Chemistry Lab curriculum. **D. Paull**

11:30 CHED 1782. Developing an open-structure paint chemistry experience to prepare students for regional employment opportunities. **P. Tandler**

11:50 CHED 1783. One-on-one technique instruction of laboratory skills in large service courses. **A. Manevich**

12:10 Panel Discussion.

Section H

Orange County Convention Center
Room W311E

General Papers

Lab Curriculum

S. A. Fleming, *Organizer*
K. N. Knust, *Presiding*

8:30 Introductory Remarks.

8:35 CHED 1784. Evaluating the economic viability of coal samples using bomb calorimetry: A problem based, interdisciplinary laboratory exercise for general chemistry students. **A.P. Bopegedera**

8:55 CHED 1785. Introducing electrochemistry with simple and fast bipolar electrochemistry experiments. S.M. Rapp, B.M. Branham, **K.N. Knust**



TECHNICAL PROGRAM

9:15 CHED 1786. Introducing crystallography and X-ray diffraction to undergraduate students in lab and lecture. **T.M. Pappenfus**

9:35 Intermission.

9:50 CHED 1787. Transforming honey into strawberries: The Fischer esterification of cinnamic acid to methyl cinnamate as an engaging experiment for the second-year organic chemistry laboratory.. **G.R. Boyce**, J.H. Steele

10:10 CHED 1788. Teaching experiment to illustrate experimental design in the investigation of a mechanism involving a novel ammonium-alkyne interaction. **E.J. St Germain**, A. Horowitz, D.J. Rucco, E.M. Rezler, S.D. Lepore

10:30 CHED 1789. Kit for experiments in electricity and electrochemistry uses a new “green” conductive material. **J. Santos**, F. Galembeck

10:50 CHED 1790. Changing freshman perception of chemistry through laboratories highlighting the traditional divisions. **D.L. Forbes**, A.B. Curtiss, C. Easley, E.E. Hardy

Bridging the (Safety) Gap between Academia & Industry

Sponsored by PRES, Cosponsored by CA, CCS, CHAS‡, CHED, PROF and YCC

TUESDAY AFTERNOON

Section A

Orange County Convention Center
Room W315A

Porphyrins & Related Macrocycles in Undergraduate Teaching & Research

J. V. Ruppel, *Organizer, Presiding*
T. Hamilton, N. Snyder, *Presiding*

1:30 Introductory Remarks.

1:35 CHED 1791. Porphyrinoids as platforms for chemical education. **C.M. Drain**, N. Bhupathiraju

1:55 CHED 1792. Colorful adventures in undergraduate research: Synthesis of novel carbaporphyrinoid systems. **T.D. Lash**

2:15 Intermission.

2:30 CHED 1793. Investigating metalloporphyrins as water oxidation catalysts with undergraduate researchers. **W.M. Ames**



TECHNICAL PROGRAM

2:50 CHED 1794. Systematic studies of syntheses of porphyrinoids with altered core structures as a challenging and enjoyable focus for undergraduate research. **G.R. Geier**

3:10 Intermission.

3:25 CHED 1795. Back to the grind: Undergraduate research and mechanochemical synthesis of porphyrins. **T.D. Hamilton**

3:45 CHED 1796. Ever-versatile porphyrin: Host-guest studies of porphyrin-based M_8Por_6 metallocubes. **J.D. Thoburn**

4:05 Intermission.

4:20 CHED 1797. Undergraduate photochemistry research: The photophysical properties of porphyrin thin films and thiazolothiazole viologens. A. Woodward, K. Sandor, J. Kassel, J. Sailer, S.M. Patberg, N. Sayresmith, M. Kaushal, **M.G. Walter**

4:40 CHED 1798. Synthesis of carbohydrate porphyrin, bacteriochlorin and phthalocyanine conjugates with therapeutic potential. J.V. Ruppel, **N.L. Snyder**

5:00 Concluding Remarks.

Section B

Orange County Convention Center
Room W312A

ACS Award for Achievement in Research for the Teaching & Learning of Chemistry

Cosponsored by PROF
D. M. Bunce, *Organizer*
C. H. Atwood, *Organizer, Presiding*

1:30 Introductory Remarks.

1:40 CHED 1799. Research Jam: An interactive experience to explore how a chemical education research experiment is conceived. **C.F. Bauer, R.S. Cole, P.L. Daubenmire, K. Havanki, R. Komperda, K.Y. Neiles, J.R. Vandenplas, A.L. Wrenne**

2:55 Intermission.

3:05 CHED 1800. Student problem-solving approaches when answering multiple-choice questions in general chemistry. **S. Lin, M.A. Teichert, D.M. Bunce, D.K. Dillner, M.J. Schroeder, R. Komperda**

3:25 CHED 1801. Pilot study investigating average students' learning on general chemistry problems from cognitive psychology and DBER perspectives. **M.D. Perry, D.M. Bunce, M.J. Cahill, R. Frey, M.A. McDaniel**

3:45 Introductory Remarks.



TECHNICAL PROGRAM

3:55 CHED 1802. Award Address (ACS Award for Achievement in Research for the Teaching and Learning of Chemistry sponsored by the ACS Exams Institute). Inclusiveness and collaboration--The keys to succeeding in chemical education research. **D.M. Bunce**

Section C

Orange County Convention Center
Room W312B

GSSPC: Artificial Molecular Machines & the Next Generation of Molecular Control

Cosponsored by COLL, I&EC, ORGN[‡], PHYS, POLY and PRES
C. Kei, J. A. Lutz, T. Myers, C. Sumner, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 CHED 1803. Engineering with biomolecular motors and enzyme cascades. **H. Hess**

2:15 CHED 1804. Molecular machines in action. **S.W. Hla**

2:55 Intermission.

3:05 CHED 1805. Making the tiniest machines. **D.A. Leigh**

3:45 CHED 1806. Radical chemistry in the design and synthesis of artificial molecular machines. **J.F. Stoddart**, Y. Qiu, Y. Feng

4:25 Concluding Remarks.

Section D

Orange County Convention Center
Room W311A

Research in Chemistry Education

S. D. Wiediger, *Organizer*
C. J. Luxford, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 CHED 1807. Comparing exam question formats and student performance data to improve assessment, instruction, and student comprehension in first semester organic chemistry. **R.R. Gokal**, R.W. Morrison

1:55 CHED 1808. Learning strategies of first semester organic chemistry students. **A.M. Clark**, J.R. Raker

2:15 CHED 1809. Analyzing the retention of knowledge among general chemistry students. **J.T. Kingsepp**, S.E. Lewis



TECHNICAL PROGRAM

2:35 CHED 1810. Investigation of students' long-term retention of general chemistry concepts in analytical chemistry. **Y. Wang**, S.E. Lewis

2:55 Intermission.

3:10 CHED 1811. Explaining for the Best Inference (EBI) and conceptual understanding of chemical phenomena using contrasting molecular animations. **A. Villalta-Cerdas**

3:30 CHED 1812. Development of an instrument to measure student representational and model competency in solving chemistry tasks related to structures. **J.M. Trate**, K.L. Murphy, J.R. Raker

3:50 CHED 1813. Coordination class theory as lens for examining students' reasoning with the idea of particulate-level energy variability in chemical kinetics. **N.M. Becker**

4:10 Concluding Remarks.

Section E

Orange County Convention Center
Room W311B

Advancing Undergraduate Research in Chemistry: Best Practices for New Frontiers

B. L. Gourley, *Organizer*
R. M. Jones, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 CHED 1814. Required research courses: Success for all? **K.L. Peterson**

1:55 CHED 1815. How undergraduates can drive research forward and create changes in research agendas. **G.C. Shields**

2:15 CHED 1816. Undergraduate research at a primarily undergraduate institution: new challenges and opportunities. **S.K. Swope**

2:35 CHED 1817. Challenges and opportunities for research at a teaching institution: My 25 years account. **A. Rahman**

2:55 CHED 1818. Unexpected benefits of attending a workshop on biochemistry, genetics and molecular biology of mitochondria: Splicing complementary programs to advance hemostasis research. **A.D. Gibson**, A. Washington

3:15 CHED 1819. Reaching out of the fishbowl. **A.V. Washington**, A.D. Gibson

3:35 Intermission.

3:45 CHED 1820. Teacher-scholar model: Paper-based devices for global health applications. **T.L. Barstis**

4:05 CHED 1821. Undergraduate research in the chemistry department at Randolph-Macon College. **S.H. Schreiner**



TECHNICAL PROGRAM

4:25 CHED 1822. Transferring a research project from independent research to the physical chemistry teaching lab using the online platform GENI-ACT. **B.J. McFarland**, J.D. Mahlum, A. Yang, G.E. Wood, P.A. Totten

4:45 CHED 1823. Design and synthesis of organic dye-sensitizers for solar cells: Advancing undergraduate research in renewable energy. **V.A. Sichula**

5:05 CHED 1824. Multidisciplinary drug discovery research model at an undergraduate institution. **B.J. Stockman**, M.A. Vanalstine-Parris, D.W. Parkin, T.M. Sonbuchner, R.V. Kumar, I. Hyatt

5:25 Concluding Remarks.

Section F

Orange County Convention Center
Room W311C

Green Chemistry as a Pillar of Safety Education

Cosponsored by CHAS
Financially supported by ACS Green Chemistry Institute; I&EC Green Chemistry Subdivision
J. E. Wissinger, *Organizer*
H. Weizman, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 CHED 1825. Green Chemistry: Where the concepts of safety and ethics meet. **G.M. Bodner**

1:55 CHED 1826. Teaching safety through a green chemistry lens. **J.E. Wissinger, A. Sitek**

2:15 CHED 1827. Incorporation of green chemistry and best safety practices in an organic chemistry laboratory curriculum. **M. Rao**, J. Vadakkan

2:35 Intermission.

2:50 CHED 1828. Combining safety and green chemistry implementation in an inorganic synthesis project. **D.C. Finster**

3:10 CHED 1829. Educational initiatives taken by Green Chemistry Network Centre (GCNC) for integrating Green Chemistry in curriculum in India. **R.K. Sharma**

3:30 Panel Discussion.

Section G

Orange County Convention Center
Room W311D

Transforming the Undergraduate Chemistry Laboratory to Teach Transferable Skills & Develop Young Scientists



TECHNICAL PROGRAM

Cosponsored by ANYL
B. Abrams, *Organizer*
R. Georgiadis, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 CHED 1830. Investigating instructor methods of addressing program outcomes in the undergraduate chemistry laboratory. **R. Harrison**, R.S. Cole

1:55 CHED 1831. Stop writing/teaching lab reports: integrating authentic research-based writing into quantitative analysis courses. **B. Abrams**

2:15 CHED 1832. Kimchi, rice beer, and color-changing sauerkraut: Incorporating writing instruction in a junior-level, capstone laboratory course. **A.M. Kiefer**, J.D. Keene, C.S. Seney

2:35 Intermission.

2:50 CHED 1833. Developing research and communication skills in a project-based physical chemistry laboratory. **J.L. Bayline**

3:10 CHED 1834. Incorporating service-learning project into writing-intensive Instrumental Analysis course. **Z. Zajickova**

3:30 CHED 1835. Coffee chemistry: A semester-long laboratory for analytical chemistry. **S. Plummer Oxley**

Section H

Orange County Convention Center
Room W311E

Perspectives on Climate Change Literacy & Education: Local to International

Cosponsored by CEI
G. P. Foy, K. E. Peterman, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 CHED 1836. Promoting climate change literacy through an interdisciplinary pop-up learning community. **A.F. Johnson**

1:55 CHED 1837. Earth's changing climate in the polar regions. **T. Watson**, G.P. Foy, K.E. Peterman

2:15 CHED 1838. Impact of water and climate change. **T. Tieu Ngo**, K.E. Peterman, G.P. Foy

2:35 CHED 1839. Why climate change activism? **A. Rizvi**, G.P. Foy, K.E. Peterman

2:55 Intermission.

3:05 CHED 1840. Climate change and its impact on health. **A. Kendrick**, K.E. Peterman, G.P. Foy



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

3:25 CHED 1841. Catalysis and sustainable energy: Lowering barriers to change. **L.I. Frye**, G.P. Foy, K.E. Peterman

3:45 CHED 1842. Diplomatic framework of global environmental issues in chemicals and waste management. **S. Toles**, G.P. Foy, K.E. Peterman

4:05 Panel Discussion.

4:20 Concluding Remarks.

WEDNESDAY MORNING

Section A

Orange County Convention Center
Room W315A

Extending the Reach of Outreach

S. K. St Angelo, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 CHED 1843. Matter in STEM: Chemistry for in-service elementary school teachers. **V. Russell**, C. Penrod, J. Dwyer

8:55 CHED 1844. Promoting girl power in the sciences: Collaboration between Georgia Gwinnett College and local middle and high schools. **G.E. Rudd, R.K. Kalman**

9:15 CHED 1845. Science and Engineering Fair Outreach: Tips to make the experience more than just a volcano. E.E. Hardy, M.L. Ewald, J.G. Marino, J.M. Lakin, H. Wada, P. Cobine, A. Landers, **V.A. Davis**

9:35 CHED 1846. Beyond lemon batteries: Broadening the extent of electrochemistry outreach. **V. Russell**, D. Caputo, S.D. Minter

9:55 Intermission.

10:05 CHED 1847. Building student success through STEAM community collaboration. **B. Kunnath**, G. Bonomo, M.M. Gillett-Kunnath, K. Ruhlandt-Senge

10:25 CHED 1848. Building a local STEAM ecosystem through partnerships and community collaboration. **M.M. Gillett-Kunnath**, G. Bonomo, N. Abrams

10:45 CHED 1849. Annotator professional development training: An outreach opportunity in STEM education and communication. **T.S. Ritchie**, M. McCartney

11:05 CHED 1850. Chemists should write like journalists and speak like cavemen. **R.C. Fortenberry**



TECHNICAL PROGRAM

11:25 CHED 1851. Communicating chemistry to adult non-scientists with concepts from *Don't Be Such a Scientist*. **S.K. St Angelo**

11:45 Discussion.

Section B

Orange County Convention Center
Room W312A

Bridging the Divide: Relating Chemistry to Biology & the Humanities

P. B. Nolibos, *Organizer*
P. M. Todebush, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 CHED 1852. Tips to help art-students distinguish justified beliefs from opinions in college chemistry classes. **B. Budy**

8:55 CHED 1853. Chemistry, art, and the impact of interdisciplinary teaching on research. **A.M. Wilson**, M.J. Samide, G.D. Smith

9:15 CHED 1854. Chemical synthesis of color in art: Curricular innovation at The Thacher School. **C. Vyhna**, E. Mahoney, Y. Lin

9:35 Intermission.

9:45 CHED 1855. Infusing cCWCS "Chemistry in Art" workshop activities into the college curriculum. **M.R. Nahm Garrett**

10:05 CHED 1856. Chemistry in art within an analytical chemistry course. **K. Jansen Labby**

10:25 CHED 1857. Perfume Chemistry: Combining artistry, science, and culture. **J.L. Bayline**

10:45 Intermission.

10:55 CHED 1858. Atomic Narratives: Exploring the Manhattan Project through writing, ethics, history, and chemistry. **A.L. Smalley**, N. Kuroiwa-Lewis

11:15 CHED 1859. Linking chemistry and political science: Topics related to weapons of mass destruction. **L. Davis**, K. Taylor

11:35 CHED 1860. Leveraging philosophy to cultivate a culture of ethical and responsible conduct in chemistry and beyond. **S.M. Kuebler**, J. Beever

11:55 CHED 1861. Humanities formation in chemistry: Evidence-based argument and Primo Levi's *The Periodic Table*. **J. Heising**, **S. Gorman**



TECHNICAL PROGRAM

12:15 Concluding Remarks.

Section C

Orange County Convention Center
Room W312B

Core Ideas, Crosscutting Concepts & Science Practices: Three-Dimensional Learning in Chemistry

K. Bain, M. Cooper, M. H. Towns, *Organizers*
J. G. Rodriguez, *Organizer, Presiding*
K. Bain, *Presiding*

8:30 Introductory Remarks.

8:35 CHED 1862. Leveraging technology to support three-dimensional instruction and assessment. **D.G. Herrington**, R.D. Sweeder, P.L. Daubenmire

8:55 CHED 1863. Promoting and identifying crosscutting concepts in an interdisciplinary first-year science program. **C. Addison**, J. Charbonneau, P. Dubois, N. Roberson

9:15 CHED 1864. Designing and evaluating a project-based, acid-base experiment that incorporates the scientific practices. **E. Villar**, N.S. Stephenson, **J.H. Carmel**

9:35 CHED 1865. Investigating the impact of three-dimensional learning on student understanding. **S.M. Underwood**, A.T. Kararo

9:55 Intermission.

10:10 CHED 1866. Assessing students' ability to create interdisciplinary connections: entropy to osmosis. **B. Martinez**, K. Parent, S.M. Underwood, R.L. Matz

10:30 CHED 1867. NGSS model lesson for materials science: Translating standards to practice. **C. Johnson**

10:50 CHED 1868. Unpacking strategies to develop three-dimensional learning activities in high school and college science.. **D.J. Wink**, B. Gane, M. Ko, L. Zeller, J. Pellegrino, S. Goldman, M. George

11:10 CHED 1869. ACS General Chemistry Performance Expectations Program: From task force to evidence-based community. **D.J. Wink**, S. Pazicni, A. Donovan

Section D

Orange County Convention Center
Room W311A

Research in Chemistry Education



TECHNICAL PROGRAM

S. D. Wiediger, *Organizer*
C. J. Luxford, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 CHED 1870. Identifying errors in Lewis structures and their connection to information processing. **C.L. Stanford**, S.M. Ruder, N. Farhat

8:55 CHED 1871. Embedding analogy in formative assessment to enhance student understanding of resonance. **D.V. Xue**, M.N. Stains

9:15 CHED 1872. Validity and reliability of a concept test to measure students' abilities to qualitatively rank acid and base strength. Y. Zhang, S. Inthof, **J.J. Stewart**

9:35 CHED 1873. Modeling the influence of constructivist learning environment factors on student outcomes in diverse chemistry courses. **R. Komperda**

9:55 Intermission.

10:10 CHED 1874. Identifying the knowledge and skills that chemists require in workplace. **Q. Cui**, J. Harshman

10:30 CHED 1875. Incorrect worked examples enhance student visual attention, engagement and retention. **V.L. Perera**

10:50 CHED 1876. Influence of delayed elaborative feedback on student performance and process with multiple-choice questions. **M.A. Teichert**, J.L. Schneider, T.S. Ritchie, J.M. Trate, K.L. Murphy, C.J. Luxford

11:10 Concluding Remarks.

Section E

Orange County Convention Center
Room W311B

Curricular Innovations in Undergraduate Chemical Education Impacted by NSF

R. K. Boggess, *Organizer*
C. A. Burkhardt, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 CHED 1877. Understanding barriers to faculty adoption of evidence-based pedagogies and the implementation of campus-based interventions to transcend those barriers. **A.L. Feig**, C.E. Hartman, P.M. Hoffmann, S.E. Kacin, K. Myhr, S. Ozgun-Koca

8:55 CHED 1878. STEM Faculty Institute: Understanding and transforming instructional decision-making. **R. Sansom**

9:15 CHED 1879. Development, implementation, and assessment of organic chemistry REActivities at a range of regional colleges and universities. **J.P. Anderson**



TECHNICAL PROGRAM

9:35 Intermission.

9:45 **CHED 1880.** Project-based chemistry laboratories for beginning and advanced students. **R. Gao, J.B. Lloyd**

10:05 **CHED 1881.** Organic chemistry, life, the universe & everything (OCLUE). **M. Cooper**, M. Klymkowsky

10:25 **CHED 1882.** Active learning organic chemistry environment with an adaptive meta-cognitive coach. **I.R. Gould**, A. Austin, K. VanLehn

10:45 Intermission.

10:55 **CHED 1883.** Partnerships and collaborations that broaden participation and impact community college student outcomes in STEM. **C.J. Foley**

11:15 **CHED 1884.** Randolph-Macon Noyce Teacher-Scholar Program: An innovative NSF-sponsored program designed to recruit, train, and retain high school chemistry, biology and physics teachers into high-need school districts.. **A. Marchetti**

11:35 **CHED 1885.** Institutional model for increasing student engagement through Course-embedded Undergraduate Research Experiences (CUREs). **J. Awong-Taylor, C. Runck, C.L. Anfuso**, A.R. D'Costa, D.P. Pursell, T. Leader, C. Achat-Mendes

11:55 Concluding Remarks.

Section F

Orange County Convention Center
Room W311C

Engaging Undergraduates with Raman Spectroscopy

M. D. Sonntag, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 **CHED 1886.** Withdrawn

8:55 **CHED 1887.** Expanding access to Raman spectroscopy using portable instrumentation. **C.J. Stromberg**, K.H. Bennett, D. Ellis, P. Wood, W. Nellis, P. Sheppard, G. Patterson

9:15 **CHED 1888.** New educational approaches for student-faculty engagement with Raman spectroscopy. **A.G. Hohreiter, R. Georgiadis**

9:35 Intermission.

9:50 **CHED 1889.** Introducing organic chemistry students to Raman spectroscopy using functional group and structural analysis. **C. Hamann**, M.P. Fares, S.R. Hange, K.P. Smith, M.D. Sonntag



TECHNICAL PROGRAM

10:10 CHED 1890. Incorporating Raman spectroscopy in forensic chemistry courses at Towson University. **K.M. Elkins,** R. Carroll, K. Gorr

10:30 CHED 1891. Multi-week project in physical chemistry lab comparing UV/vis, IR, fluorescence, and Raman spectroscopies. **J.M. Wiester**

10:50 CHED 1892. Incorporating Raman spectroscopy and computational chemistry into the undergraduate physical chemistry curriculum. **W. Adams,** M.D. Sonntag

11:10 Intermission.

11:25 CHED 1893. Raman spectroscopy in undergraduate research projects. **E.E. Mojica,** Z. Dai

11:45 CHED 1894. Experiential learning with open-source hardware: Application to Raman spectroscopy. **J. Alexander,** A.G. Taylor, R.A. Bloodworth, C. Vincent, R. Diegan

12:05 CHED 1895. Designer pigment libraries: Synthesis and analysis of pigments derived from naphthol AS-G by Raman and LDI-MS. **J.F. Lomax,** S.Q. Lomax

12:25 Concluding Remarks.

Section G

Orange County Convention Center
Room W311D

Research on Learning in the Laboratory

S. Sandi-Urena, *Organizer*
M. J. Chrzanowski, *Organizer, Presiding*
S. Sandi, *Presiding*

8:30 Introductory Remarks.

8:35 CHED 1896. Using laboratory notebook quizzes to improve student record-keeping. **C.A. Sarisky, T.W. Johann,** K.E. Anderson, W.E. Brenzovich, E.E. Hardy, W.G. Hollis, S. Hughes, J.R. Ingle, R.B. Keithley, S.R. Kennedy, S. Livingston

8:55 CHED 1897. Using the lens of inclusive excellence to redesign and assess the general chemistry laboratory experience. **S.A. Kennedy,** A.C. Curtis

9:15 CHED 1898. Beyond gate-keeping: Improving the first-semester general chemistry laboratory experience. **L.J. Doody**

9:35 CHED 1899. Multimodal laboratory environment: phenomenology of learning of experimental chemistry mediated by varied instructional styles. **S. Sandi-Urena, M.J. Chrzanowski**

9:55 Intermission.



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

10:05 CHED 1900. Laboratory reform using multi-dimensional learning based on the NRC *Framework for K-12 Science Education* practices and the *MCAT 2015* competencies.. **D.J. Wink**, L. Huma, H. Zhang

10:25 CHED 1901. Emergence of mindfulness and mindlessness in multiple, diverse laboratory environments and its impacts on evidence-based curricula design. **M.J. Chrzanowski**

10:45 CHED 1902. Development of a Peer-Led Undergraduate Research Initiative (PLURI) Module in organic chemistry teaching laboratory. **S. Laulhe, R.E. Minto**, A. Chase

11:05 CHED 1903. *Cross-Disciplinary Practice Focused Undergraduate Laboratory Transformation* . **J.P. Walker**, F. Li, K. Callis-Duehl

11:25 Concluding Remarks.

Section H

Orange County Convention Center
Room W311E

Students as Informal Educators: Student use of NISE Net Explore Science: Let's Do Chemistry Kits

L. Raines, D. F. Sittenfeld, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 CHED 1904. Museum: Chemist collaborations with explore science: Let's do chemistry kits at 250 events in the United States. **C. McCarthy**

8:55 CHED 1905. Saturday morning science: Building student confidence through community outreach. **A.H. Shelton**, P.A. Shelton

9:15 CHED 1906. Student-led outreach and implementation of the Explore Science: Let's do Chemistry Kit in a majority-minority middle school. **R. Hulet**

9:35 CHED 1907. Binghamton University's Chemistry Outreach Program 2018 NCW Celebration with NISE Network Let's Do Chemistry kit. **V. Van Nostrand**, B. Turnpenny, A.S. Silva

9:55 CHED 1908. Training high school students to lead Let's Do Chemistry activities through two ACS outreach channels: ACS science coaches and ACS high school chem clubs. **G.W. Ruger, J.L. Maclachlan, M.L. Agan**

10:15 Intermission.

10:25 CHED 1909. Improve your outreach activities with the explore science: Let's do chemistry digital kit. **P. Galvan**

10:45 CHED 1910. NCW Kit provides a host of ways to encourage STEAM encounters. **M. Gulotta**

11:05 CHED 1911. Informal science education through STEM outreach events by the northeastern section of American Chemical Society and Museum of Science & Boston Children's Museum, Boston: A low cost and high impact program for student success. **J. Ranga**, A. Daniels, D.F. Sittenfeld, R. Lam, E. Hostetler



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

11:25 CHED 1912. Out of the box outreach: Gordon College's utilization of the Let's do Chemistry Kits. **Q. Dougherty, V. Ganss, L. Atlas, A.H. Kjellson, H. Gordon, D. McGibbon, I.J. Levy**

11:45 CHED 1913. Withdrawn

12:05 CHED 1914. Teaching chemistry organically: Adjusting teaching practices to make chemistry accessible to all ages. **M.R. Packer, D.F. Sittenfeld, A. Daniels**

12:25 Concluding Remarks.

WEDNESDAY AFTERNOON

Section A

Orange County Convention Center
Room W315A

Fundamentals of Chemistry Outreach Education: From Program Design to Assessment

Cosponsored by CCA, LSAC, SOCED and YCC
E. J. Brush, S. Nellutla, *Organizers*
E. S. Garcia Segal, *Organizer, Presiding*
S. Nellutla, *Presiding*

1:30 Introductory Remarks.

1:40 CHED 1915. Middle school girls and chemistry: 4 years in the making. **S.M. Taylor**

2:00 CHED 1916. Randolph-Macon STEM Consortium: A novel partnership between STEM-focused industry, non-profits, governmental organizations, and academia designed to increase the quality of STEM education in central Virginia. **A. Marchetti, R.R. Michelsen**

2:20 CHED 1917. Princeton University Materials Academy new initiatives. **D.J. Steinberg, S. Rodriguez Martinez**

2:40 CHED 1918. Chemistry and the college experience: A partnership with Project SEED to enrich underserved communities. **G. Bonomo, B. Kunnath, M.M. Gillett-Kunnath, K. Ruhlandt-Senge**

3:00 Intermission.

3:15 CHED 1919. Curricular cartography with cCWCS: Remapping course content with computational chemistry and case studies for student success and satisfaction. **S.M. Brothers**

3:35 CHED 1920. Museums collaborating with chemists on public outreach events nationwide using Explore Science: Let's Do Chemistry kit activities. **C. McCarthy**

3:55 CHED 1921. Symposium workshop on the fundamentals of chemistry outreach education. **E.J. Brush, S. Nellutla, E.S. Garcia Segal**

4:35 Discussion.



TECHNICAL PROGRAM

Section B

Orange County Convention Center
Room W312A

Bridging the Divide: Relating Chemistry to Biology & the Humanities

P. B. Nolibos, *Organizer*

P. M. Todebush, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 CHED 1922. Creative strategies at the interface of chemistry and biology: Making it real with cCWCS. **E.J. Banner**

1:55 CHED 1923. Content alignment for pre-nursing track science courses at Georgia Gwinnett College. **R.K. Kalman, X. Li**

2:15 CHED 1924. Increasing student engagement through the use of medical examples in an upper-division biochemistry course. **T.W. Johann**

2:35 Intermission.

2:45 CHED 1925. Enticing majors to integrate concepts through food chemistry. **J.P. Ellis**

3:05 CHED 1926. Forensic science for non-majors: Training problem-solvers for the humanities. **F.L. Musko**

3:25 Concluding Remarks.

Section C

Orange County Convention Center
Room W312B

Core Ideas, Crosscutting Concepts & Science Practices: Three-Dimensional Learning in Chemistry

M. Cooper, M. H. Towns, *Organizers*

K. Bain, J. G. Rodriguez, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 CHED 1927. Characterizing instruction in undergraduate science courses: The three-dimensional learning observational protocol. **K. Bain**, R.L. Matz, C.L. Fata-Hartley, M.D. Caballero, D.G. Herrington, D. Ebert-May, E.M. Duffy, J. Stoltzfus, J.T. Laverty, J. Carmel, L. Bender, L.A. Posey, M. Urban-Lurain, R. Stowe, R.D. Sweeder, S.M. Underwood, S. Tessmer, M. Cooper

1:55 CHED 1928. Faculty perceptions of science practices in undergraduate chemistry laboratory courses. **C. Schnoebelen**, T.J. Bussey, S. Brydges



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

2:15 CHED 1929. Innovative and effective methods of engaging organic chemistry students in 3-dimensional learning: Building success in the classroom and preparing students to become active participants in new frontiers of science. **B. Van Kuiken**

2:35 CHED 1930. Causal mechanistic reasoning in organic chemistry. **O.M. Crandell**, M. Cooper

2:55 Intermission.

3:10 CHED 1931. "I made an educated guess": Students' responses to scientific practices assessment tasks. **N.S. Stephenson**, J.H. Carmel, E.M. Duffy, D.G. Herrington, M. Cooper

3:30 CHED 1932. Exploring students' proficiency with selected scientific practices in traditional and reformed laboratory environments. **N.S. Stephenson**, **J.H. Carmel**, E.M. Duffy, D.G. Herrington, M. Cooper

3:50 CHED 1933. Impact of guided-inquiry approaches in physical science laboratory curriculum for k-8 teachers. **A. Sangha**, D. Donnelly

4:10 CHED 1934. Crosscutting concepts: critical component or red headed stepchild of 3D-learning? **M. Cooper**

Section D

Orange County Convention Center
Room W311A

Research in Chemistry Education

C. J. Luxford, *Organizer*

S. D. Wiediger, *Organizer, Presiding*

1:30 Introductory Remarks.

1:55 CHED 1935. Open-note chemistry exams as opportunities for meaningful learning and assessment. **E. Yuriev**, M. Lazarus, D. Malone

2:15 CHED 1936. Development of an instrument to characterize faculty conceptions of writing in the classroom. **S.A. Finkenstaedt-Quinn**, A. Moon, J.R. Raker, A. Gere, G.V. Szymczak Shultz

2:35 Intermission.

2:50 CHED 1937. Exploring teacher noticing, interpreting and acting in response to written student work. **S.A. Murray**, H. Sevan

3:10 CHED 1938. On the value of studying faculty's instructional practices and mindsets. **M.N. Stains**

3:30 CHED 1939. Challenges and lessons learned during the initial propagation of a curriculum. **A.T. Kararo**, S.M. Underwood

3:50 Concluding Remarks.



TECHNICAL PROGRAM

Section E

Orange County Convention Center
Room W311B

Curricular Innovations in Undergraduate Chemical Education Impacted by NSF

C. A. Burkhardt, *Organizer*
R. K. Boggess, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 **CHED 1940.** National Science Foundation programs that support undergraduate chemistry education. **J.E. Lewis, D. Rickey**

1:55 Discussion.

2:15 **CHED 1941.** Implementation of polymer instruction by crosslinking the chemistry curriculum. **B.P. Quillian, S. Gray, G. Guillet, N. Shank, M. Weiland, S.K. Zingales, C.W. Padgett, C.E. MacGowan, R. Groom**

2:35 Intermission.

2:45 **CHED 1942.** Deepening conceptual understanding through chemical demonstrations. **D. Wiegand, T. Francis**

3:05 **CHED 1943.** Tale of two studies that explored how students made sense of contrasting animations of video recorded chemical reaction events. **R.M. Kelly, S.J. Hansen**

3:25 **CHED 1944.** Modeling for the Enhancement of Learning Chemistry (ModEL-C): Using biometric and eye tracking data to characterize learner cognitive processes during 3D modeling tasks across general, organic and biochemistry courses. **C. Terrell, K.J. Linenberger Cortes**

3:45 Intermission.

3:55 **CHED 1945.** Results from a linked, organic to analytical, course-based undergraduate research experience - ChemCUREs. **J.P. Walker, W.E. Allen, A.M. Kennedy**

4:15 **CHED 1946.** Simulating the real-world research experience through course clustering. **R.G. Aslanian, M. Bendaoud, R. Carroll**

4:35 **CHED 1947.** Modeling interdisciplinary collaborations through a Course-based Undergraduate Research Experience (CURE). **R. Roberts, S. Price, J. Koeppel, P. Craig**

4:55 Concluding Remarks.

Section F

Orange County Convention Center
Room W311C



TECHNICAL PROGRAM

Coexistence of Joy, Motivation, & Learning in Chemistry Classrooms

I. Eilks, *Organizer*
O. Gulacar, *Organizer, Presiding*

1:30 Introductory Remarks .

1:35 CHED 1948. Learning is an emotional experience. **R.E. Gibbons**

2:15 CHED 1949. Peer enhanced experiential research in general chemistry. **K.T. Nicholson**, P. Acioli, J. Hibdon, E. Head, R.E. Trana

2:35 Intermission.

2:45 CHED 1950. Development of basic chemistry and math activities to facilitate student success in general chemistry. **C. Kelleher**, B. Turnpenny, A.S. Silva

3:05 CHED 1951. Organic chemistry choice project to tap into students' intrinsic motivation for learning. **J.J. Stewart**, E.J. Maxwell

3:25 CHED 1952. Removing walls around science: The efforts that make chemistry meaningful again. **O. Gulacar**, I. Eilks, C. Zowada, A. George

3:45 Concluding Remarks.

Section G

Orange County Convention Center
Room W311D

Designs to Improve Learning Outcomes in an Allied-Health Chemistry Course

C. E. Brown, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 CHED 1953. Use of adaptive learning courseware in a GOB course: A report on the impact on student performance and attitude towards chemistry. **D.K. Jean**, A. Agah

1:55 CHED 1954. Flipping and restructuring an OB course: Improved student performances and positive longitudinal student survey responses. **D.M. Schirch**

2:15 CHED 1955. Strategies to promote engaged learning in the allied-health chemistry classroom. **S.C. Silver**

2:35 Intermission.

2:45 CHED 1956. Withdrawn



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

3:05 CHED 1957. Metabolism in the context of a GOB chemistry course. **C.E. Brown**

3:25 Concluding Remarks.

3:30 Discussion.

THURSDAY MORNING

Section A

Orange County Convention Center
Room W223A

General Papers

Fun Topics to Teach

S. A. Fleming, *Organizer*
T. A. Russell, *Presiding*

8:00 Introductory Remarks.

8:20 CHED 1958. Incorporation of green and environmental chemistry into the general chemistry curriculum and laboratory: Lessons learned from cWCSC Green Chemistry and Environmental Chemistry workshops. **D.W. Carpenetti**

8:40 CHED 1959. Lake Michigan Ozone Study: Characterization and sources of airborne particles. **A. Milani**, D. Hughes, E.A. Stone

9:00 CHED 1960. Fun with forensic chemistry. **A.A. Hazari**

9:20 Intermission.

9:40 CHED 1961. Teaching about climate chemistry in chemistry courses. **R.F. Hirsch**

10:00 CHED 1962. Nitrates and nitrites in cured and uncured meats. **R. Indralingam**, R. Slater

10:20 CHED 1963. Incorporating food science into the chemistry curriculum. **T.A. Russell**

10:40 CHED 1964. Two new models of protein dynamics for use in a non-majors biochemistry course.. **K.E. Theisen**

Section B

Orange County Convention Center
Room W312A

General Papers



TECHNICAL PROGRAM

Curriculum Issues

S. A. Fleming, *Organizer*
L. Aronne, *Presiding*

8:00 Introductory Remarks.

8:20 CHED 1965. Exploring the effectiveness of the use of lecture outlines in teaching General Chemistry. **C.J. Ohrenberg**

8:40 CHED 1966. Exploring the use of a flipped classroom, mid-semester in a general chemistry trailer course.. **J. Beres**

9:00 CHED 1967. Withdrawn

9:20 CHED 1968. Using WileyPLUS Concept Mastery assignments and ORION adaptive practice to give students ownership over their learning and ultimately their success in organic chemistry lecture. **S.P. Hickey**

9:40 Intermission.

10:00 CHED 1969. Withdrawn

10:20 CHED 1970. Withdrawn

10:40 CHED 1971. Withdrawn

11:00 CHED 1972. Withdrawn

Section C

Orange County Convention Center
Room W312B

General Papers

S. A. Fleming, *Organizer*
M. Dunphy, *Presiding*

8:00 Introductory Remarks.

8:05 CHED 1973. Replacing the Bohr atomic model with an accessible picture of how atoms and light truly interact. **B. Abrams**

8:25 CHED 1974. Counting orbitals: A beautiful way to teaching quantum numbers and hybrids. **J.F. Lomax**

8:45 CHED 1975. Benefits of collaboration between colleges and high schools. **L. Aronne**

9:05 Intermission.



TECHNICAL PROGRAM

9:20 CHED 1976. Leadership development and applied soft skills in the Walsh University chemistry curriculum. **M. Dunphy, J.A. Lupica, P. Tandler**

9:40 CHED 1977. Active learning in stressed classroom environments. **A.M. Gonzalez-Mederos**

10:00 CHED 1978. Adapting specifications grading into an introductory biochemistry course to assess learning outcomes. **H.J. Fletcher**

10:20 CHED 1979. International research experience for undergraduate students. C. Wilson, M. Hirtz, P. Levkin, **A.E. Holmes**

Section D

Orange County Convention Center
Room W311A

Research in Chemistry Education

C. J. Luxford, *Organizer*
S. D. Wiediger, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 CHED 1980. Analyzing mathematics fluency, course averages, and algorithmic and conceptual common question scores: What picture is given by statistical modeling. **W.K. Willis, V.M. Williamson**

8:25 CHED 1981. Adapting chemistry assessments for greater equitability among cohorts of differential preparation in mathematics. **V.R. Ralph, S.E. Lewis**

8:45 CHED 1982. Embedded math in chemistry: A case study of students' attitudes and mastery. **A.M. Preininger**

9:05 Intermission.

9:20 CHED 1983. Exploring the student-home identity nexus for general chemistry students. **G.N. Leon-Lozano, N.S. Stephenson, J.H. Carmel**

9:40 CHED 1984. Withdrawn

10:00 CHED 1985. Testing of a model of the impact of enjoyment and anxiety on performance as mediated by motivation. **A.J. Dood, K.B. Fields, J.R. Raker**

10:20 Concluding Remarks.

Section E

Orange County Convention Center
Room W311B



TECHNICAL PROGRAM

Observing & Measuring Classroom Instructional Practices

E. Saitta, *Organizer, Presiding*

8:00 Introductory Remarks .

8:05 CHED 1986. Using student interaction rubrics to assess the development of workplace skills in large enrollment courses. **C.L. Stanford**, S.M. Ruder, C.F. Bauer, R.S. Cole, J. Lantz, G.J. Reynders

8:25 CHED 1987. Impact of Peer-led Team Learning on students' long-term retention of general chemistry concepts. **M. Rahman**, S.E. Lewis

8:45 CHED 1988. Exploring the impact of General Chemistry curriculum reform on underrepresented minorities. **M.L. Head**, K.J. Linenberger Cortes

9:05 CHED 1989. Withdrawn

9:25 Intermission.

9:35 CHED 1990. Environmental, technological, pedagogical, and content knowledge (ETPCK): A new framework for teacher knowledge. **J. Donnelly**, L. Berry

9:55 CHED 1991. Twenty-four/seven window into an inquiry classroom: An anytime resource for classroom observation. **C.F. Bauer**

10:15 CHED 1992. Establishing a practice-based learning community of general chemistry GTAs through video club and design-based research. **M.M. Wu**, M. Ryu

10:35 Intermission.

10:45 CHED 1993. Observations from afar: The role of survey research in characterizing instructional practices. **J.R. Raker**, K.L. Murphy

11:05 CHED 1994. Investigating biochemistry instructors' teaching practices through the use of classroom observations and interviews: A qualitative approach. **F.K. Lang**, G.M. Bodner

11:25 CHED 1995. Considering classroom practice. **R.S. Cole**

11:45 Concluding Remarks.

CHAS

Division of Chemical Health & Safety

J. Pickel and D. Decker, *Program Chairs*



TECHNICAL PROGRAM

SUNDAY AFTERNOON

Section A

Orange County Convention Center
Room W232C

Educating the Educators

Cosponsored by CCS
S. B. Sigmann, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 CHAS 1. Safety education: *Not* the same as safety training. **R.H. Hill**

2:00 CHAS 2. Creative tension between safety education and training. **R. Stuart**

2:25 CHAS 3. Communicating facility limitations: Lab design and beyond. **S.M. Hick**, B. Butkus, C. Collier, R. Michel

2:50 CHAS 4. Engaging students to gain understanding of chemical safety information. **E. Sweet**

3:15 Intermission.

3:25 CHAS 5. Easy implementation of risk assessment. **M.R. Wilhelm**

3:50 CHAS 6. Dissemination of a RAMP toolbox to K-12 teachers through NSTA workshops. **M.U. Gmurczyk**, J. Bishoff, I.G. Cesa, S.B. Sigmann

4:15 CHAS 7. Using a “mock safety sort” to raise the many issues a high school science teacher may face. **S.D. Wiediger**

4:40 CHAS 8. New break-out safety activity for educating educators safe laboratory practices. **R. Sunasee**, S. Nephew

MONDAY MORNING

Section A

Orange County Convention Center
Room W232C

A Decade Later: The Death of Sheri Sangji as a Catalyst for a Change in Safety Culture

Cosponsored by CCS and PROF
H. Weizman, *Presiding*



TECHNICAL PROGRAM

8:00 Introductory Remarks.

8:05 CHAS 9. Evaluating the perspective of chemistry graduate students' on the 2008 UCLA incident. **H. Weizman**

8:30 CHAS 10. Review of progress and challenges in promoting enhance safety instruction. **D.C. Finster**

8:55 CHAS 11. Transitioning from graduate student researcher to safety professional. **B. Armstrong**

9:20 CHAS 12. A decade later: Moving safety culture forward in the University of California. **D.M. Decker**

9:45 Intermission.

10:00 CHAS 13. Using safety climate surveys to measure the impact of faculty engagement and leadership on laboratory safety. **C.A. Merlic**

10:25 CHAS 14. Managing chemical safety as a social construct: A paradigm shift in chemistry. **S.B. Sigmann**, R. Stuart

10:50 CHAS 15. Collaboration in laboratory safety. **E. Sweet**

11:15 CHAS 16. Using acid etch safety to promote collaboration between university professions. **E. Chartier**

MONDAY AFTERNOON

Section A

Orange County Convention Center
Room W232C

Cannabis Chemistry's First Annual ElSohly Award Symposium

K. Boyar, E. M. Pryor, *Presiding*

1:30 Opening Remarks.

1:35 CHAS 17. Constituents of cannabis: Less is more? **S. Goldman**

2:00 CHAS 18. Analytical expressions for viscosity of concentrated cannabis oils. **M.T. Coffin**

2:25 CHAS 19. Brief synopsis of basic propagation and breeding techniques in cannabis. **B.A. Jones**

2:50 Intermission.

3:00 CHAS 20. Old wine in new bottles: The health and safety implications of the cannabis access law on the prescription drug epidemic. **J. Marcu**, J. Roberts

3:25 CHAS 21. Innovation involves inspiration. **M. Vialpando**

3:50 CHAS 22. Frontiers in the development of cannabis-based therapeutics. **M.A. Elsohly**



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

The Chemistry of Disasters

Sponsored by PRES, Cosponsored by CCS and CHAS⁺

Chemistry in Space: Future Directions

Sponsored by YCC, Cosponsored by AGFD, ANYL, BIOT, BMGT, CHAS, ENVR, FLUO, GEOC, HIST, I&EC, MEDI, POLY and PROF

MONDAY EVENING

Section A

Orange County Convention Center
West Hall C

Sci-Mix

J. M. Pickel, *Organizer*

8:00 - 10:00

CHAS 23. Developing SOPs for hazardous chemical manipulations. **T. Chandra**

CHAS 24. Division of Chemical Health and Safety Poster. **J.M. Pickel**

CHAS 25. Impacts of various acids on thermal decomposition of tetrahydrocannabinolic acid (THCA) and tetrahydrocannabinol (THC) in methanol and ethanol. **M.N. Bauer**, B.M. Canfield

CHAS 26. Database of pharmacokinetic time-series data and parameters for evaluating the safety of environmental chemicals. R. Sayre, J. Wambaugh, **C. Grulke**

TUESDAY MORNING

Section A

Orange County Convention Center
Room W232C

Cannabis Chemistry's First Annual ElSohly Award Symposium

K. Boyar, E. M. Pryor, *Presiding*



TECHNICAL PROGRAM

9:00 Opening Remarks.

9:05 CHAS 27. Chemical barcoding for cannabis source identification. **D.J. Boston**, C.A. Kinney, J. Carsella

9:30 CHAS 28. Formulation of customized cannabis concentrates. **T. Trah**

9:55 CHAS 29. Cannabis microbiome sequencing and its implications for cannabis safety testing. **K. Boyar**

10:20 CHAS 30. How a cannabis CRO can support cannabis LPs in their processing optimization needs. **M. Roggen**, J. Hein, G. Sammis

10:45 CHAS 31. Development of an efficient method for the extraction and isolation of cannabidiol (CBD) from bulk industrial hemp using pressurized liquid extraction (PLE) and flash chromatography. **C.A. Kinney**, D. Seifried

Bridging the (Safety) Gap between Academia & Industry

Sponsored by PRES, Cosponsored by CA, CCS, CHAS[‡], CHED, PROF and YCC

TUESDAY AFTERNOON

Section A

Orange County Convention Center
Room W232C

Improving Academic Safety Culture: Undergraduate & Graduate Student Leadership in Laboratory Safety

Cosponsored by CCS and PROF
K. A. Miller, *Presiding*

1:30 Introductory Remarks.

1:35 CHAS 32. Leadership and empowerment: How to ask and answer safety questions well. **R. Stuart**

2:00 CHAS 33. Building a stronger, sustainable safety culture at the University of Chicago. **J. Ting**, R.J. Menssen, S.R. Zinn, J. Lettow, B. Slaw, L. Pulido, Q. Wu, J.H. Wright, K. Mormann

2:25 CHAS 34. Design your own safety education. **K.P. Fivizzani**

2:50 CHAS 35. How effective is safety training in undergraduate teaching labs? **K. Mesa**

3:15 CHAS 36. Student-led safety inspections of chemistry teaching and research laboratories. **B.J. Stockman**

Section A

Orange County Convention Center
Room W232C



TECHNICAL PROGRAM

Ask Doctor Safety about New Materials, Processes & Products

Cosponsored by CCS
H. J. Elston, *Presiding*

3:50 CHAS 37. Controlling safety when you just don't know. **H.J. Elston**

4:15 CHAS 38. From Walmart to Target: Current initiatives to remove toxic chemicals from personal care products. **F. Umesiri**

4:40 CHAS 39. Inserting green chemistry considerations into RAMP. **D.C. Finster**, R.H. Hill, J. MacKellar

Green Chemistry as a Pillar of Safety Education

Sponsored by CHED, Cosponsored by CHAS

WEDNESDAY MORNING

Section A

Orange County Convention Center
Room W232C

New Frontiers in Cannabis: Analytical Tools, Post-Processing, & Policy Directions

A. R. Wise, *Organizer, Presiding*
J. Bramante, *Presiding*

9:00 Opening Remarks.

9:05 CHAS 40. Using ImageJ for automated counting of colony forming units of yeast and molds in cannabis flowers. N. Stolze, A. Sutlief, **A.E. Holmes**

9:30 CHAS 41. Standardizing the Entourage Effect: Regulating terpenes & flavor additives for inhalable cannabis products without throwing the baby out with the bathwater. **B. Douglass**, J.C. Raber

9:55 CHAS 42. Chemistry of cannabis concentrate aerosolization. **J. Meehan-Atrash**, R.M. Strongin

10:20 CHAS 43. Chemical and genetic origins of strain-specific aroma in *Cannabis sativa* L.. **A. Gilbert**

10:45 Intermission.

10:55 CHAS 44. Gas chromatography-mass spectrometry and tandem-mass spectrometry for cannabinoid analysis and discovery. **A. Leghissa**, Z. Hildenbrand, K. Schug

11:20 CHAS 45. Novel formation of THC isomers in cannabis oil distillate. **N. Mosely**, Z. Iszard



TECHNICAL PROGRAM

11:45 CHAS 46. Fundamental chemistry research from a collaborative cannabis research venture. **M. Roggen**, G. Sammis, J. Hein

CINF

Division of Chemical Information

R. Bienstock and S. Cardinal, *Program Chairs*

SUNDAY MORNING

Section A

Orange County Convention Center
West Hall B4 - Theater 10

Drug Discovery: Informatics Approaches

Cosponsored by MEDI
E. Davis, *Organizer, Presiding*

8:30 CINF 1. Analysis of billions of Synthetically Accessible Virtual Inventory (SAVI) compounds as to their drug potential. **H. Patel**, W. Ihlenfeldt, M. Nicklaus

8:55 CINF 2. Drug repurposing is a common phenomenon: Bibliometric and cheminformatics evidence based on PubMed data. **N.C. Baker**, S. Ekins, A.J. Williams, A. Tropsha

9:20 CINF 3. Biology scale modeling in chemical-proteomics: Data management and analytics. **H. Wang**

9:45 CINF 4. Monomer.org. **D.J. Milton**

10:10 Intermission.

10:20 CINF 5. Extensive data-driven modeling of food-derived bioactive peptides that inhibit the angiotensin I-converting enzyme. **D.P. Russo**, Y. Zhang, H. Zhu

10:45 CINF 6. BIOFACQUIM: A compound database of natural products from Mexico. **B.A. Pilon-Jimenez**, J. Medina-Franco

11:10 CINF 7. Analysis of tautomeric transforms in chemical databases in the context of redesign of handling of tautomerism for InChI V2. **D. Dhaked**, M. Nicklaus

11:35 CINF 8. Kinase inhibitor selectivity data analysis. **Z. Luo**, V. Ulshoefer



TECHNICAL PROGRAM

Section B

Orange County Convention Center
West Hall B4 - Theater 11

Partnering Up in the New Frontier: Libraries & External Partners Working Together

S. K. Cardinal, *Organizer*
M. Qiu, *Organizer, Presiding*

8:30 Introductory Remarks.

8:40 CINF 9. Universities and scholarly publishers collaborating to help students and postdocs advance their research and get published. **G. Baysinger, S. O'Reilly**

9:10 CINF 10. Partnership between librarians and non-profit stakeholders in research information ecosystem: WikiEdu and carpentries. **Y. Li**

9:40 CINF 11. FAIR chemical data for health and safety: Connecting the dots with cheminformatics and librarianship. **L.R. McEwen, E. Bolton**

10:10 Intermission.

10:20 CINF 12. 30 years of Reaxys: Chemical information for the chemists. **J.N. Currano, J. Dolenc, O. Renn, J. Swienty-Busch**

10:50 CINF 13. PubChem as a resource for chemical information training. **S. Kim, E. Bolton**

11:20 Panel Discussion.

11:50 Concluding Remarks.

Data Science for Catalysis Research

Sponsored by CATL, Cosponsored by CINF, COMP and ENFL

Advances in Methods for Comparing Molecular & Supramolecular Simulations to Experiments

Sponsored by CATL, Cosponsored by CINF, COMP and PHYS

SUNDAY AFTERNOON

Section A



TECHNICAL PROGRAM

Orange County Convention Center
West Hall B4 - Theater 10

Drug Discovery: Informatics Approaches

Cosponsored by MEDI
E. Davis, *Organizer, Presiding*

1:30 CINF 14. SuCOS: A pharmacophoric-shape overlap metric for comparing binding modes. **S. Leung**, M. Bodkin, F. von Delft, P. Brennan, G.M. Morris

1:55 CINF 15. LigandNet: A machine-learning-based toolkit for predicting ligand activity to proteins. M. Hassan, D. Castaneda, D. Shrestha, I. Salama, **S. Sirimulla**

2:20 CINF 16. Machine learning-based prediction of compound profiling matrices. **R. Rodríguez Pérez**, J. Bajorath

Section A

Orange County Convention Center
West Hall B4 - Theater 10

Collaborations & Data Sharing in Rare & Orphan Disease Drug Discovery

Cosponsored by MEDI
R. J. Bienstock, *Organizer, Presiding*

3:20 CINF 17. Collaborations and data sharing in rare disease. **R.J. Bienstock**

3:40 CINF 18. Genetic and Rare Diseases (GARD) information center treatment profiles. **Q. Zhu**, D. Nguyen, N. Southall, A. Chen, E. Sid, A. Pariser

4:05 CINF 19. Biomedical data translator: Supporting data integration and rare disease research. **N. Southall**, C. Colvis

4:30 CINF 20. Data-driven drug discovery for rare diseases: tales from the trenches. **F. van den Broek**

Section B

Orange County Convention Center
West Hall B4 - Theater 11

Careers in Chemical Information

Cosponsored by SCHB
N. Bharti, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 CINF 21. Computational chemistry and chemoinformatics career opportunities at the NIH (NIEHS). **R.J. Bienstock**



TECHNICAL PROGRAM

1:55 CINF 22. Careers in publishing chemical information: From the lab bench to the editorial office to the database. **G. Jones**

2:15 CINF 23. Water-quality data and publications for careers in chemistry information. **E.C. Wild**

2:35 CINF 24. Scientist in EH&S: Changing the tradition in laboratory safety. **S. Singh, N. Bharti**

2:55 Intermission.

3:05 CINF 25. Antony Williams, the ChemConnector: A career path through a diverse series of roles and responsibilities. **A.J. Williams**

3:25 CINF 26. Careers in science: Science policy and general advice. **E. Dunlea**

3:45 CINF 27. How interests and experience led to a career in chemical literature informatics. **N.C. Baker**

4:05 CINF 28. Lab to library: A career in chemistry librarianship. **N. Ruhs**

Frontiers in Cyber Security

Sponsored by SCHB, Cosponsored by CINF

Data Science for Catalysis Research

Sponsored by CATL, Cosponsored by CINF, COMP and ENFL

Advances in Methods for Comparing Molecular & Supramolecular Simulations to Experiments

Sponsored by CATL, Cosponsored by CINF, COMP and PHYS

SUNDAY EVENING

Section A

Orange County Convention Center
West Hall C

CINF Scholarships for Scientific Excellence: Student Poster Competition

Cosponsored by PROF
Financially supported by American Chemical Society, Publications Division
E. Alvaro, M. Qiu, *Organizers*



TECHNICAL PROGRAM

6:30 - 8:30

CINF 29. Computational-aided design of diversity: Chemical libraries based on natural products. **F. Saldivar**, E. Lenci, A. Trabocchi, J. Medina-Franco

CINF 30. Classification models of pesticides by mode of action. A. Osnaya-Hernandez, **G. Gómez-Jiménez**, D. Chavez, F. Cortes-Guzman, A. Madariaga, K. Martinez Mayorga

CINF 31. Understanding stereoselectivity in radical cation Diels-Alder reactions using quasi-classical dynamics. **J. Tan**, R.S. Paton

CINF 32. Application of *ab initio* molecular dynamic simulation in 4D fingerprints. **Y. Tu**, Y. Tseng, M. Appell

CINF 33. ASKCOS: Data-driven synthetic route design and validation for small organic molecules. **C.W. Coley**, H. Gao, W.H. Green, K.F. Jensen

CINF 34. Hierarchical H-QSAR modeling method that integrates binary/multi classification and regression models for predicting acute oral systemic toxicity. **X. Li**, D. Fourches

CINF 35. *In silico* platform as an alternative to animal testing for acute toxicity. **J. Borba**, V.M. Alves, A.C. Silva, K. Overdahl, S. Capuzzi, E. Overdahl, D. Korn, R. Silva, S. Hall, R. Braga, N. Kleinstreuer, C.H. Andrade, E. Muratov, A. Tropsha

CINF 36. BDEDB: A bond-dissociation energy database and instant prediction. **Y. Guan**, R.S. Paton

MONDAY MORNING

Section A

Orange County Convention Center
West Hall B4 - Theater 10

Web-Based Chemoinformatics Platforms

J. L. Medina-Franco, *Organizer, Presiding*
K. Martinez Mayorga, *Presiding*

8:00 Introductory Remarks.

8:05 **CINF 37.** Designing drug candidates and chemical probes in cyberspace. **B. Villoutreix**

8:35 **CINF 38.** Cheminformatics tools and applications on the web: Challenges, examples, and the future. **D. Fourches**

9:05 **CINF 39.** SynSpace: A user-friendly web- and cloud-based design platform to expand synthetically-enabled scaffold and lead analogue space for medicinal chemistry and AI-assisted drug discovery. **G. Makara**, G. Pocze, L. Kovacs, O. Demeter, I. Szabo



TECHNICAL PROGRAM

9:35 CINF 40. Exploring an expanded chemical universe using www.chemmaps.com. **A. Borrel**, D. Fourches, N. Kleinstreuer

10:05 Intermission.

10:20 CINF 41. Exploring chemical space at gdb.unibe.ch. D. Probst, M. Awale, A. Thakkar, **J. Reymond**

10:50 CINF 42. Developing an integrated model management solution to assure quality of predicted data at the US EPA's National Center of Computational Toxicology. **C. Grulke**, A.J. Williams, A. Singh, J. Edwards

11:20 CINF 43. US-EPA CompTox chemicals dashboard: A web-based data integration hub for environmental chemistry data. **A.J. Williams**, C. Grulke, R. Judson, J. Wambaugh, J. Dunne, J. Edwards

Section B

Orange County Convention Center
West Hall B4 - Theater 11

Creating a Common Language for Chemistry: IUPAC's Past, Present & Future Roles

Cosponsored by HIST
Financially supported by International Union of Pure and Applied Chemistry (IUPAC)
H. A. Lawlor, L. R. McEwen, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 CINF 44. IUPAC Commission on Isotopic Abundances and Atomic Weights: Its history, role, and work. **J. Meija**

9:00 CINF 45. Archives of the international union of pure and applied chemistry at the Science History Institute. **R.S. Brashear**

9:25 CINF 46. "A" in IUPAC: Applying the common language for chemistry to meet world needs. **M.C. Cesa**

9:50 Intermission.

10:05 CINF 47. Accidental nomenclaturest: A journey from bench chemist to ACS-NTS and IUPAC member. **M.M. Rogers**

10:30 CINF 48. iGROW: IUPAC global recognition opportunities for women. F. Meyers, C. Ribes, **A.K. Wilson**

10:55 CINF 49. Role of IUPAC Committee on Chemistry Education in communicating chemistry. **M.H. Towns**

11:20 CINF 50. Short history of IUPAC InChI algorithm. **S.R. Heller**

11:45 Concluding Remarks.

Data Science for Catalysis Research



TECHNICAL PROGRAM

Sponsored by CATL, Cosponsored by CINF, COMP and ENFL

MONDAY AFTERNOON

Section A

Orange County Convention Center
West Hall B4 - Theater 10

Web-Based Chemoinformatics Platforms

J. L. Medina-Franco, *Organizer, Presiding*
K. Martinez Mayorga, *Presiding*

1:10 Introductory Remarks.

1:15 **CINF 51.** Web Force-Field (WebFF) repository: Molecular dynamics force-field data for soft materials at multiple levels of granularity. **F.R. Phelan**, H. Sun

1:45 **CINF 52.** CavityPlus: A web server for protein cavity detection with pharmacophore modelling, allosteric site identification, and covalent ligand-binding ability prediction. **J. Pei**

2:15 **CINF 53.** iSpiEFP: Automating the computational workbench. **Y. Bui**, L.V. Slipchenko

2:45 **CINF 54.** ProteinsPlus and SMARTSviewer: Two web applications for the modeling and cheminformatics community. R. Fährrolfes, R. Schmidt, **M. Rarey**

3:15 Intermission.

3:30 **CINF 55.** D-Peptide Builder: A web-based application to enumerate the chemical space of peptides. **B. Diaz Eufrazio**, J. Medina-Franco, O. Palomino-Hernández, A. Arredondo-Sanchez

4:00 **CINF 56.** Freely available online resource for prediction of novel multitarget anti-HIV agents. **D. Druzhilovskiy**, D. Filimonov, L. Stolbov, P. Savosina, V. Poroikov, M.C. Nicklaus

4:30 **CINF 57.** ZINC15.docking.org: Over 1.5 billion compounds you can search and buy; 550 million lead-like you can dock. **J.J. Irwin**

Section B

Orange County Convention Center
West Hall B4 - Theater 11

Creating a Common Language for Chemistry: IUPAC's Past, Present & Future Roles

Cosponsored by HIST
Financially supported by International Union of Pure and Applied Chemistry (IUPAC)
H. A. Lawlor, L. R. McEwen, *Organizers, Presiding*



TECHNICAL PROGRAM

1:30 Introductory Remarks.

1:35 **CINF 58.** Towards a “Digital IUPAC”: Coordinating community needs for digital data standards. **L.R. McEwen**, D. Martinsen, H.A. Lawlor

2:00 **CINF 59.** Renovating the IUPAC gold book for the digital era and the next 100 years. **S.J. Chalk**

2:25 **CINF 60.** ISMC: IUPACs interdivisional sub-committee on materials chemistry. **C.K. Ober**, V. Gubala

2:50 Intermission.

3:05 **CINF 61.** FAIR data in the 21st century: The role of scientific unions in facilitating interdisciplinary data science in Chemistry and the Earth Sciences. **S. Stall**, **L.R. McEwen**

3:30 **CINF 62.** Top ten emerging technologies in chemistry: A new initiative from IUPAC and *Chemistry International*. **F. Gomollon-Bel**, J. Garcia Martinez, H.A. Lawlor

3:55 **CINF 63.** IUPAC and its next century: A secretary general’s perspective. **R. Hartshorn**

4:20 Panel Discussion.

4:50 Concluding Remarks.

MONDAY EVENING

Section A

Orange County Convention Center
West Hall C

Sci-Mix

R. J. Bienstock, *Organizer*

8:00 - 10:00

29-36. See previous listings.

CINF 774. Analyzing the effectiveness of a pilot community service learning project in the undergraduate chemistry laboratory. **H.H. Grewal**, **J. Khalil**, C.C. Lovallo, K. Ho

TUESDAY MORNING

Section A

Orange County Convention Center
West Hall B4 - Theater 10



TECHNICAL PROGRAM

Web-Based Chemoinformatics Platforms

J. L. Medina-Franco, *Organizer, Presiding*
K. Martinez Mayorga, *Presiding*

8:00 Introductory Remarks.

8:05 CINF 64. 3decision®: Bringing structural data analytics to the masses. **G. Jonasson**

8:35 CINF 65. Leveling the playing field: Illuminating understudied targets with Pharos. **T. Sheils**, D. Nguyen, N. Southall, T.I. Oprea, V. Siramshetty

9:05 CINF 66. Chembench: A publicly-accessible, integrated cheminformatics portal. **E. Muratov**, S. Capuzzi, V.M. Alves, V. Tkachenko, A. Korotcov, D. Korn, W. Lam, T. Thornton, D. Pozefsky, A. Tropsha

9:35 CINF 67. K4DD database: Ligand binding kinetics at its best. **G.F. Ecker**, L. Richter

10:05 Intermission.

10:20 CINF 68. MOEsaic: The application of matched molecular pair analysis to SAR exploration. **G. Fortin**

10:50 CINF 69. ARENA360: An integrated informatics solution for drug discovery. **C. Betton**, Z. Luo, V. Ulshoefer

11:20 CINF 70. Delivering computational chemistry to cheminformatics: collaborative drug discovery with LiveDesign. **E. Davis**

11:50 Concluding Remarks.

Section B

Orange County Convention Center
West Hall B4 - Theater 11

Deep Learning

Cosponsored by COMP
K. Martinez Mayorga, *Organizer*
J. L. Medina-Franco, *Presiding*

8:00 Introductory Remarks.

8:05 CINF 71. Advances in deep learning and their applied utility toward chemical informatics & drug discovery. **E. Clark**, **W.E. Hahn**, R. St Clair, P. Morris, M. Teti

8:35 CINF 72. How much can we learn from smiles as text? **H. Sun**

9:05 CINF 73. Novel, active learning approach for deep learning of chemical data: Extracting more chemical insights by choosing less. **M. Haghghatlari**, J. Hachmann



TECHNICAL PROGRAM

9:35 **CINF 74.** Application of machine learning to skin cancer detection and classification. **A.C. Terentis**, J. Strasswimmer

10:05 Intermission.

10:20 **CINF 75.** Deep learning for the characterization and identification of small molecules. **S. Colby**, J. Nunez, N. Hodas, C. Corley, R. Renslow

10:50 **CINF 76.** Virtual high-throughput screening: A combined deep-learning approach. **P. Morris**, **R. St Clair**, **M. Teti**, E. Clark, W.E. Hahn

11:20 **CINF 77.** Learn deep before deep learning. **K. Martinez Mayorga**, G. Gómez Jiménez, A. Madariaga-Mazon

TUESDAY AFTERNOON

Section A

Orange County Convention Center
West Hall B4 - Theater 10

Assessing Chemistry Outreach

Cosponsored by YCC
M. R. Hartings, *Organizer, Presiding*

1:15 **CINF 78.** Going beyond popular: Assessing *SciPop Talks!* **R.M. Burks**, K. Deards, E. DeFrain

1:35 **CINF 79.** Understanding interest, relevance, & self-efficacy: Chemistry at the museum and beyond. **E.L. Howell**, S. Yang, D.A. Scheufele

1:55 **CINF 80.** Collecting, understanding, and utilizing audience feedback to increase interest, relevance, and self-efficacy related to hands-on chemistry activities in a museum. **G.M. Haupt**

2:15 **CINF 81.** Advancing inclusive excellence in academic chemistry departments from the top down through a discipline-based evidenced-based approach. **R. Hernandez**, D. Stallings, S.K. Iyer

2:35 **CINF 82.** Science outreach: What does it mean to be successful, and how do we know? **J. Garbarino**

2:55 Intermission.

3:10 **CINF 83.** Amplifying your social impact: A collaborative approach to chemistry outreach. **M.T. Gallardo-Williams**, **G. Van Den Driessche**, A. Malico

3:30 **CINF 84.** Evaluating impact. **S. Kundu**

3:50 **CINF 85.** How can I measure the success of my online outreach? **D. Reeser**, S. Hadden, M. Ruhl, A.T. Yarnell

4:10 **CINF 86.** Mapping the chemistry Twitter community: A reproduction of academic power structures or an opportunity to empower marginalized voices? **P. Vincent-Ruz**, D. Reeser, M.R. Hartings



TECHNICAL PROGRAM

Section B

Orange County Convention Center
West Hall B4 - Theater 11

Deep Learning

Cosponsored by COMP
K. Martinez Mayorga, *Organizer*
J. L. Medina-Franco, *Presiding*

1:30 Introductory Remarks.

1:35 **CINF 87.** Interpretable molecular design based on layer-wise relevance propagation. **Y. Kwon**, K. Kim, I. Kim, J. Yoo, W. Son, Y. Choi, H. Lee, J. Shin

2:05 **CINF 88.** Machine-learned model for molecular simulations of liquid and water vapor. T. Loeffler, T. Patra, H. Chan, **S. Sankaranarayanan**

2:35 **CINF 89.** Prediction of chemical reactivity with a graph-convolutional neural network model. **C.W. Coley**, W. Jin, L. Rogers, T.F. Jamison, T. Jaakkola, W.H. Green, R. Barzilay, K.F. Jensen

3:05 Intermission.

3:20 **CINF 90.** Predicting bond dissociation energies through deep learning. **Y. Guan**, Y. Kim, P. St. John, S. Kim, R.S. Paton

3:50 **CINF 91.** Multitask prediction of site selectivity in aromatic C-H functionalization reactions. **T.J. Struble**, C.W. Coley, K.F. Jensen

4:20 **CINF 92.** Molecular transformer for chemical reaction prediction and uncertainty estimation. **P. Schwaller**, T. Laino, T. Gaudin, C. Bekas, A.A. Lee

WEDNESDAY MORNING

Section A

Orange County Convention Center
West Hall B4 - Theater 10

Applications of Cheminformatics to Environmental Science

Cosponsored by ENVR
A. J. Williams, *Organizer, Presiding*

8:00 Introductory Remarks.



TECHNICAL PROGRAM

8:05 CINF 93. Environmental chemical information in PubChem. **J. Zhang**, E. Bolton

8:25 CINF 94. EPA CompTox chemicals dashboard: An online resource for environmental chemists. **A.J. Williams**, C. Grulke, J. Dunne, J. Edwards

8:45 CINF 95. Mapping of chemical identifiers to DSSTox to enable data integration in the US-EPA CompTox Chemicals Dashboard. **C. Grulke**, I. Thillainadarajah, P. Browne, A.J. Williams, A. Richard

9:05 CINF 96. Consistency checking the experimental data available from the USEPA NCCT CompTox database. **S.J. Chalk**, A.J. Williams, C. Grulke

9:25 Intermission.

9:40 CINF 97. Literature-based cheminformatics for research in chemical toxicity. **N.C. Baker**, A.J. Williams, T. Knudsen

10:00 CINF 98. Green chemistry and open data. **J. Zhang**, E. Bolton

10:20 CINF 99. Development of the alternatives assessment dashboard webtool. L. Vegosen, **T. Martin**

10:40 CINF 100. Application of chemical informatics to alternatives assessment. **W. Barrett**, S.R. Takkellapati, K. Tadele, L. Vegosen, M.A. Gonzalez

11:00 CINF 101. Prediction of toxicity using WebTEST (Web-services Toxicity Estimation Software Tool). **T. Martin**, A.J. Williams, **V. Tkachenko**

11:20 CINF 102. Case study in quantitative GenRA predictions using repeated dose toxicity studies from ToxRefDB v2.0. **G. Helman**, G. Patlewicz, I. Shah, K. Paul Friedman, L. Pham, S. Watford

11:40 CINF 103. Enhancement of acute toxicity prediction by multi-task learning. **S. Sosnin**, D. Karlov, I.V. Tetko, M.V. Fedorov

Section B

Orange County Convention Center
West Hall B4 - Theater 11

Deep Learning

Cosponsored by COMP
K. Martinez Mayorga, *Organizer*
J. L. Medina-Franco, *Presiding*

8:00 Introductory Remarks.

8:05 CINF 104. Prediction of toxicity: Deep learning with small and imbalanced datasets. **G.F. Ecker**, J. Hemmerich, E. Asilar

8:35 CINF 105. Imputing compound activities based on sparse and noisy data. T. Whitehead, B. Irwin, P.A. Hunt, **M.D. Segall**, G. Conduit



TECHNICAL PROGRAM

9:05 **CINF 106.** Machine learning in the context of bioactivity. J. Sieg, **M. Rarey**

9:35 **CINF 107.** ML and AI in the design of new drug lead compounds. **S. Keinan**, W.J. Shipman, E.H. Frush, E. Addison

10:05 Intermission.

10:20 **CINF 108.** Influence of compound profiling matrix density on the performance of multi-task deep neural networks and random forest models. **R. Rodríguez Pérez**, J. Bajorath

10:50 **CINF 109.** Many possible roles of deep learning in drug discovery: Separating truth from hype. **R. Abel**, K. Leswing, K. Marshall, J. Staker, C. McQuaw, S. Jerome, S. Mondal, S. Bhat

11:20 **CINF 110.** Industry perspective: Deep learning for QSAR models. **J. Shen**

11:50 Concluding Remarks.

WEDNESDAY AFTERNOON

Section A

Orange County Convention Center
West Hall B4 - Theater 10

Applications of Cheminformatics to Environmental Science

Cosponsored by ENVR
A. J. Williams, *Organizer, Presiding*

1:15 **CINF 111.** OPERA models for physicochemical properties, environmental fate and toxicological endpoints to support regulatory purposes. **K. Mansouri**, R. Judson, A.J. Williams, N. Kleinstreuer

1:35 **CINF 112.** Applications of a chemotype-enrichment approach to the ToxCast data landscape and beyond: Inverting the SAR paradigm. **A. Richard**, R. Lougee, C. Grulke, N.C. Baker, J. Wang, A.J. Williams

1:55 **CINF 113.** Framing chemical safety and risk management: Ontological perspectives from laboratory procedures and incident reports. C.M. Shimizu, **L.R. McEwen**

2:15 **CINF 114.** Evaluation of the chemotype-enrichment workflow as a tool for independent evaluation biological activity thresholds and a comparison with traditional QSAR methods. **R. Lougee**, A. Richard, C. Grulke

2:35 **CINF 115.** Case study in quantitative GenRA predictions using acute oral toxicity. **G. Helman**, I. Shah, G. Patlewicz

2:55 **CINF 116.** Comprehensive computational approach for predicting human skin sensitization as suggested alternative to animal testing. **E. Muratov**, V.M. Alves, J. Borba, R. Braga, S. Capuzzi, A.C. Silva, N. Kleinstreuer, C.H. Andrade, A. Tropsha

3:15 Intermission.



TECHNICAL PROGRAM

3:25 CINF 117. Predicting chemical-assay interference using Tox21 qHTS data. **A. Borrel**, R. Huang, M. Xia, K. Houck, R. Judson, N. Kleinstreuer

3:45 CINF 118. Methods for *in silico* screening of use and exposure data in authority databases. **S. Fischer**

4:05 CINF 119. Novel nanodescriptors applied in QNAR: Combination of virtual nanomaterial library and geometrical structure of nanomaterial. **X. Yan**, A. Sedykh, W. Wang, B. Yan, H. Zhu

4:25 CINF 120. Reaction library for predicting direct phototransformation products of aquatic organic contaminants. **C. Yuan**, C.T. stevens.caroline@epa.gov, E.J. Weber

4:45 CINF 121. Cheminformatics and non-targeted analysis: A two-way street. **E.M. Ulrich**, J. Sobus, S. Newton, C. Grulke, A. Richard, R. Singh, A. McEachran, K. Phillips, K. Mansouri, J. Wambaugh, K.K. Isaacs, A.J. Williams

5:05 CINF 122. Elucidation of chemical dark matter using 'standards-free' small molecule identification. **R. Renslow**, S. Colby, D. Thomas, J. Nunez, Y. Yesiltepe, N. Govind, J.R. Cort, J. Teeguarden

5:25 Concluding Remarks.

CHAL

Division of Chemistry and the Law

K. Bianco and K. McIntyre, *Program Chairs*

SUNDAY AFTERNOON

Section A

Orange County Convention Center
Room W308D

Strengthening Your Patent Rights in Light of Recent Federal Circuit Court Decisions

Cosponsored by PROF
X. Pillai, *Organizer, Presiding*

2:00 CHAL 1. Strengthening your future patent rights in light of recent Federal Circuit court and UPTO decisions. **X. Pillai**

MONDAY MORNING



TECHNICAL PROGRAM

Section A

Orange County Convention Center
Room W308D

The Many Faces of CHAL: Where Chemistry Meets the Law

K. L. McIntyre, *Organizer*

K. E. Bianco, *Organizer, Presiding*

10:00 CHAL 2. Monitoring Hg emissions from gold shops in Peru: Science vs policy. **A.M. Kiefer**, M. Silva González, C.S. Seney, K.H. Moody, K. Hasan, V. Blakeman, L. Hicks, D. Loving, S. Aljic, C. McMahan, M.E. Moore

10:45 CHAL 3. Strategies for monetization of patent portfolios in chemical fields. **K.A. Rubino**

11:15 CHAL 4. Post-grant proceedings of bio & pharma patents: A brief overview and analysis of noteworthy cases since implementation of the America Invents Act. **K.A. Rubino**

MONDAY AFTERNOON

Section A

Orange County Convention Center
Room W308D

Beyond the Bench: Non-Traditional Careers in Chemistry

Cosponsored by BMGT, PROF and YCC

J. L. Kennedy, *Organizer*

J. Carver, *Presiding*

2:00 CHAL 5. Beyond the bench: Non-traditional careers in chemistry. **J. Carver, S. Santos, K.E. Bianco, K. Lavoie**

MONDAY EVENING

Section A

Orange County Convention Center
Room West Hall C

Sci-Mix

K. E. Bianco, K. L. McIntyre, *Organizers*

8:00 - 10:00

CHAL 6. Chocolate: Food of the gods. **H.M. Peters, S.B. Peters**



TECHNICAL PROGRAM

CHAL 7. National Inventors Hall of Fame. **H.M. Peters, S.B. Peters**

TUESDAY MORNING

Section A

Orange County Convention Center
Room W308D

Patent Insights for Pharmaceutical Companies

Cosponsored by PROF
S. K. Cyr, *Organizer, Presiding*

9:30 CHAL 8. Patent prosecution and portfolio management in the pharmaceutical industry. **D. Weingarten**

10:00 CHAL 9. Patent litigation under the Hatch-Waxman Act. **S.K. Cyr**

10:30 CHAL 10. Post-grant review in Hatch-Waxman litigation. **D. Weingarten**, K. Leonard

11:00 CHAL 11. Trade secret strategies for pharmaceutical innovations. **S.K. Cyr**, M. Meyers

COLL

Division of Colloid and Surface Chemistry

R. Nagarajan, *Program Chair*

SUNDAY MORNING

Section A

Orange County Convention Center
West Hall B4 - Theater 1

Understanding the Inorganic-Organic Interface in Colloidal Nanomaterials

Characterization of the Ligand Coating on Nanocrystal Surfaces

V. M. Rotello, *Organizer*



TECHNICAL PROGRAM

H. M. Mattoussi, *Organizer, Presiding*
Z. Hens, *Presiding*

8:30 Introductory Remarks.

8:45 **COLL 1.** Colloidal nanocrystal surface chemistry: A perspective based on NMR spectroscopy. **Z. Hens**

9:15 **COLL 2.** Characterization of semiconductor nanocrystals using advanced NMR spectroscopy. **L. Piveteau**, T. Ong, B.J. Walder, D.N. Dirin, D. Moscheni, B. Schneider, L. Protesescu, N. Masciocchi, A. Guagliardi, L. Emsley, C. Coperet, M. Kovalenko

9:35 **COLL 3.** Atomic-level structures of the organic-inorganic interface by NMR crystallography. **L. Emsley**

10:05 Intermission.

10:25 **COLL 4.** Ligand and surfactant distribution on inorganic nanoparticles. **L. Liz Marzan**

10:55 **COLL 5.** X-ray-mediated release of molecules and engineered proteins from nanostructure surfaces. M. Su, K. Guggenheim, J. Lien, J.B. Siegel, **T. Guo**

11:15 **COLL 6.** Impact of pH on the orientation of antibody adsorbed onto gold nanoparticles. **J.D. Driskell**, G. Ruiz, K. Tripathi

11:35 **COLL 7.** Biomimetic self-assembly of functional gold nanoparticles. **N. Nonappa**, P. Engelhardt

Section B

Orange County Convention Center
West Hall B4 - Theater 2

Biomaterials & Biointerfaces

Advances in Biomaterials

Y. Lapitsky, *Organizer*
R. Wylie, *Organizer, Presiding*
J. Moran-Mirabal, *Presiding*

8:30 **COLL 8.** Molecular mechanical characterization of bioinspired catecholamine polymers at interfaces. K. Malollari, P. Delparastan, **P.B. Messersmith**

9:00 **COLL 9.** Role of membrane lipid asymmetry in regulating nanoparticle-plasma membrane interactions. S. Nazemidashtarjandi, **A. Farnoud**

9:20 **COLL 10.** Functionalizing silk fibroin with fluorocarbons via F-capping chemistry to create multiuse inks. **M.J. Hawker**, J. Fountain, V. Montanari, K. Kumar, D.L. Kaplan

9:40 **COLL 11.** Effect of shape on buckling instability of multilayer hydrogel microcapsules in solutions. **N. Gupta**, V.A. Kozlovskaya, E.P. Kharlampieva



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

10:00 COLL 12. pH-Driven hierarchical assembly of DNA origami nanostructures. **S. Yang**, W. Liu, R. Wang

10:20 COLL 13. Single-step synthesis of alginate microbeads with a PEG shell: A new way to protect encapsulated cells. **S. Ahn**, W.E. Bentley, S.R. Raghavan

10:40 COLL 14. Fluorescent artificial lipoprotein with improved thermal stability for cell imaging and drug delivery. **J. Ding**, C.V. Kumar

11:00 COLL 15. Linking the kinetics of calcium carbonate formation and crystallization to the mechanical response of mineralized hydrogels. **J. Lopez-Berganza**, R.M. Espinosa-Marzal

11:20 COLL 16. One-pot synthesis of hybrid MoS₂/graphene nanosheet suspensions in water for bioelectronic and sensing applications. **M. Puglia**, C.V. Kumar

Section C

Orange County Convention Center
West Hall B4 - Theater 3

Quantitative Particle Cell Interaction

N. Feliu, L. Liz Marzan, W. J. Parak, *Organizers, Presiding*

8:30 COLL 17. Self-assembly of biomimetic nanoparticles with amyloid proteins: Concept and functions. **N. Kotov**, Y. Wang, U. Kadiyala, Z. Qu, P. Elvati, C. Altheim, A. Violi, J. VanEpps

9:00 COLL 18. Next-generation of quantum dot sensing. **H. Weller**

9:30 COLL 19. Elucidating the nanoparticle-cell interface. **M. Stevens**

10:00 COLL 20. Harvesting immunogenic cell death-inducing nanocarriers and catalytically active redox-active nanomaterials for nano-enabled breast and pancreas cancer immunotherapy. **A. Nel**

10:30 COLL 21. Nanoengineering of poly(ethylene glycol) particles for stealth and targeting. **F. Caruso**

11:00 COLL 22. Nanoparticles interaction with viruses. **F. Stellacci**

11:30 COLL 23. Utilizing meta-analysis to understand the cellular toxicity of quantum dots. **I. Medintz**, M. Bilal, E. Oh, R. Liu, H. Liu, J. Breger, Y. Cohen

Section D

Orange County Convention Center
West Hall B4 - Theater 4

Novel Functionalization Methods for Textiles & Fibers



TECHNICAL PROGRAM

M. Richards, *Organizer*
N. Pomerantz, *Organizer, Presiding*
M. Richards, *Presiding*

8:30 COLL 24. Water-based environmentally benign flame retardant nanocoatings for textiles. **J.C. Grunlan**, S. Lazar

9:00 COLL 25. Microencapsulation of flame retardants: A new approach for imparting fire resistance to nylon-cotton fabric blends. **R. Sharma**, J.D. Ogilvie-Battersby, D. Hari, J. Kumar, R. Mosurkal, N. Orbey, R. Nagarajan

9:30 COLL 26. Functional, biobased poly(phosphazene) flame-retardant coatings for textiles. **A. Pich**, A. Deniz

10:00 COLL 27. Functionalized fabrics for chemical protection. **B.J. Johnson**, B.J. Melde, M.H. Moore

10:30 COLL 28. Zinc oxide nanoparticles on polypropylene fibers and films: Adhesion and surface segregation. S. Kim, O. Grimm, E.A. Welsh, R. Pang, P.J. Stenhouse, D.M. Steeves, J.W. Soares, **J.E. Whitten**

11:00 COLL 29. Decontamination of toxic organophosphates using metal hydroxide/polymer textiles: Particle aggregation and its effects on material performance. **D.B. Dwyer**, J. Gomez, A. Davoodabadi, T. Tovar, W. Bernier, J. DeCoste, W.E. Jones

11:30 COLL 30. Aminated polyacrylonitrile fiber coated with Fe_2O_3 as a high-capacity adsorbent for phosphorus removal. **J. Youngkyun**, T. Do, Y. Ko, U. Choi

Section E

Orange County Convention Center
West Hall B4 - Theater 5

Nanomaterials

Applications: Colloid & Surface Chemistry Influencing Function

J. A. Hollingsworth, *Organizer*
R. Nagarajan, *Organizer, Presiding*

8:30 COLL 31. Hybrid dual-functional Ag@Au based nanofilms with high sensitivity for in-situ SERS monitoring of catalytic reaction. **S. He**, F. Tian

8:50 COLL 32. Degradation studies on organophosphate methyl parathion mediated by silver-titania core-shell nanoparticles. **S. Talebzadeh Farooji**, F. Forato, B. Bujoli, S. Trammell, S. Grolleau, H. Pal, c. queffelec, D. Knight

9:10 COLL 33. Self-assembled monolayer of 2D metal oxides: Applications in gas sensing. **J. Miao**, L. Meng, C. Chen, J.Y. Lin

9:30 COLL 34. Hydrophilic/hydrophobic self-converting nanoreactors. **H. Jia**, J. Gohy

9:50 COLL 35. Encoding molecular information to plasmonic gold nanostars for anti-counterfeiting. **Y. Huo**, S. Curry, C. Jiang



TECHNICAL PROGRAM

10:10 COLL 36. Constructing transferrable electronics on functionalized graphene. **K.E. Whitener**, W. Lee, J.T. Robinson, P. Sheehan

10:30 COLL 37. Impact of solvent quality on graphene transfer process: Toward optimizing graphene transfer onto transparent polymer films. **A.J. Carr**, J. Andrade, S. Bhatia, M. Eisaman

10:50 COLL 38. Highly stable boron nitride nanotube (BNNT) dispersions and pastes for thin film coatings and fibers. **H. Lim**, B.J. Kim, S. Jang

11:10 COLL 39. Paper-derived SiC sheet with high-density stacking faults for high-performance electromagnetic wave absorption. **Z. Wang**

11:30 COLL 40. Gate-enhanced photocurrent of (6,5) single-walled carbon nanotube based field effect transistor. **K. Park**, S. Lee, F. Toshimitsu, J. Lee, S. Park, T. Fujigaya, J. Jang

Section F

Orange County Convention Center
West Hall B4 - Theater 6

Surface Chemistry

Growth, Reactivity & Catalysis

S. L. Tait, *Organizer*

N. Baig, A. V. Teplyakov, *Presiding*

8:30 COLL 41. Surface chemistry of metal deposition and atomic layer etching. **A.V. Teplyakov**

8:50 COLL 42. Epitaxial growth and characterization of Ru (0001) supported hexagonal MoN thin films. **A. Khaniya**, M. Sajid, W. Kaden

9:10 COLL 43. Electrochemical control of the thermal stability of atomically thin Ag films on Au(111). **J. Phillips**, L.K. Harville, H. Morgan, L.E. Jackson, G. LeBlanc, E.V. Iski

9:30 COLL 44. Electrochemically generated superhydrophobic meshes for efficient separation of oil from water. **N. Baig**, T. A. Saleh

9:50 COLL 45. Computational modeling of graphene oxidation. **J. Graña-Otero**, S. Schmitt, A. Kumar

10:10 COLL 46. Dynamic adsorption of airborne contaminants on graphite. **M. Salim**, M. Montgomery, H. Liu

10:30 COLL 47. Local changes to the structure and chemistry of thick MoS₂ flakes due to heating. U. Ukegbu, W. Spychalski, M. Pisarek, **R. Szoszkiewicz**

10:50 Intermission.

11:00 COLL 48. Copper-supported single layer MoS₂ for higher alcohol synthesis from syngas: A DFT + kMC study. T.B. Rawal, **D. Le**, T.S. Rahman



TECHNICAL PROGRAM

11:20 COLL 49. Theoretical study on the conversion mechanism of methane on surface single atom catalysts. **Y. Liu**

11:40 COLL 50. Key details of nerve-agent decomposition on single site Zr-based polyoxometalates revealed by a correlated multimodal approach. **Y. Tian**, A. Plonka, A. Ebrahim, R. Palomino, S.D. Senanayake, A. Balboa, W.O. Gordon, D. Troya, J. Musaev, J.R. Morris, M.B. Mitchell, D. Collins-Wildman, C.L. Hill, A. Frenkel

12:00 COLL 51. Investing MOFs as a potential filtration media for the adsorption and decontamination of chemical warfare agents using *operando* synchrotron techniques. **A. Ebrahim**, A. Plonka, Y. Tian, A. Frenkel

Section G

Orange County Convention Center
West Hall B4 - Theater 7

Colloidal Nanoparticle Synthesis & Assembly

O. Chen, T. Li, *Organizers*
F. Bai, H. Fan, *Organizers, Presiding*

8:30 COLL 52. Synthesis and assembly of dendrimer-nanocrystal hybrid superstructures. **C.B. Murray**, K.C. Elbert, D. Jishkariani, N. Gogotsi, J. Park, H. Zhang, M.M. Taheri, J.B. Baxter

9:00 COLL 53. Mechanism of nanocrystal self-assembly at an interface, followed by oriented attachment. **D. Vanmaekelbergh**

9:30 COLL 54. N- and P-doped colloidal nanocrystal and nanowire assemblies. **C.R. Kagan**

10:00 Intermission.

10:10 COLL 55. Synthesis and plasmonic properties of colloidal metal oxide nanocubes. **D.J. Milliron**

10:40 COLL 56. *In situ* observation of nanocrystal chemistry. **H. Weller**

11:10 COLL 57. Synthesis and properties of imperfect nanomaterials. **E. Shevchenko**

11:40 COLL 58. Stoichiometric preparations of iron oleate to improve the reproducibility of iron oxide nanoparticle syntheses. **D. Huber**, S. Ivanov, E.C. Vreeland, J.D. Watt

Section H

Orange County Convention Center
West Hall B4 - Theater 8

Biomembrane Synthesis, Structure, Mechanics & Dynamics

J. Katsaras, S. Muralidharan, M. Nieh, A. N. Parikh, *Organizers*
M. L. Longo, J. Nickels, *Presiding*



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

8:30 COLL 59. Molecular simulations of separations of enantiomer using chiral stationary phases. **X. Wang**, C. Jameson, S. Murad

8:50 COLL 60. Dynamics of phospholipid membranes beyond thermal undulations. **G.J. Schneider**, S. Gupta, J.U. De Mel, R. Perera

9:15 COLL 61. Peptoid structure impacts adsorption of water-soluble peptoids to lipid bilayers. **G.Y. Stokes**, A.A. Fuller, M.R. Landry, J. Rangel, V. Dao, M.A. MacKenzie, A. Calkins, F.L. Gutierrez

9:40 COLL 62. Lipid motion reflects additive-induced effects on the dynamic and phase state of phospholipid membranes. **E. Mamontov**, V. Sharma

10:05 COLL 63. Vascular smooth muscle cells: Key players in arterial aging. **A. Trache**, H. Sreenivasappa, S. Padgham, S. Shin, J. Trzeciakowski, C. Woodman

10:30 COLL 64. Liposome delivery and release driven by molecular recognition. **M. Best**, J. Lou, X. Zhang, A.J. Carr, A.J. Watson

10:55 COLL 65. Solute partitioning and solvation in lipid membranes: Microscopic origins of bioaccumulation. **R.A. Walker**, C.A. Gobrogge, K. Duncan

11:20 COLL 66. Dynamic interplay between PA and DGPP regulates lipid negative charge and protein-lipid interactions. **E. Kooijman**

11:45 COLL 67. From lipid vesicles to lipid onions: A molecular-dynamics simulation study. **J. Carrillo**, D. Bolmatov, M. Lavrentovich, J. Katsaras, B. Sumpter

Section I

Orange County Convention Center
West Hall B4 - Theater 9

Surface Chemistry of Colloidal Nanocrystals

S. Neretina, D. Qin, *Organizers*
J. Chen, X. Xia, *Organizers, Presiding*

8:30 COLL 68. Porous shells on gold nanorods. **C.J. Murphy**

9:00 COLL 69. Impact of surface chemistry in multimetallic nanoparticle synthesis and performance. **J. Millstone**

9:30 COLL 70. Deconstructing nanoconstructs. **T.W. Odom**

10:00 Intermission.

10:15 COLL 71. Crystal growth and surface chemistry of metal halide perovskite nanomaterials. **S. Jin**, M. Hautzinger

10:45 COLL 72. Surface versus solution chemistry: Manipulating nanoparticle shape and composition through metal-thiolate interactions. **S.E. Skrabalak**



TECHNICAL PROGRAM

11:15 COLL 73. Leaching of metal nanostructures through oxidative etching and its influence on the catalytic reduction of 4-nitrophenol. **R. Hughes**, R.D. Neal, T.D. Demille, S. Neretina

Engineered Lignocellulosic Materials & Multiphase Systems: Anselme Payen Award Symposium in Honor of Orlando Rojas

Sustainable Nanofibers

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Molecular Processes at Mineral-Water Interfaces: Predictions via Linking Theory & Experiments

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SUNDAY AFTERNOON

Section A

Orange County Convention Center
West Hall B4 - Theater 1

Understanding the Inorganic-Organic Interface in Colloidal Nanomaterials

Ligand Arrangements

H. M. Mattoussi, V. M. Rotello, *Organizers*
C. J. Murphy, J. S. Owen, *Presiding*

2:00 COLL 74. Surface chemistry of colloidal lead halide perovskite nanocrystals. **M. Kovalenko**

2:30 COLL 75. Characterizing the organic coating of quantum dots using NMR spectroscopy. C. Zhang, G. Palui, **H.M. Mattoussi**



TECHNICAL PROGRAM

2:50 COLL 76. Dynamic ligand exchange and surface charge density modulate the optical properties of CdSe quantum dots in water as a function of pH. **D.E. Westmoreland**, E. Weiss

3:10 COLL 77. Gold nanoparticle-blood serum interaction assay reveals humoral immunity development and immune status of animals from neonates to adults. **Q. Huo**, T. Zheng

3:30 Intermission.

3:50 COLL 78. Affinity of neutral Lewis bases and ion pairs for colloidal nanocrystal surfaces. N.C. Anderson, P. Chen, J. De Roo, **J.S. Owen**

4:20 COLL 79. Optoelectronic impacts of surface chemistry in small noble metal nanoparticles. **J. Millstone**

Section B

Orange County Convention Center
West Hall B4 - Theater 2

Biomaterials & Biointerfaces

Immuno & Adhesive Materials

Y. Lapitsky, R. Wylie, *Organizers, Presiding*

2:00 COLL 80. Enhancing humoral immunity to subunit vaccines through engineered immunogen binding to aluminum hydroxide adjuvant. **D.J. Irvine**

2:30 COLL 81. Engineered materials as tools to study immune function. **C. Jewell**

3:00 COLL 82. Nanoparticle immunotherapy: Towards a cancer-curative vaccine. **A. Nouredine**, L. Tang, R. Serda, J. Brinker

3:20 COLL 83. Macrophage-mediated delivery of bioorthogonal nanozymes for targeted cancer therapy. **R. Das**, J. Hardie, M.E. Farkas, V.M. Rotello

3:40 COLL 84. Long term delivery of antibodies from hydrogels for local cancer immunotherapy. **V. Huynh**, R. Wylie

4:00 COLL 85. Electrical “suturing” of polyelectrolyte hydrogels to reseal cut or damaged tissues. **L.K. Borden**, A. Gargava, S.R. Raghavan

4:20 COLL 86. Thermo-reversible bioadhesives based on cohesive failure. **B. Li**, M.E. Thompson

Section C

Orange County Convention Center
West Hall B4 - Theater 3

Quantitative Particle Cell Interaction



TECHNICAL PROGRAM

N. Feliu, L. Liz Marzan, W. J. Parak, *Organizers, Presiding*

2:00 COLL 87. State of nanoparticle active tumour cell targeting. **W. Chan**

2:30 COLL 88. Protein nanoparticles as multifunctional drug delivery carriers. **J. Lahann**

3:00 COLL 89. Ultrafast single micron to sub-micron particle detection method based on a half-bowtie coplanar waveguide. **R. Blick**, P. Gwozdz, A. Bhat, A. Guse, B. Diercks, L.C. Hernandez, U. Singh

3:30 COLL 90. How does nano-silver get inside bacteria? Mechanistic studies using AgAu alloy nanoparticles. **C. Rehbock**, C. Streich, J. Jakobi, S. Grade, M. Kühnel, V. Migunov, T. Knura, B. Sures, m. Stiesch, S. Barcikowski

3:50 COLL 91. Nanotoxicology: Exploring nanoparticle-model membrane interactions. C. Bailey-Hytholt., E. Kamaloo, K. Waterman, K. Swana, T.A. Camesano, **R. Nagarajan**

4:20 COLL 92. Multi-hierarchically profiling the biological effects of various metal-based nanoparticles in macrophages under low-exposure doses. **S. Liu**

4:50 COLL 93. Degradation of hybrid nanoparticles. **W.J. Parak**

5:10 COLL 94. Human serum protein coronas greater alter interactions between nanoparticles and a model red blood cell membrane. **G.D. Bothun**, N. Ganji

Section D

Orange County Convention Center
West Hall B4 - Theater 4

Novel Functionalization Methods for Textiles & Fibers

N. Pomerantz, M. Richards, *Organizers, Presiding*

2:00 COLL 95. Ionically crosslinked polymers for antimicrobial textiles. **H.B. Nulwala**, X. Zhou

2:30 COLL 96. Preparation of functional polymers and fibers through controlled radical graft polymerization processes. **G. Sun**

3:00 COLL 97. 3-Mercapto-1,2-propanediol modified robust polyester nonwoven for stabilization of zero-valent iron nanoparticles for multifunctional application. **M. Morshed**, N. Behary, N. Bouazizi, V. Nierstrasz

3:30 COLL 98. Perfluoropolyether-based molecular bottlebrush as water/oil repellent additive for fiber forming thermoplastics. **L. Wei**, P. Brown, I.A. Luzinov

4:00 COLL 99. Environmentally-friendly superhydrophobic and superoleophobic fabrics prepared from water-based suspensions. **R. Cai**, B. Nysten, K. Glinel, A.M. Jonas

4:30 COLL 100. Superhydrophilic, wrinkle-free cotton fabrics via plasma and nanofluid treatment. **L. Lao**, L. Fu, G. Qi, E.P. Giannelis, J. Fan



TECHNICAL PROGRAM

5:00 COLL 101. Microencapsulation of natural insect repellents for protective coatings on fabrics. **J.D. Ogilvie-Battersby**, R. Sharma, N. Orbey, R. Nagarajan, J. Kumar, R. Mosurkal

Section E

Orange County Convention Center
West Hall B4 - Theater 5

Nanomaterials

J. A. Hollingsworth, R. Nagarajan, *Organizers*
C. Shih, *Presiding*

2:00 COLL 102. Interfacial self-assembly of hierarchically structured nanoparticles with photocatalytic activity. **H. Fan**

2:30 COLL 103. Photophysics and electronic structure of metal-organic frameworks. **N.B. Shustova**

3:00 COLL 104. Structural and mechanical properties of self-supporting covalent organic framework membranes obtained via two different preparation routes. N. Turangan, Y. Xu, H. Spratt, L. Rintoul, S. Bottle, **J. MacLeod**

3:20 COLL 105. Rigid rod vs semiflexible chain construction through connection of computationally designed coiled coil peptides using Thiol-Michael *click* reaction. **N. Sinha**, D. Wu, R. Guo, C.J. Kloxin, J.G. Saven, D.J. Pochan

3:40 COLL 106. Locking-in 1-dimensional π -conjugated superstructures to regulate the formation of well-defined nanoscale objects. A. Ashcraft, c. Liu, K. Liu, A. Mukhopadhyay, T. Phan, D. Husainy, **O. Jean-Hubert**

4:00 COLL 107. Controllable, wide-ranging n- and p-doping of monolayer transition-metal disulfides and diselenides. **S. Zhang**, H.M. Hill, A.R. Hight Walker, S. Barlow, S.R. Marder, S.J. Pookpanratana, C.A. Hacker

4:20 COLL 108. Continuous and ultrafast production of exfoliated 2D nanomaterials using compressible flows. M. Islam, R. Sheikh, M. Islam, D. Messer, **R. Rizvi**

4:40 COLL 109. Fluid-like reconfigurable graphene matrix with superlubricity. **I. Jeon**, T.M. Swager

5:00 COLL 110. Dispersion, characterization, and diffusion of boron-nitride nanotubes in water. A.D. Smith McWilliams, Z. Tang, C. de los Reyes, S. Ergulen, M. Pasquali, **A.A. Marti**

Section F

Orange County Convention Center
West Hall B4 - Theater 6

Supramolecular Assemblies at Surfaces: Non-covalent, Covalent & Coordination Bonding

Cooperative Self-Assembly

F. Rosei, S. L. Tait, *Organizers*
U. Mazur, M. Stoehr, *Presiding*



TECHNICAL PROGRAM

2:00 Introductory Remarks.

2:10 **COLL 111.** Temperature-induced transformation of amphiphilic thermo-sensitive hyperbranched poly(ionic liquid)s. **H. Lee**, V. Korolovych, A. Erwin, O. Stryutsky, V. Shevchenko, V.V. Tsukruk

2:30 **COLL 112.** Counting charges on surface-bound peptides. **F. Geiger**

2:50 **COLL 113.** Parent Zn and Ni metalloporphyrins form bilayers at the air/water interface. M. Jovanovic, V. Schlutz, J. Bozzone, W. Bu, T.F. Magnera, P.I. Dron, **J. Michl**

3:20 Intermission.

3:40 **COLL 114.** On-surface assembly and reactivity of oligo/polythiophenes. **D.F. Perepichka**

4:10 **COLL 115.** Standing, lying, and sitting: Unique properties of diyne phospholipid striped phases in templating inorganic and organic nanomaterials. **S.A. Claridge**

4:40 **COLL 116.** Leveraging a step-wise, sequence-specific synthesis of shape-persistent macrocycles to control hierarchical self-assembly on surfaces. **J. Dobscha**, A.H. Flood

5:00 **COLL 117.** BioNanoarchitectonics and the dynamics of *alive* functional surfaces. **M. Lingenfelder**

5:30 **COLL 118.** Puzzling electrical conduction in ionic surface channels fabricated by interfacial electron beam chemical patterning of highly ordered *n*-alkylsilane monolayers on silicon - a synthetic single-layer material. R. Maoz, B. Gogoi, **J. Sagiv**

Section G

Orange County Convention Center
West Hall B4 - Theater 7

Colloidal Nanoparticle Synthesis & Assembly

F. Bai, O. Chen, *Organizers*
H. Fan, T. Li, *Organizers, Presiding*

2:00 **COLL 119.** From colloidal synthesis to integration: Hybrid materials for infrared nanophotonics. **J.A. Hollingsworth**

2:30 **COLL 120.** Colloidal CdSe 0-dimension nanocrystals and their self-assembled 2-dimension structures. **K. Yu**

3:00 **COLL 121.** Colloidal superparticles from crystallization of artificial atoms. **Y. Cao**

3:30 **COLL 122.** Looking at lead salt nanocrystals one by one at low temperature and under high magnetic field. **H. Htoon**

4:00 Intermission.

4:10 **COLL 123.** Orientational order in self-assembled nanocrystal superlattices. **M. Gruenwald**, Z. Fan



TECHNICAL PROGRAM

4:40 COLL 124. Aptamer-based rapid whole cell detection and quantification of pathogens. **L. Stanciu**

5:10 COLL 125. Safe-by-design hybrid nanoparticles of antimicrobial silver, aminocellulose, and quorum quenching acylase eradicate bacteria and their biofilms. **A. Ivanova**, K. Ivanova, T.J. Heinze, T. Tzanov

Section H

Orange County Convention Center
West Hall B4 - Theater 8

Biomembrane Synthesis, Structure, Mechanics & Dynamics

J. Katsaras, M. Nieh, A. N. Parikh, *Organizers*
S. Muralidharan, *Organizer, Presiding*
A. B. Subramaniam, *Presiding*

2:00 COLL 126. Understanding the dynamics of phospholipid membranes using field cycling NMR. **J.U. De Mel**, M. Rosenberg, S. Gupta, M. Hofmann, M.F. Roberts, G. Schneider

2:20 COLL 127. Light triggered, cell-specific liposome fusion and drug delivery *in vivo*. **A. Kros**

2:45 COLL 128. Functional biomembranes entrapped within mesoporous silica and titania gels. W. Zeno, K. Johnson, S. Gakhar, C. Tan, S. Risbud, **M.L. Longo**

3:10 COLL 129. Functionalized lipid carriers for nucleic-acid and drug therapeutics. **C.R. Safinya**, V.M. Steffes, E.A. Wonder, K.K. Ewert

3:35 COLL 130. Stressful process of patterning fluid-solid membrane domains. **M.M. Santore**

4:00 COLL 131. Lateral organization in live cells and model biomembranes. **J. Nickels**

4:25 COLL 132. Phase-forming mechanism in multicomponent lipid mixtures. **M. Zhernenkov**

4:50 COLL 133. Undulated films of conformationally asymmetric binary lipids and polymer blends. **R. Kumar**

Section I

Orange County Convention Center
West Hall B4 - Theater 9

Surface Chemistry of Colloidal Nanocrystals

J. Chen, D. Qin, X. Xia, *Organizers*
S. Neretina, *Organizer, Presiding*

2:00 COLL 134. High-index facet particle shape regulation by dealloying. **C.A. Mirkin**



TECHNICAL PROGRAM

3:00 COLL 135. Controlling the surface of dilute bimetallic nanoparticles via halide-mediated metal ion reduction. **M.L. Personick**

3:30 Intermission.

3:45 COLL 136. Engineering of colloidal nanocrystals for multifunctional coatings. **H. Fan**

4:15 COLL 137. Chemical potential of metal atoms in supported and unsupported nanoparticles: Dependence upon particle size and support. **C.T. Campbell**

4:45 COLL 138. Spectral-selective plasmonic polymer nanocomposites. **G. Liu, A.U. Khan, Y. Guo, X. Chen**

Engineered Lignocellulosic Materials & Multiphase Systems: Anselme Payen Award Symposium in Honor of Orlando Rojas

Cellulose Nanocrystals Enabling Sustainable Materials

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SUNDAY EVENING

Section A

Orange County Convention Center
West Hall C

Fundamental Research in Colloids, Surfaces & Nanomaterials

R. Nagarajan, *Organizer*



TECHNICAL PROGRAM

6:00 - 8:00

COLL 139. Preparation and characterization of a new erlotinib polymorph. **S.A. Nickel**, R. Quinones

COLL 140. Manipulation of gold nanostructures for imaging applications using a single-beam optical trap. **K. Langford**, K. Meyers, T. Szekerczes, **M. Devadas**

COLL 141. Modification of Inorganic Oxides with Poly(hydridomethyl)siloxanes as an Approach to Mixed Functional Surfaces. **G. Fardella**, **R. Perez**, J.W. Krumpfer

COLL 142. Solution-based green amplified spontaneous emission from colloidal perovskite nanocrystals exhibiting high stability. **J. Tan**, Y. Wang, Y. Chan

COLL 143. Graphene oxide-metal hybrid systems for sensing and catalysis. **H. Kelani**, **M. Devadas**

COLL 144. Synthesis and characterization of a conductive biomimetic hydrogel nanocomposite for responsive wound management technologies. **A.N. Linhart**, W. Chura, J.J. Keleher

COLL 145. pH-Responsive nanoparticle embedded catalysts for imaging of biofilm-associated infections. **A. Gupta**, R. Das, V.M. Rotello

COLL 146. Sum frequency generation imaging microscopy of self-assembled monolayers on metal surfaces: Factor analysis of multicomponent mix monolayers. **A. Pikalov**, D.T. Ngo, H. Lee, T. Lee, S. Baldelli

COLL 147. Preparation of sol-gel GeO₂ and GeO₂-SiO₂ nanoparticles for use in 3D printed optics. **A.C. Vahle**, J.F. Destino

COLL 148. Biomimetic, peptide-directed synthesis of size-controlled iron oxide nanoparticles. **A. Eyler**, L. Leon

COLL 149. Synthesis, modification, and integrity of zinc oxide nanoparticles for RNA delivery. **A. Freese**, C. Hernandez, A. Wanekaya

COLL 150. Development of pH-responsive microgels for nanoparticle-based detection methodologies. **A. Silva**, **J. Lo**, S.R. Emory, D.A. Rider

COLL 151. Tailoring the material properties of surface-anchored metal-organic frameworks. **A.J. VanZanten**, A.J. Osterbaan, M.J. Maraugh, A.E. Trojniak, M.E. Anderson

COLL 152. Silver selenide nanoparticles as a gateway to diverse quantum dot compositions. **A. Fall**, P.G. Van Patten

COLL 153. High-precision measurements of the surface tension and viscosity of high-viscosity liquids using surface light scattering spectroscopy and pendant drop tensiometry. **A.R. Titus**, N.K. Thapa, E. Mann, E. Kooijman

COLL 154. Modification of silica surface by Suzuki coupling. **A.A. Kuvayskaya**, A. Vasiliev

COLL 155. Self-assembly of micron-sized polystyrene colloids via Langmuir-Blodgett technique for highly reproducible fabrication of large-area gold microcavity arrays. **A. Schaum**, A. Baride, P. May

COLL 156. Synthesis of FeCo nanoparticles for magnetic hyperthermia. **A. Sergides**, A. LaGrow, P. Lecante, C. Amiens, N. Thanh



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- COLL 157.** Chemically modified titanium boride nanosheets: High yield synthesis and macrostructure assembly. **A.L. James**, M. Lenka, N. Pandey, K. Jasuja
- COLL 158.** NaYF₄: Yb, Er upconversion nanoparticles (UCNPs) with an active NaYF₄: Yb, Nd shell for dual-wavelength excitation. **A. Chov**, P. May, A. Baride
- COLL 159.** Investigating the physical and electrical properties of copper-paddlewheel surface-anchored metal-organic frameworks. **A.E. Trojniak**, **M.J. Maraugh**, A.J. VanZanten, A.J. Osterbaan, M.E. Anderson
- COLL 160.** Antibacterial coating on aluminum alloy: SERS detection. **B. Baruah**
- COLL 161.** Switchable single-walled carbon nanotube-polymer composites for CO₂ sensing. **B. Yoon**, S. Choi, T.M. Swager, G.F. Walsh
- COLL 162.** Fabrication and application of aluminum nanocrescents for surface enhanced infrared absorption spectroscopy. **C. Coplan**, M.M. Swartz, J.S. Shumaker-Parry
- COLL 163.** Identifying critical parameters of silica coating of silver nanoparticles using ruggedness test. **C. Jabs**, M.M. Roca
- COLL 164.** Novel statistical analysis of Langmuir monolayers. L.W. Stephenson, **C. Van Cleave**, B.J. Peters, D.C. Crick, D.C. Crans, J.L. Sharp
- COLL 165.** Manipulating plasmon resonances in In₂O₃ by bandgap tuning and dual-doping. **C.R. Conti**, D.A. Hardy, G.F. Strouse
- COLL 166.** Multi-functional coatings formed from the electrostatic self-assembly of glycerol-based carbon nanoparticles and *Moringa oleifera* Cationic Protein (MOCP). **C.B. Perry**, F. Webster
- COLL 167.** Carbon-dots-based biosensors for the selective detection of biomarkers. **C. Choi**, S. Jeon, T. Kang, L. SIN, J. Kim
- COLL 168.** Study the energy transfer in organic-inorganic two-dimensional hybrid materials. **C. Liao**, J. Phan, M. Herrera, M.A. Mahmoud
- COLL 169.** Study of the influence of antifoaming additives on the crude oil/air interface by rheology. **C.E. Mansur**, M. Mendes, L. Palermo
- COLL 170.** Electrochemical scanning tunneling microscopy studies on the adsorption and assembly of benzenecarboxylic acids at electrode/electrolyte interfaces. **C. Leasor**
- COLL 171.** Programmable self-assembly of functionalized tricarbazolo triazolophane macrocycles at interfaces. **C. Trainor**, H.D. Castillo, J. Dobscha, A.H. Flood, S.L. Tait
- COLL 172.** Synthesis mechanism of mesoporous titanium dioxide from industrial titanyl sulfate solution. **C. Tian**
- COLL 173.** Analyzing molecular structure of liquid crystals to develop wavelength independent films to mitigate laser attacks on aircraft. **D. Maurer**, P. Nevarez, J. Hofmann, J.J. Keleher



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- COLL 174.** Probing the influence of surface dipoles on the structure of contacting liquids with sum frequency generation spectroscopy. **D. Rodriguez**, M.D. Marquez, O. Zenasni, T. Lee, S. Baldelli
- COLL 175.** Silver nanowire/graphene oxide conducting films on antireflective/superhydrophilic substrates. **D.W. Fox**, A. Schropp
- COLL 176.** Synthesis and nanopatterning of core-shell nanoparticles encapsulated with porphyrins. **D. Hebert**, N. Kuruppu Arachchige, J.C. Garno
- COLL 177.** Selective electrodeposition of polyaniline on transparent indium tin oxide electrodes using magnetic nanoparticles and magnet arrays. **D. Wirth**, G. LeBlanc, K. Burch, M.J. Petty
- COLL 178.** Preserving silver nanoparticle color in solutions and films using silica coating. **D. Donelson**, M.M. Roca
- COLL 179.** Novel patterning method of silver nanowire-based transparent electrode by selective hydrophilic treatment of substrate. **D. Ko**, S. Chu, Y. Ma, G. Sim, J. Kim
- COLL 180.** Dewetting conditions and morphologies of poly(vinyl alcohol) thin films fabricated on polydimethylsiloxane substrates. **E. Hazen**, W. Chen
- COLL 181.** Amphiphilic peptoid polymers for directing the assembly of gold nanoparticles at the oil-water interface. **E.J. Robertson**, H. Paneth, E. Whitney
- COLL 182.** Examining the effect of functional groups on ligand substitution dynamics. **E.A. Reasoner**, B. Nelson, M. Wilker
- COLL 183.** Road to custom engineered nanocrystal surface chemistry: Changes without exchanges. **E. Little**, J. Niezgoda
- COLL 184.** Mechanical properties of soft samples measured by AFM indentation: Effects of probe shape models. **F. Bodowara**, **B.B. Akhremitchev**
- COLL 185.** Polyethylene glycol and RGD immobilized binary colloidal crystal nanostructures as tunable substrates for cell culture. **F.S. Diba**, P. Wang, H. Thissen, P. Kingshott
- COLL 186.** Reduction of CO₂ on early Earth using UV radiation. **F. Ileaasu**, M. Dooling, S.E. Maurer
- COLL 187.** Fabrication and evaluation of hydrophobic anti-icing coating with thixotropic lubricant gel. **G. IMAI**, T. Yamazaki, H. Nakamura, S. Shiratori
- COLL 188.** Venturi effect: A novel way to obtain nanodispersions by solvent displacement. **G. Garcia Salazar**, D. Quintanar-Guerrero
- COLL 189.** Quantifying adsorption of chlorpromazine and clozapine to phospholipid membranes using second-harmonic generation. **G.E. Gadbois**, C.A. Read, G.Y. Stokes
- COLL 190.** Solution-phase synthesis and thermoelectric characterization of n- and p-type tetrahedrite nanoparticles. **G. Kunkel**, J.P. Rogers, D.P. Weller, D.T. Morelli, M.E. Anderson
- COLL 191.** Investigating nanoparticle-protein interactions with hybrid lipid-coated gold nanoparticles. **G.W. Marquart**, F. Zhou, M.R. Mackiewicz



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- COLL 192.** Investigating adsorption dynamics of serum proteins onto gold nanoparticles. **G. Ruiz**, N. Ryan, J.D. Driskell
- COLL 193.** Sonochemical functionalization of boron nitride nanomaterials. **H. Harrison**, A. Kelkar, J. Alston
- COLL 194.** Hydrogel-stabilized radioluminescent colloidal crystalline arrays: Fine-tuning color characteristics via Förster Resonance Energy Transfer (FRET) pairing. **H.W. Jones**, M. Burdette, I. Bandera, S.H. Foulger
- COLL 195.** Design of cholera toxin B-conjugated gold nanoparticles to target retinal ganglion cells in the eye. **H. Sawab**, M.R. Mackiewicz
- COLL 196.** Magnetic microdroplets as a method to extract antibodies from their growth media. **H.H. Al-Terke**
- COLL 197.** Teasing apart how specific features of silver nanoparticles contribute to toxicity. **H. Wu**, A. Engstrom, B. Harper, S. Harper, M.R. Mackiewicz
- COLL 198.** Colloidal synthesis of hexagonal FeIn₂S₄ and its layer-dependent band structures. **H. Kim**, h. LEE
- COLL 199.** UiO-66-NH₂ on functionalized graphene oxide (GO). **H. Jung**, S. Jang, Y. Jin, H. Jung
- COLL 200.** Surface growth of UiO-66-NH₂ on cotton fabric for toxic chemical degradation. **H. Jung**, M. Kim, S. Ryu, M. Park
- COLL 201.** Investigation of the effects on stability of silver nanoparticles. **I.I. Niyonshuti**, M. Alqahtany, Y. Wang, J. Chen
- COLL 202.** Calcium-triggered release of contents from liposomes for drug delivery applications. **J. Lou**, A.J. Carr, A.J. Watson, S.I. Mattern-Schain, M. Best
- COLL 203.** Dopamine surface adhesion via spin casting. **J. Byun**, Y. Zhou, M. Le, W. Chen
- COLL 204.** Thermoelectric characterization and thermostability of doped-tetrahedrite nanoparticles synthesized by modified polyol process. **J.P. Rogers**, **E. Garcia-Ponte**, G. Kunkel, D.P. Weller, D.T. Morelli, M.E. Anderson
- COLL 205.** Tyrosine-assisted fluorescent gold nanoclusters for sensing Fe³⁺ and Cu²⁺. **J. Youn**, P. Kim, P. Kang, Z. Qin, J. Lee
- COLL 206.** Synergistic oxygen generation of manganese ferrite and ceria nanoparticles potentiates M2 polarization of macrophages for rheumatoid arthritis treatment. **J. Kim**
- COLL 207.** Monitoring reactive oxygen species production at the single DNA level. **J.R. Pyle**, J. Chen
- COLL 208.** Validating Raman spectroscopy for the detection of surface molecules on silver nanoparticles. **J. Danischewski**, M.M. Roca
- COLL 209.** Gold nanoparticle colorimetric detection of estrogen and estrogen mimics. **J.M. Montgomery**, A. Stadler
- COLL 210.** Preparation of a glycerol-based carbon / magnetic iron nanocomposite for the removal of contaminants in aqueous systems. **J. Daniels**, F. Webster



TECHNICAL PROGRAM

- COLL 211.** Interaction of molecular oxygen with surface defects on single-particle organolead halide perovskites. **J.R. Vicente**
- COLL 212.** Characterization of yellow-colored colloids in the Manasquan Watershed, NJ. **J. Ha**
- COLL 213.** Metal-assisted and microwave-accelerated germination. J. Guy, M. Stevenson, A. Souffrant, A. Bigio, E. Bonyi, **K. Aslan**
- COLL 214.** Metal-assisted and microwave-accelerated decrystallization of pseudo-tophaceous aggregates in human joint models. **K. Aslan, Z. Boone-kukoyi**, K. Moody, C. Nwawulu, R. Auriori, H. Ajifa, G. McLemore
- COLL 215.** Magnetism and luminescence property of Mn²⁺-doped and Cu⁺ doped (CdSe)₁₃ clusters. **K. Tsai, Y. Liu**
- COLL 216.** Uncovering key nanoparticle/chemistry adsorption mechanisms relevant to shallow trench isolation (STI) and copper (Cu) chemical mechanical planarization (CMP) performance. **K.M. Wortman-Otto, A.M. Mikos**, C.F. Graverson, J.J. Keleher
- COLL 217.** Multi-point alignment of 6,5 carbon nanotubes on DNA origami substrates. **K. Pitton**, D. Neff, **M.L. Norton**
- COLL 218.** Photo-degradation of organic contaminants using a novel nano-carbon / TiO₂ layer-by-layer composite. **K.M. Mankowski**, F. Webster
- COLL 219.** Predicting size dependence of CdSe quantum dot net charge using modified charge equilibration methods. N. Weeks, **K.C. Tvrđy**
- COLL 220.** Metal-assisted and microwave-accelerated treatment and prevention of bacterial infections. **K.E. Walker**, E. Bonyi, H. Ajifa, C. Nwawulu, R. Auriori, Z. Boone-Kukoyi, **K. Aslan**
- COLL 221.** Semiconducting Langmuir-Blodgett films of copper paddle-wheel frameworks. **K. Ishihara**, F. Tian
- COLL 222.** Effects of stabilizing ligands on nanoparticle sintering during calcination in supported nanoparticle catalysts. **K.N. Bryant**, S.R. Saunders
- COLL 223.** Time-resolved temperature measurements of gold nanorods on surfaces in different media. **K. Shrestha**, L. Khosravi Khorashad, H.H. Richardson
- COLL 224.** Patterned perovskite thin film and single microcrystal arrays on a chemically patterned flat substrate. **K. Sy Piecco**, J. Chen
- COLL 225.** 2D nanosheets with binding multivalency for the optical detection of pathogenic bacteria. **L. SIN**, T. Kang, I. Hwang, S. Jeon, C. Choi, J. Kim
- COLL 226.** Metal-ligand self-assembly on powdered supports: A novel strategy towards heterogeneous single-site catalysts. **L. Chen**, I.S. Ali, X. Zhou, G.E. Sterbinsky, S.L. Tait
- COLL 227.** Assembling gold nanorods using secondary structure transitions in electrostatically adsorbed poly-L-lysine. **L.B. Thompson**, C.F. Benstead, S.E. Kotchey, F.E. McFeaters
- COLL 228.** Emulsions stabilized by chemically heterogeneous nanoparticles. **L.D. Capre**, C. Acevedo



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- COLL 229.** Anion exchange and extinction coefficient determination of cesium lead halide nanocubes. **L. Holtzman**, R. Alam
- COLL 230.** CTAB-controlled silica coating on nanorods and its impact on surface plasmon resonance. **M. Wang**, **A. Hoff**, Y. Bao
- COLL 231.** Towards tunable nanostructures using electroactive amphiphiles. **M. Alotaibi**
- COLL 232.** Surface alignment transitions in liquid crystals induced by exposure to formaldehyde gas. M. Thomas, **M. Bedolla-Pantoja**
- COLL 233.** Exploiting directed assembly to obtain precise coupling between colloidal silica whispering gallery mode resonators. **M.J. Smith**, S. Yu, V.V. Tsukruk
- COLL 234.** Partial molar volumes and volume of mixing of salts and osmolytes. **M.M. Pozhilenko**, W.H. Vakay, Y. Zhang
- COLL 235.** Size control on zeolitic imidazolate framework-8 particles for gas sensing. **M. Weber**, T. Baker, C. Kwon, F. Tian
- COLL 236.** Shiga and cholera toxins induce roll-up of membranes. **M. Berg Klenow**, J. Camillus Jeppesen, A.C. Simonsen
- COLL 237.** Self-assembly of surfactants at air-liquid interfaces. **M. Khan**, U.I. Premadasa, K. Kotturi, E. Masson, K.A. Cimatu
- COLL 238.** End-group functionalized polymer ligands for QD-based luminescent solar concentrators. **M.C. Plummer**, Y. Chen, K. Koch, M. Boxx, D.L. Patrick, D.A. Rider
- COLL 239.** Improving the functionality of carbon dots via doping and functionalization. **M. Prado**
- COLL 240.** Deuterium NMR spectroscopy in colloid and surface chemistry. T.R. Molugu, S. Lee, K. Mallikarjunaiah, J. Kinnun, C. Job, H.I. Petrache, **M.F. Brown**
- COLL 241.** Quasielastic and elastic neutron scattering of membrane proteins. S.M. Perera, U. Chawla, U.R. Shrestha, D. Bhowmik, A.V. Struts, S. Qian, X. Chu, **M.F. Brown**
- COLL 242.** Flexible surface model for lipid-protein interactions. A.R. Eitel, S.D. Fried, S.M. Perera, N. Weerasinghe, C.E. Norris, A.V. Struts, **M.F. Brown**
- COLL 243.** CdSe quantum shells growth on CdS core nanocrystals. **M. Galindo**
- COLL 244.** Designing glycocalyx-mimetic interfaces for blood-contacting biomaterials: New insights from single-molecule microscopy. **M. Hedayati**, N. Rapp, D. Krapf, M. Kipper
- COLL 245.** Synthesis and characterization of Gd:InP/ZnS quantum dots for an MRI-active Parkinson's disease probe. **M. Duszynski**, M. Ellis, K. Fichter
- COLL 246.** Adsorption of water-soluble peptoids to synthetic phospholipid membranes monitored by Second Harmonic Generation (SHG). **M.A. MacKenzie**, J. Rangel, M.R. Landry, V. Dao, G.Y. Stokes



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

COLL 247. Zigzag-shaped silver nanoplates: Synthesis, growth mechanism, and their application to highly sensitive strain sensors. D. Kim, J. Kim, **M. Kim**

COLL 248. Metal nanocrystal-based sensing platform for the quantification of water in water-ethanol mixtures. D. Kim, **M. Kim**

COLL 249. Exciton dynamics in colloidal covalent organic frameworks. **N. Flanders**, A.M. Evans, M.S. Kirschner, L.X. Chen, W.R. Dichtel

COLL 250. Porphyrin macrocycles linked to surfaces by centrally coordinated Si-O bridges. **N. Kuruppu Arachchige**, P.C. Chambers, J.C. Garno

COLL 251. Tuning the sensing performance of multilayer plasmonic core-satellite assemblies for rapid detection of targets from lysed cells. **N. Le**, J. Chen, C. Peng, G. Ye

COLL 252. Influence of calcite on uranium(VI) sorption onto montmorillonite clay. **N. Hall**, A.C. Shaw, D.N. La, C. Tournassat, R.M. Tinnacher

COLL 253. Synthesis and design of biomimetic conductive nanocomposites to enhance key surface adsorption phenomena in microbial fuel cells. **N.E. Yuede**, A.D. Dunne, H.J. Khan, S.A. Boetscher, M.D. Puckett, J.J. Keleher

COLL 254. Comparing the optical properties of Au₂₅ icosahedral and bi-icosahedral clusters. **N. Hondrogiannis**, B. Hutson, **K. Langford**, **M. Devadas**

COLL 255. Self-assembled monolayer functionalization of gold nanostar particles with a custom designed carboxylate-terminated dithiol as a linker for bioconjugation. **P. Ansari**, T. Lee, R.C. Willson

COLL 256. Methane hydrate formation and dissociation: On the effects of different porous materials. **P. Rangsunvigit**

COLL 257. Synthesis of germanium nanoparticles by rapid inductive heating. **P. Sharma**

COLL 258. Effect of *Ficus tikoua* leaves extract as an eco-friendly inhibitor of carbon steel in HCl solution. **Q. Wang**, X. Li

COLL 259. Analyzing the surface Interactions of a myelin sheath Langmuir model membrane system with the addition of quercetin. **R. Book**, **M.L. Jarju**, A. Sostarecz

COLL 260. Heterogeneous catalytic upgrading of long-chain alkenones derived from microalgae. **R. Kowaleski**, R.H. Hagmann, G.W. O'Neil, M.E. Bussell

COLL 261. Transition metal mediated bioorthogonal catalysis with controlled localization and kinetics for nanotheranostics. **R. Das**, R.F. Landis, G.Y. Tonga, P. Puangpoy, M. Knapp, V.M. Rotello

COLL 262. Continuous and scalable synthesis of Pt multipods with enhanced electrocatalytic activity toward oxygen reduction reaction. **R. Chen**, Z. Cao, Z. Lyu, M. Xie, Y. Shi, Y. Xia

COLL 263. Study of structure-property relationships of methoxylated sucrose soyate polyol self-assembly. **R.P. Chitemere**, B. Rasulev, D.C. Webster, M.A. Quadir

COLL 264. Design of a supramolecular photocatalytic nanocomposite for the remediation of heterogenous wastewater. **S.J. Baker**, **J.L. Tabert**, F.M. Byrne, R.K. McDonough, J.J. Keleher



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- COLL 265.** Seed-mediated synthesis of bimetallic copper-nickel nanoparticles for catalysis. **S. Powell**, S. Jeong, X. Ye
- COLL 266.** Core-size conversion of plasmonic gold nanomolecules. **S. Eswaramoorthy**
- COLL 267.** Growth and characterization of bimetallic metallic-organic framework films. **S. Farzandh**, A. Brandt, E. Dolgoplova, O. Ejegbavwo, D.M. Shakya, N.B. Shustova, D.A. Chen
- COLL 268.** Tuning the surface ordering of self-assembled ionic surfactants on semiconducting single-walled carbon nanotubes: Concentration, tube diameter, and centerions. **S. Algoul**, S. Sengupta, T. Bui, L.A. Velarde
- COLL 269.** Stabilizing enzyme on carbon nanotubes with metal-organic frameworks for enzyme delivery and biocatalysis applications. **S. Neupane**, Y. Pan, Z. Yang
- COLL 270.** Immobilized antioxidants and their radical scavenging activity. **S. Muráth**, A. Szerlauth, D. Kádár, D. Sebök, I. Szilágyi
- COLL 271.** Dynamic self-assembly of quasi-1D and 3D structures in rotating fluids. **T. Lee**, K. Gizynski, Y. Sobolev, O. Cybulski, B.A. Grzybowski
- COLL 272.** Probing the interactions between polymeric filtration media and nanoparticle dispersions relevant to copper (Cu) Chemical Mechanical Planarization (CMP). **T. Zubi**, K.M. Wortman-Otto, C.F. Graverson, C. Saucedo, M.G. Salinas, J.J. Keleher
- COLL 273.** Self-assembly of functionalized carbon nanoparticles on polyurethane foam for low-cost water purification. **T. Riffle**, F. Webster
- COLL 274.** Synthesis and antibacterial enhancement of biomimetic hydrogel matrices for wound management applications. **T.J. Beckmann**, D. Danhausen, W. Chura, J.J. Keleher
- COLL 275.** Investigating adsorption of methylene blue on single-walled carbon nanotubes using vibrational sum-frequency generation. **T.T. Bui**, S. Algoul, L.A. Velarde
- COLL 276.** Detection of mercury ion using surface functionalized gold nanorods. **t. Iuan**
- COLL 277.** Use of dynamic light scattering for accurate sizing of gold nanoparticles with particular application to chemical and biological sensing. **T. Zheng**, Q. Huo
- COLL 278.** Synthesis of all-inorganic Cd-doped CsPbCl₃ perovskite nanocrystals with dual-wavelength emission. **T. Cai**
- COLL 279.** Broad bandwidth excitation profile acquisition for interfacial rhodamine dyes by doubly resonant vibrational-electronic difference-frequency generation spectroscopy. **T.J. Santiago**, L.A. Velarde
- COLL 280.** Self-assembly, thermal properties and gelation studies of acridine based cholesteryl carbamate as low molecular mass gelators. **T. Sawyer**, A.V. Mallia
- COLL 281.** Fluorescence detection of Fe³⁺ using Salecan-derived nitrogen and phosphorus doped carbon dots and cell imaging. **W. Dong**, **G. Zuo**
- COLL 282.** Stability of spin cast poly(vinyl alcohol) thin films on polydimethylsiloxane. **W. Wang**, W. Chen



TECHNICAL PROGRAM

COLL 283. Assembly of amphiphilic homopolymers into controlled nanoscale particles. **W. Jang**, S. Swan, P.N. Eyimegwu, J. Kim

COLL 284. Functional dual drug-loaded dendrimer/carbon dot nanohybrids for cancer cell fluorescence imaging and enhanced therapy. D. Li, Y. Fan, M. Shen, **X. Shi**

COLL 285. Investigation of ceria-nickel-containing aerogels for catalytic converter applications. **X.P. Li**, M.K. Carroll, A.M. Anderson, B.A. Bruno

COLL 286. Boronic acid materials: Applications in glycoprotein recognition and enhanced cellular delivery. **X. Zhang**, D. Santana Alves, S. Zhang, S. Baek, F.N. Barrera, M. Best

COLL 287. Metal-ligand coordination for single-site catalysts on oxide surfaces. **X. Zhou**, S.L. Tait

COLL 288. Cr (VI) removal with porous Fe/C microspheres prepared from glycerol via ultrasonic spray pyrolysis. **Y. Cui**, J.D. Atkinson

COLL 289. Seed-mediated growth in shape-controlled synthesis of copper nanocrystals. **Z. Lyu**, Y. Xia

COLL 290. Simulations of grain boundaries between ordered colloidal hard sphere domains: Impurity and gravity confinement. **Z. Guo**, J. Kindt

Section B

Orange County Convention Center
West Hall C

Novel Functionalization Methods for Textiles & Fibers

Posters

N. Pomerantz, M. Richards, *Organizers*

6:00 - 8:00

COLL 291. Antimicrobial surface textile treatments. **C.S. Carfagna**

COLL 292. Novel durable, flame retardant textile treatments for nylon/cotton blends. **S. Beck**, F. Mazzini, A. Mullins, B.E. Koene

Section C

Orange County Convention Center
West Hall C

Supramolecular Assemblies at Surfaces: Non-covalent, Covalent & Coordination Bonding

Posters



TECHNICAL PROGRAM

F. Rosei, S. L. Tait, *Organizers*

6:00 - 8:00

COLL 293. Molecular self-assembly at surfaces: Dynamics, interactions, and design. **H.D. Castillo**, J.M. Espinosa Duran, S. Kim, J. Dobscha, S. Debnath, R.D. Mortensen, S.R. Schrecke, M. Lee, K. Raghavachari, A.H. Flood, D. Lee, P. Ortoleva, S.L. Tait

MONDAY MORNING

Section A

Orange County Convention Center
West Hall B4 - Theater 1

ACS Award in Surface Chemistry: Symposium in Honor of Hajo Freund

Cosponsored by CATL⁺ and PHYS
F. C. Calaza, W. Kaden, R. J. Meyer, A. Savara, *Organizers*
J. A. Boscoboinik, *Organizer, Presiding*
R. Meyer, *Presiding*

8:00 Intermission.

8:30 COLL 294. Interface materials on the nanoscale: Dominant media of chemical change and evolution. **G.A. Somorjai**

9:05 COLL 295. Heats of formation of adsorbed catalytic intermediates on well-defined surfaces by single crystal adsorption calorimetry. **C.T. Campbell**

9:40 COLL 296. Model interfaces constructed from ordered oxide films: From heterogeneous catalysis to electrocatalysis, photoelectrocatalysis, and organic-oxide hybrid materials. **J. Libuda**

10:15 Intermission.

10:35 COLL 297. Vinyl acetate formation pathways and selectivity on model metal and alloy catalyst surfaces. **W.T. Tysoe**

11:10 COLL 298. Polarons on TiO₂ and their affinity for water. **G. Thornton**

Section B

Orange County Convention Center
West Hall B4 - Theater 2

Biomaterials & Biointerfaces

Biomimetic & Bioactive Materials



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

Y. Lapitsky, R. Wylie, *Organizers, Presiding*

8:30 COLL 299. Bioinspired materials synthesis in microenvironments formed by liquid-liquid phase separation. **C.D. Keating**

9:00 COLL 300. Nature-inspired elastic capsules, tubes and hairy surfaces. **S.R. Raghavan**

9:30 COLL 301. Thermophoretic manipulation of biomaterials mechanical properties in microfluidics. **A. Kosmidis, D. Vigolo**

9:50 COLL 302. Integration of cells with silicon devices for *in vitro* tissue engineering of functional systems for preclinical drug discovery and toxicology. **J.J. Hickman**, C. Long, C. McAleer, C. Oleaga, J. Rumsey, A. Goswami, X. Guo, M.L. Shuler

10:10 COLL 303. Designing biomimetic interfaces for blood-contacting biomaterials: New insights from single-molecule microscopy. **M. Hedayati**, D. Krapf, M. Kipper

10:30 COLL 304. Studying the response of human macrophage-like cells to surface chemistry with diazonium-modified polystyrene substrates. **E. Buck**, S. Lee, L. Stone, M. Cerruti

10:50 COLL 305. Functional microgels for decoration of biointerfaces. **A. Pich**

11:10 COLL 306. Phase-separated liposomes for enhanced chemotherapeutic delivery. **A. Trementozzi**, Z.I. Imam, M. Mendicino, J. Stachowiak

Section C

Orange County Convention Center
West Hall B4 - Theater 3

Quantitative Particle Cell Interaction

N. Feliu, L. Liz Marzan, W. J. Parak, *Organizers, Presiding*

8:30 COLL 307. Enhanced delivery of quantum dots and gold nanocrystals to live cells. **H.M. Mattoussi**

9:00 COLL 308. Analytical ultracentrifugation of nanocrystals and fullerenes for biolabelling. **P. Mulvaney**

9:30 COLL 309. Gold nanoparticles for specific binding and internalization in cells. **A. Mews**, M. Mutas, L. Prisner, P. Witthöft, C. Strelow, T. Kipp

10:00 COLL 310. Gold nanoparticle-cell interactions. **A. Kanaras**

10:30 COLL 311. Plasmonic nanoparticle assemblies for real-time reaction monitoring. **X. Ling**

11:00 COLL 312. Surface modification strategies for interfacing metal nanoparticles with biological systems. **I. García**, M. Henriksen, J. Mosquera, J. Langer, L. Liz Marzan



TECHNICAL PROGRAM

11:30 COLL 313. Nanoparticle-cell interactions: Implications on nanomedicine. **N. Feliu**, W.J. Parak

Section D

Orange County Convention Center
West Hall B4 - Theater 4

ACS Award in Colloid Chemistry: Symposium in Honor of Naomi Halas

Cosponsored by PHYS
C. J. Murphy, *Organizer*
M. Moskovits, *Presiding*

8:30 COLL 314. Novel concepts in plasmonics. **P.J. Nordlander**

9:00 COLL 315. Probing molecule-plasmon dynamics with ultrafast SERS. **R.R. Frontiera**

9:30 COLL 316. Shifting the plasmon resonance of gold nanoparticles with incident light intensities as low as those encountered in ordinary UV-visible spectroscopy. **M. Moskovits**

10:00 Intermission.

10:30 COLL 317. Charge injection properties in plasmonic nanocomposites and thin films. **B.G. DeLacy**, Y. Rao, D.L. Kuhn

11:00 COLL 318. Nanotechnology enables hot gold nanorods to kill cancer cells and to stop alive sick cells from migrating to other places in the body. **M.A. El-Sayed**

11:30 COLL 319. Light years: Combined optical and environmental electron microscopy to visualize photonic processes with atomic-scale resolution. **J. Dionne**

Section E

Orange County Convention Center
West Hall B4 - Theater 5

Nanomaterials

Advanced Nanoscale Characterization: In Situ TEM & Beyond

R. Nagarajan, *Organizer*
J. A. Hollingsworth, *Organizer, Presiding*

8:30 COLL 320. Matter in motion by liquid cell TEM: Phase transitions, diffusion, collisions, and growth mechanisms. **N.C. Gianneschi**

9:00 COLL 321. 3D structure study of colloidal nanocrystals using liquid phase TEM. **J. Park**, B. Kim, J. Heo, S. Kim



TECHNICAL PROGRAM

9:30 COLL 322. *In situ* look at interfacial controls over nucleation and growth of nanostructured materials. **J.J. De Yoreo**, G. Zhu, M.L. Sushko, B.A. Legg, M.D. Baer, S. Huang, Y. Zhang, J.A. Soltis, C.J. Mundy, Y. Min, J. Chun, G.K. Schenter

10:00 COLL 323. Investigating magnetic nanoparticle interactions with Cryo-TEM. **J.D. Watt**, A. Begay, D. Huber

10:30 COLL 324. Gentle etching of metal from polymeric three-dimensional structures: Making scanning electron microscopy a non-destructive technique. **S.M. Kuebler**, R. Sharma

10:50 COLL 325. Two types of water on free-standing reduced graphene oxide revealed by neutron scattering. **Z. Liu**, J. Huang, L. Zhang, V.G. Sakai, C. Yang, L. Hong

11:10 COLL 326. Interface and dynamic indentation of crosslinked polyester films. **S. Ahuja**

Section F

Orange County Convention Center
West Hall B4 - Theater 6

Supramolecular Assemblies at Surfaces: Non-covalent, Covalent & Coordination Bonding

Self-Assembly in 2D

F. Rosei, S. L. Tait, *Organizers*
L. Chi, M. Lingenfelder, *Presiding*

8:30 COLL 327. Complexity in metal-organic redox assembly at surfaces: Bimetallic sites and redox isomer surface structures. T.W. Morris, D. Wisman, I.J. Huerfano, C. Tempas, M. Wang, N. Din, D. Skomski, D. Le, T.S. Rahman, K.G. Caulton, **S.L. Tait**

9:00 COLL 328. Chemical self-assembly strategies for designing molecular electronic circuits. D. Olson, **W.T. Tysoe**

9:30 COLL 329. Balancing noncovalent interactions in self-assembly of nonplanar aromatic carboxylic acid linkers at the solution/solid interface: Progress toward 2D SURFMOFs synthesis. **U. Mazur**, K. Hips

10:00 COLL 330. Conformal surface-anchored metal-organic frameworks: Characterization of thin film growth, porosity, and electronic transport. **M.E. Anderson**

10:30 Intermission.

10:50 COLL 331. H-bonded and metal-organic coordination networks on graphene. **M. Stoehr**

11:20 COLL 332. Role and tracking of weak interactions in adsorbed layers on surfaces. **A. Rochefort**

11:50 COLL 333. Organic, 2D transition metal dichalcogenide interface. **A. Wee**

Section G



TECHNICAL PROGRAM

Orange County Convention Center
West Hall B4 - Theater 7

Colloidal Nanoparticle Synthesis & Assembly

O. Chen, T. Li, *Organizers*
F. Bai, H. Fan, *Organizers, Presiding*

8:30 COLL 334. Topology and electronic coupling in the assembly of nanoparticle superlattices. I. Coropceanu, E.M. Janke, M. Boles, X. Lan, **D. Talapin**

9:00 COLL 335. Synthesis of morphology controlled Zn-chalcogenide nanocrystals: A few surprises. **U. Banin**

9:30 COLL 336. Surface chemistry of lead halide perovskites nanocrystals. **L. Manna**

10:00 Intermission.

10:10 COLL 337. Synthesis and assembly of chiral nanoparticles. **N. Kotov**

10:40 COLL 338. Making nanoscale chemistry matter: Synthesis & assembly. **S.W. Cranford**

11:10 COLL 339. Colloidal cesium and formamidinium lead halide perovskite nanocrystals: Genesis, properties and applications. **M. Kovalenko**

11:40 COLL 340. Strong plasmon-exciton coupling in colloially assembled Au quantum-dot structures. Y. Luo, **J. Zhao**

Section H

Orange County Convention Center
West Hall B4 - Theater 8

Biomembrane Synthesis, Structure, Mechanics & Dynamics

J. Katsaras, S. Muralidharan, M. Nieh, A. N. Parikh, *Organizers*
D. Daleke, K. Morigaki, *Presiding*

8:30 COLL 341. Simple class of responsive liposomes that transform into micelles upon heating. **N. Agrawal**, S.R. Raghavan

8:50 COLL 342. Annexins induce membrane curvature near hole edges during plasma membrane repair. T. Boye, J. Nylandsted, **A.C. Simonsen**

9:15 COLL 343. Molecular interactions between cell membranes and surface immobilized peptides. **Z. Chen**

9:40 COLL 344. Lipid self-assembly in bulk and at interfaces: Non-lamellar phases and biomolecular interactions. M. Valdeperas, N. Mahmoudi, S. Teixeira, M. Talaikis, I. Matulaitiene, G. Niaura, J. Barauskas, A. Svendsen, **T. Nylander**



TECHNICAL PROGRAM

10:05 COLL 345. Mapping membrane receptor dynamics, self-association, and oligomerization: Applications of homo-FRET and super-resolution microscopy. **C. Yip**

10:30 COLL 346. Direct comparison between molecular lateral diffusion constant and lipid membrane viscosity using quasi-elastic neutron scattering techniques. **M. Nagao**, E.G. Kelley, T. YAMADA, A. Faraone, K. Shibata, P. Butler

10:55 COLL 347. Understanding the mechanism of antimicrobial peptides using small-angle x-ray and neutron scattering techniques: The lipid's point of view. J. Eilsoe Nielsen, V. Bjornestad, **R. Lund**

11:20 COLL 348. Heterogeneous dielectric implicit membrane model for the calculation of MMPBSA binding free energies. **R. Luo**, D. Greene

11:45 COLL 349. Growing supergiant liposomes on nanocellulose paper and regenerated cellulose membranes. **A.B. Subramaniam**, J. Pazzi

Section I

Orange County Convention Center
West Hall B4 - Theater 9

Surface Chemistry of Colloidal Nanocrystals

D. Qin, X. Xia, *Organizers*
J. Chen, S. Neretina, *Organizers, Presiding*

8:30 COLL 350. Self-assembly of nanoparticles into two-dimensional arrays for catalytic applications. **S. Sun**

9:00 COLL 351. Use of ligand-binding to form low-index facet metal nanocrystals for catalysis. **R. Tilley**

9:30 COLL 352. Tailoring surface structures of spongy metallic nanoparticles toward optimization of electrocatalysis. **H. Wang**

10:00 Intermission.

10:15 COLL 353. Surface-driven magnetism of Fe-oxide nanocrystals. **J.A. De Toro**, P.S. Normile, E.H. Sánchez, S. Lee, M. Vasilakaki, M.S. Andersson, K.N. Trohidou, R. Mathieu, J. Nogués

10:45 COLL 354. Carbon nitride compounds for heterogeneous photocatalysis. **P. Ricci**

11:15 COLL 355. Surface-modified magnetic nanoparticles as efficient adsorbents for heavy metal removal from wastewater: Progress and prospects. **M.O. Ojemaye**, O.O. Okoh, **A. Okoh**

Molecular Processes at Mineral-Water Interfaces: Predictions via Linking Theory & Experiments

Sponsored by GEOC, Cosponsored by COLL



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

Engineered Lignocellulosic Materials & Multiphase Systems: Anselme Payen Award Symposium in Honor of Orlando Rojas

Creating Sustainable Polymers & Composites

Sponsored by CELL, Cosponsored by ANYL and COLL

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Sponsored by PROF, Cosponsored by AGFD, ANYL, BIOL, BIOT, CARB, CELL, CHED, CMA, COLL, COMP, ENVR, GEOC, I&EC, MEDI, MPPG, NUCL, ORGN, PHYS, PMSE, POLY, PRES, WCC and YCC

Interdisciplinary Chemistry for New Frontiers in Biology and Medicine

Biomarker Discovery

Sponsored by ANYL, Cosponsored by BIOL, COLL[‡], MPPG, PHYS[‡] and PMSE[‡]

MONDAY AFTERNOON

Section A

Orange County Convention Center
West Hall B4 - Theater 1

ACS Award in Surface Chemistry: Symposium in Honor of Hajo Freund

Cosponsored by CATL[‡] and PHYS
J. A. Boscoboinik, R. J. Meyer, A. Savara, *Organizers*
F. C. Calaza, W. Kaden, *Organizers, Presiding*

1:30 Intermission.

2:00 **COLL 356.** Rearrangement of bimetallic alloys: understanding through surface science models. **C.M. Friend**, M. van Spronsen, K. Duanmu, P. Sautet, R. Madix

2:35 **COLL 357.** Control of charge transfer into large organic molecules on ultrathin MgO(001) films. **M. Sterrer**

3:10 **COLL 358.** Highly active FeNi bimetallic phosphide catalyst gives unprecedented selectivity to the direct desulfurization pathway. **S.T. Oyama**, H. Zhao, K. Asakura



TECHNICAL PROGRAM

3:45 Intermission.

4:05 COLL 359. Ionic liquid adsorption and ion exchange processes at single crystal surfaces. **H. Steinrueck**

4:40 COLL 360. Selectivity in hydrogenation catalysis. **F. Zaera**

Section B

Orange County Convention Center
West Hall B4 - Theater 2

Biomaterials & Biointerfaces

Cellular Interactions with Colloids

R. Wylie, *Organizer*
Y. Lapitsky, *Organizer, Presiding*
S. C. Owen, *Presiding*

2:00 COLL 361. Engineered nanomaterials for cancer immunotherapy. **J.J. Moon**

2:30 COLL 362. Glycodendron modified HES nanocapsules for targeting of dendritic cells. **M. Frey**, M. Krumb, J. Pereira, V. Mailänder, T. Opatz, K. Landfester

2:50 COLL 363. Local reprogramming of antigen presenting cell function using synthetic depots to promote tolerance. **H. Eppler**, C. Jewell

3:10 COLL 364. Transient membrane pore-forming conjugated polymer nanoparticles. P. Manandhar, F. Chen, J. He, **J. Moon**

3:30 COLL 365. Designing biodegradable lipid nanoparticles for enhanced intracellular delivery and genome editing. **M. Wang**

3:50 COLL 366. Intracellular cytotoxic peptide release triggered by *in situ* hybridization of complementary, DNA-conjugated, multicolor carbon dots. **I. Srivastava**, S.K. Misra, K.A. Boateng, J. Soares, A. Schwartz-Duval, D. Pan

4:10 COLL 367. Lipid corona formation from nanoparticle interactions with bilayers. **F. Geiger**

4:30 COLL 368. Erythrocyte membrane-coated piezoelectric sensor for studying the interactions between nanoparticles and surfaces of red blood cells. **T. Islam**, O. Chesnokova, A. Oleinikov, P. Yi

4:50 COLL 369. Polysaccharide coated nanoparticles for biological detection. **X. Huang**, S. HossainiNasr, C. Qian

5:10 COLL 370. Noncovalent protein coating onto porous nanoparticles to prevent protein corona enhances *in vivo* therapeutic efficacy. **J. Ryu**

Section C



TECHNICAL PROGRAM

Orange County Convention Center
West Hall B4 - Theater 3

Quantitative Particle Cell Interaction

N. Feliu, L. Liz Marzan, W. J. Parak, *Organizers*
R. A. Alvarez-Puebla, *Presiding*

2:00 COLL 371. Aluminum nanostructures with strong visible-range SERS activity for versatile micropatterning of molecular security labels. **I. Phang**

2:30 COLL 372. Degradation of protein coronas exposed to proteolytic environment of pancreatic tumor cells. C. Rodriguez-Quijada, G. Cramer, C. Yelleswarapu, J. Celli, **K. Hamad-Schifferli**

3:00 COLL 373. Combination of SERS and fluorescence for detection and/or characterization in biological systems. **R.A. Alvarez-Puebla**

3:30 COLL 374. Quantitative super-resolution imaging of self-assembled nanocarriers via spectroscopic single molecule localization microscopy (sSMLM). **J. Davis**, Y. Zhang, S. Yi, K. Song, E. Scott, C. Sun, H. Zhang

3:50 COLL 375. Synthesis of highly brilliant SERS-encoded nanoparticles: Plasmonic core-satellites structures. **N. Pazos-Perez**, R.A. Alvarez-Puebla

4:20 COLL 376. Using single-particle spectroscopy to probe nanoparticle uptake by mammalian cells. **C.M. Hill**, J.W. Hill

4:40 COLL 377. TiO₂ nanoparticles, in the absence of light, oxidize the protein corona leading to an oxidative stress response in cells. **D.T. Jayaram**, S. Runa, M.L. Kemp, C.K. Payne

5:00 COLL 378. Nitroxide-liquid crystal nanoparticle conjugates for the protection of cells against reactive oxygen species. **O.K. Nag**, J. Delehanty, J. Naciri

Section D

Orange County Convention Center
West Hall B4 - Theater 4

ACS Award in Colloid Chemistry: Symposium in Honor of Naomi Halas

Cosponsored by PHYS
C. J. Murphy, *Organizer*
D. Zhao, *Presiding*

2:00 COLL 379. Ligand dynamics and chemistry on plasmonic nanoparticle surfaces: Insights from plasmon-enhanced spectroscopy. **H. Wang**

2:30 COLL 380. Commercialization of gold nanoshells. **S. Oldenburg**

3:00 COLL 381. Rational metamaterial design through colloidal crystal engineering. **C.A. Mirkin**



TECHNICAL PROGRAM

3:30 COLL 382. Correlating carrier density and emergent plasmonic features in Cu_{2-x}Se nanoparticles. **J. Millstone**

4:00 COLL 383. From the beaker to an engineering platform: Scale-up, functionalization, and assembly of plasmonic nanoparticles. K. Park, Y. Yi, C. Mahoney, J. Streit, **R.A. Vaia**

4:30 COLL 384. Quantification of the optical properties of colloidal nanoparticles in solutions: Challenges and opportunities. **D. Zhang**

Section E

Orange County Convention Center
West Hall B4 - Theater 5

Nanomaterials

New Colloidal Nanomaterials: Fundamentals, Synthesis, Integration & Properties

J. A. Hollingsworth, R. Nagarajan, *Organizers*
B. J. Wiley, *Presiding*

2:00 COLL 385. Synthesis and characterization of perovskites for energy applications. **S.S. Wong**

2:30 COLL 386. Perovskite colloidal quantum wells: Self-assembly and physics. **C. Shih**

3:00 COLL 387. Sonochemical synthesis of polymorphic lead halide perovskite microcrystals in polar solvents. **S. Cho**, S. Yun

3:20 COLL 388. Boron cluster building blocks for the development of hybrid materials. **A.M. Spokoyny**

3:40 COLL 389. Novel nanohybrids of chemically active boron based nanosheets with gold nanoparticles and graphene: Assembling mixed dimensional heterostructures in solution. **A.L. James**, S. Khandelwal, A. Dutta, K. Jasuja

4:00 COLL 390. Influence of nanoparticle dimensionality on rates of electron transfer between semiconductor nanoparticles. **A. Brumberg**, B. Diroll, G. Nedelcu, M. Sykes, M. Kovalenko, R. Schaller

4:20 COLL 391. Colloidal semiconductor CdS magic-size clusters: Thermally induced reversible structural isomerization. **K. Yu**

4:40 COLL 392. SnGe alloys: Full compositional range at nanoscale. K. Ramasamy, M. Brumbach, N. Modine, P. Kotula, J.M. Pietryga, **S. Ivanov**

5:00 COLL 393. Self-assembly of CdSe nanoplatelets into twisted threads. **B. Abecassis**, S. Jana, P. Davidson

Section F

Orange County Convention Center
West Hall B4 - Theater 6



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

Supramolecular Assemblies at Surfaces: Non-covalent, Covalent & Coordination Bonding

On-Surface Synthesis

F. Rosei, S. L. Tait, *Organizers*
E. Barrena, D. F. Perepichka, *Presiding*

2:00 COLL 394. Self-assembly of aryl halides for various degrees of dehalogenation. L. Grossmann, M. Fritton, M. Lischka, **M. Lackinger**

2:30 COLL 395. Two-dimensional porphyrin networks: From nucleobase driven self-assembly to covalent-organic frameworks. **M.O. Blunt**, C. Nowicka-Dylag, Y. Hu, N. Goodeal, A.M. Ganose, A. Slater, R.G. Palgrave, C. Toft, W. Lewis, H. Bronstein, N.R. Champness

3:00 COLL 396. On-surface synthesis: strategies towards the targeted products. T. Wang, **J. Zhu**

3:30 COLL 397. Long-range ordered and atomic-scale control of graphene hybridization by photocycloaddition. **M. Yu**

4:00 Intermission.

4:20 COLL 398. Bottom-up fabrication of atomically precise molecular nanostructures through on-surface reactions. **S. Maier**

4:50 COLL 399. Assemblies and reactions of small carboxylated molecules on metal surfaces: diverse chemical and structural outcomes from simple precursor molecules. **J. MacLeod**

5:20 COLL 400. Selective activation of chemical bonds in on-surface chemistry. **L. Chi**

Section G

Orange County Convention Center
West Hall B4 - Theater 7

Colloidal Nanoparticle Synthesis & Assembly

O. Chen, T. Li, *Organizers*
F. Bai, H. Fan, *Organizers, Presiding*

2:00 COLL 401. Synthesis and directed assembly plasmonic nanostructures. **D.S. Ginger**

2:30 COLL 402. Organizing nanorods end to end. **C.J. Murphy**

3:00 COLL 403. *In-situ* scattering techniques to study synthesis and crystallization processes of colloidal nanocrystals. **M. Cargnello**, L. Wu, J. Qin, C. Tassone

3:30 COLL 404. Templated evaporative self-assembly as a powerful tool for creating functional superstructures and patterns. **E. Zubarev**



TECHNICAL PROGRAM

4:00 Intermission.

4:10 **COLL 405.** *In situ* high-energy XRD studies on the nucleation, growth, and 3D atomic structure of ultrathin Au nanowires in solution. **V. Petkov**

4:30 **COLL 406.** Understanding the role of soft ligands on nanoparticle assembly using small angle x-ray and neutron scattering techniques. **B. Lee**, E. Shevchenko

5:00 **COLL 407.** Nanoisland deposition on colloidal nanoparticle substrates. **J. Millstone**

Section H

Orange County Convention Center
West Hall B4 - Theater 8

Biomembrane Synthesis, Structure, Mechanics & Dynamics

J. Katsaras, S. Muralidharan, *Organizers*
M. Nieh, A. N. Parikh, *Organizers, Presiding*

2:00 **COLL 408.** Protein corona formation on nanoparticles and its effect on interaction with biological membranes. **L. Wang**, N. Malmstadt

2:20 **COLL 409.** Substrate specificity of P4-ATPases. **D.L. Daleke**, S. Smiriti, M.L. Zimmerman, D. Dudek

2:45 **COLL 410.** Fatty acid flip-flop in lipid membranes. V. Cheng, D. Kimball, **J.C. Conboy**

3:10 **COLL 411.** Consequences of oxidation of plasma membrane lipids. **N. Malmstadt**

3:35 **COLL 412.** Compositional and biophysical asymmetry in mammalian membrane bilayers. **I. Levental**

4:00 **COLL 413.** Supported membranes as a platform for dynamic phenotyping of primary human cells: Quantifying the effect of intrinsic and extrinsic factors. **M. Tanaka**

4:25 **COLL 414.** Physical properties of simple sphingolipids in phospholipid bilayers: Wild, tamed, and caged tigers. **F.M. Goni**, A. Alonso

4:50 **COLL 415.** Correlation of an antimicrobial peptide's potency and its influences on membrane elasticity. W. Chang, S. Chen, **Y. Chen**

Section I

Orange County Convention Center
West Hall B4 - Theater 9

Surface Chemistry of Colloidal Nanocrystals



TECHNICAL PROGRAM

J. Chen, D. Qin, *Organizers*
S. Neretina, X. Xia, *Organizers, Presiding*

2:00 COLL 416. Quantifying the formation of functional colloidal nanoparticles through the understanding of surface chemistry. **H. Yang**

2:30 COLL 417. Manipulation of surface capping for controlled growth, transformation, and assembly of nanocrystals. **Y. Yin**

3:00 COLL 418. Single-crystal electrochemistry reveals why nanowires grow. M.S. Kim, Z. Chen, K.A. Fichthorn, **B.J. Wiley**

3:30 Intermission.

3:45 COLL 419. Temperature-dependent photoluminescence and stability of perovskite nanocrystal superlattices. Y. Zhang, C. Thomas, M. Abney, **B.A. Korgel**

4:15 COLL 420. Autocatalytic surface reduction and its role in the synthesis of metal nanocrystals. **Y. Xia**

4:45 COLL 421. Importance of surface chemistry in synthesis, transformations, and sensing applications of plasmonic metal nanoparticles. **V.V. Kitaev**, N. Cathcart, N. Murshid

Engineered Lignocellulosic Materials & Multiphase Systems: Anselme Payen Award Symposium in Honor of Orlando Rojas

Creating 21st Century Sustainable Materials from Lignin

Sponsored by CELL, Cosponsored by ANYL and COLL

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Sponsored by PROF, Cosponsored by AGFD, ANYL, BIOL, BIOT, CARB, CELL, CHED, CMA, COLL, COMP, ENVR, GEOC, I&EC, MEDI, MPPG, NUCL, ORGN, PHYS, PMSE, POLY, PRES, WCC and YCC

Interdisciplinary Chemistry for New Frontiers in Biology and Medicine

DNA/RNA & Disease Diagnosis

Sponsored by ANYL, Cosponsored by BIOL, COLL, PHYS and PMSE

MONDAY EVENING



TECHNICAL PROGRAM

Section A

Orange County Convention Center
West Hall C

Sci-Mix

R. Nagarajan, *Organizer*

8:00 - 10:00

139, 144-152, 154-157, 160, 165-166, 168, 170-172, 174-175, 177, 181, 183-186, 193, 196-197, 201, 205, 214-217, 219-223, 226-228, 230, 232-237, 242, 245-246, 249-252, 255, 257-258, 261- 263, 268-270, 272, 274-280, 287-290. See previous listings.

TUESDAY MORNING

Section A

Orange County Convention Center
West Hall B4 - Theater 1

ACS Award in Surface Chemistry: Symposium in Honor of Hajo Freund

Cosponsored by CATL⁺ and PHYS
W. Kaden, R. J. Meyer, A. Savara, *Organizers*
J. A. Boscoboinik, F. C. Calaza, *Organizers, Presiding*

8:00 Intermission.

8:30 COLL 422. Surface action spectroscopy: A new tool for the spectroscopy of surface vibrations. **H. Kuhlenbeck**, Z. Wu, A. Plucienik, Y. Liu, H. Freund

9:05 COLL 423. Extracting chemistry from the analysis of core-level spectra. **P.S. Bagus**, C.J. Nelin

9:40 COLL 424. Metal oxide – water interface: Quantum chemical studies compared to experiment. **J. Sauer**

10:15 Intermission.

10:35 COLL 425. Composition and chemistry of liquid/vapor interfaces studied by liquid-jet x-ray photoelectron spectroscopy and molecular dynamics simulations. **J.C. Hemminger**

11:10 COLL 426. Chemical dynamics in heterogeneous catalysis. **R. Schloegl**

Section B



TECHNICAL PROGRAM

Orange County Convention Center
West Hall B4 - Theater 2

Biomaterials & Biointerfaces

Biomolecular Interactions

Y. Lapitsky, R. Wylie, *Organizers, Presiding*

8:30 COLL 427. Structuring of organic solvents at biointerfaces and its ramifications for antimalarial inhibition of hemozoin crystallization. **J.D. Rimer**, J.C. Palmer, P.G. Vekilov

9:00 COLL 428. Real-time chemical imaging of carbon-dot-templated tubulin-polymerization. **I. Srivastava**, P. Mukherjee, R. Bhargava, D. Pan

9:20 COLL 429. Catechin-mediated restructuring of a bacterial toxin inhibits activity. **E. Chang**, J. Huang, Z. Lin, A.C. Brown

9:40 COLL 430. Molecular dynamics simulation study of the effect of lignin dimers on the gel to liquid-crystalline transition temperature in DPPC bilayers. **X. Tong**, M. Moradipour, B. Novak, B. Knutson, S. Rankin, B. Lynn, D. Moldovan

10:00 COLL 431. Multiscaling method for systematic investigation of nanostructure-biointerface interactions in crowded biological media. **S.A. Hassan**

10:20 COLL 432. Functionalization of cotton fabric substrate for enhanced sequestration of Doxorubicin (DOX) chemotherapeutic agent. **O. Wadsworth**, M. Bardot, L. Dehart, S. Kala, M.D. Schulz

10:40 COLL 433. Blood filtration: Materials to modulate systemic immune responses. **R. Wylie**

11:00 COLL 434. Homogeneous immunoassay for the detection of EGFR-HER2 heterodimerization on cell surfaces. **S.C. Owen**

11:20 COLL 435. Structure and orientation of a small protein on a gold nanoparticle surface. **Y. Perera**, A. Huges, N. Fitzkee

11:40 COLL 436. Reducing protein adsorption on biomimetic superhydrophobic surfaces: Hybrid hydrophilic-hydrophobic arrays prepared by 3D printing. **B. Mondal**, Q. Xu, A.M. Lyons

Section C

Orange County Convention Center
West Hall B4 - Theater 3

Quantitative Particle Cell Interaction

L. Liz Marzan, W. J. Parak, *Organizers*
N. Feliu, *Organizer, Presiding*



TECHNICAL PROGRAM

- 8:30 COLL 437.** Gold nanoparticle imaging in complex mammalian cell cultures. **M. Henriksen**, D. Jiménez de Aberasturi, J. Langer, I. Garcia, L. Liz Marzan
- 9:00 COLL 438.** Live-cell encoding by single-nanoparticle FRET multiplexing. **C. CHEN**, N. Hildebrandt
- 9:20 COLL 439.** Unraveling the origin of plasmon-coupled circular dichroism from gold nanorod-protein complexes at single-particle level. **Q. Zhang**, T. Hernandez, K.W. Smith, S.H. Jebeli, L. Warning, R. Baiyasi, L.A. McCarthy, H. Guo, C.F. Landes, S. Link
- 9:40 COLL 440.** Engineering nanomaterials for imaging and therapy of bacteria and biofilm-associated infections. **A. Gupta**, R.F. Landis, R. Das, V.M. Rotello
- 10:00 COLL 441.** Magnetic iron oxide nanoparticles grafted with a thermosensitive polypeptide brush: Uptake by tumor cells and cytotoxicity upon magnetic hyperthermia. G. Hemery, C. Genevois, S. Lacomme, S. MacEwan, F. Couillaud, E. Gontier, A. Chilkoti, S. Lecommandoux, **E.B. Garanger**, O. Sandre
- 10:20 COLL 442.** How the toxicity of nanomaterials towards different species could be simultaneously evaluated: A multi-nano-read-across approach. **B. Rasulev**
- 10:40 COLL 443.** Real-time monitoring of “soft” and “hard” protein corona in carbon dots via a microfluidic setup. **I. Srivastava**, M.S. Khan, K. Dighe, T. Ghonge, L.M. Grove, D. Pan
- 11:00 COLL 444.** Deciphering uptake and trafficking of nanostructured materials built from immune signals. **M.L. Bookstaver**, C. Jewell
- 11:20 COLL 445.** Understanding the effects of surface coating and nanocrystal shape on corona formation for gold colloids. **W. Perng**, Z. Jin, L. Du, H.M. Mattoussi

Section D

Orange County Convention Center
West Hall B4 - Theater 4

ACS Award in Colloid Chemistry: Symposium in Honor of Naomi Halas

Cosponsored by PHYS
C. J. Murphy, *Organizer*
R. Bardhan, *Presiding*

- 8:30 COLL 446.** Carrier dynamics in plasmonic nanostructures. **S. Link**
- 9:00 COLL 447.** How adsorbates influence plasmon dephasing and relationships to photocatalysis. **P. Christopher**
- 9:30 COLL 448.** Gold nanorods: SAXS studies of their growth and the effects of hydrostatic pressure. **P. Mulvaney**
- 10:00** Intermission.
- 10:30 COLL 449.** Gold nanorods with ultranarrow LSPR bands. **L. Liz Marzan**
- 11:00 COLL 450.** Next-generation anisotropic and optical materials: Imaging. **C.J. Murphy**



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

11:30 COLL 451. Cancer diagnosis and response to treatment with plasmonic nanoprobcs. **R. Bardhan**

12:00 Concluding Remarks.

Section E

Orange County Convention Center
West Hall B4 - Theater 5

Understanding the Inorganic-Organic Interface in Colloidal Nanomaterials

Nanocrystals Interfaced with Biology

H. M. Mattoussi, *Organizer*
V. M. Rotello, *Organizer, Presiding*
G. F. Strouse, *Presiding*

8:30 COLL 452. Protein adsorption on inorganic nanoparticles in complex environments. **W.J. Parak**

9:00 COLL 453. Integrating nanoparticles and transition metal catalysts for boorthogonal chemistry: Imaging and therapeutics using engineered nanoparticle 'nanozymes'. **V.M. Rotello**

9:30 COLL 454. Tailor-made surface modifications of nanocrystals for applications in materials and life sciences. **H. Weller**

10:00 Intermission.

10:20 COLL 455. Surface peptide mediated quantum dot/ gold uptake. **G.F. Strouse**

10:50 COLL 456. Influence of composition and surface state on the toxicity and fate of indium phosphide quantum dots. **P. Reiss**

11:20 COLL 457. Multiply-binding polymeric imidazole ligands: Influence of molecular weight and monomer sequence on colloidal quantum dot stability. **J.H. Dunlap**, A.F. Loszko, R.A. Flake, Y. Huang, B.C. Benicewicz, A.B. Greytak

Section F

Orange County Convention Center
West Hall B4 - Theater 6

Supramolecular Assemblies at Surfaces: Non-covalent, Covalent & Coordination Bonding

2D to 3D & Biomolecular Assemblies

F. Rosei, S. L. Tait, *Organizers*
M. Lackinger, J. MacLeod, *Presiding*



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

8:30 COLL 458. Combining electrospray ionisation deposition and scanning tunnelling microscopy to investigate the surface assembly of macromolecules. **G. Costantini**

9:00 COLL 459. Programmable supramolecular self-assembly of DNA at surfaces. **T. Ye**, H. Cao, G. Abel

9:20 COLL 460. Diverse self-assemblies of protein 2D crystalline at solid-liquid interface. **S. Zhang**, R. Alberstein, F.A. Tezcan, J. De Yoreo

9:40 COLL 461. Molecular mechanism of peptide assembly propensity studied with STM. **C. Wang**

10:10 Intermission.

10:20 COLL 462. Chiral organization and charge redistribution in molecular layers on surfaces beyond the monolayer. **E. Barrena**

10:50 COLL 463. Building the next layer. C. Fang, J. He, L. Wilczek, H. Zhu, O. Chen, **M.B. Zimmt**

11:20 COLL 464. Sub-molecular tunneling barrier measurements of molecular adlayers at the solution-graphite interface. **J.A. Olson**, J.C. Baum, M.J. Novak, K. Sriraman

11:40 COLL 465. Understanding cooperative interactions in the polymorphs of self-assembled macrocycles. **S. Debnath**, J. Yang, H.D. Castillo, J. Dobscha, S.L. Tait, A.H. Flood, P. Ortoleva, K. Raghavachari

12:00 COLL 466. Order/disorder phase boundary in supramolecular self-assembly of macrocycles at surfaces. **H.D. Castillo**, J. Yang, S. Debnath, J. Dobscha, C. Trainor, R.D. Mortensen, K. Raghavachari, A.H. Flood, P. Ortoleva, S.L. Tait

12:20 Concluding Remarks.

Section G

Orange County Convention Center
West Hall B4 - Theater 7

Colloidal Nanoparticle Synthesis & Assembly

F. Bai, O. Chen, H. Fan, *Organizers*

T. Li, *Organizer, Presiding*

Y. Jiang, *Presiding*

8:30 COLL 467. Multi-layered metal-organic framework microcrystals as a host to control the guest-to-host and guest-to-guest interactions. **C. Tsung**

9:00 COLL 468. Nanostructured electrode materials for Li/Na ion storage. **A. Yan**

9:30 COLL 469. Advanced *in situ* X-ray diffraction in revealing the structural changes of high voltage cathode under the effect of different electrolytes. M. He, **M. Cai**

10:00 Intermission.



TECHNICAL PROGRAM

10:10 COLL 470. From interfacial studies to high-performing catalysts: Synthetic design at nanoscale. **Y. Huang**

10:40 COLL 471. Toward total synthesis of thiolate-protected metal nanoclusters. **J. Xie**

11:10 COLL 472. Synthesis and functionalization of NIR-to-NIR upconversion nanophosphors for oil reservoir application. **W. Wang**

11:40 COLL 473. Investigating the effects of phase transfer procedures on the photoluminescence of aqueous quantum dots. **J.C. Schwabacher**, M.S. Kodaimati, E. Weiss

Section H

Orange County Convention Center
West Hall B4 - Theater 8

Biomembrane Synthesis, Structure, Mechanics & Dynamics

J. Katsaras, S. Muralidharan, M. Nieh, A. N. Parikh, *Organizers*
R. Ashkar, N. Malmstadt, *Presiding*

8:30 COLL 474. Design efficacious targeting lipid nanoparticles. **M. Nieh**, A.T. Rad, C. Ching-Wen, W. Aresh, P. Lai

8:55 COLL 475. Assembly of receptor tyrosine kinases in the plasma membrane regulates function at the protein, cell and organism levels. S. Kim, X. Shi, **A.W. Smith**

9:20 COLL 476. Mechanism of toxin enrichment in bacterial outer membrane vesicles. J.B. Nice, **A.C. Brown**

9:45 COLL 477. Spin labeling of cysteines for EPR structural studies on type II cannabinoid receptor CB₂. A. Yeliseev, L.T. Hooper, W.E. Teague Jr, K.G. Hines, R.L. Beckner, L. Zoubak, **K. Gawrisch**

10:10 COLL 478. Self-spreading of a phospholipid bilayer in the scaffold of polymerized lipid bilayer. **K. Morigaki**, F. Tamura, Y. Tanimoto, R. Nagai, M. Yamada, F. Hayashi

10:35 COLL 479. Fatty acids of Gb₃ influence its partition in phase separated lipid membranes as well as Shiga toxin binding. **C. Steinem**

11:00 COLL 480. Peering into the lipid world. **N.K. Devaraj**

11:25 COLL 481. Lateral diffusion and fluorescence quenching in lipid bilayer membranes on graphene oxide. **R. Tero**

11:50 COLL 482. Domain dynamics and shape adaptations in osmotically stressed giant lipid vesicles. **A.N. Parikh**

Section I

Orange County Convention Center
West Hall B4 - Theater 9

Surface Chemistry of Colloidal Nanocrystals



TECHNICAL PROGRAM

J. Chen, X. Xia, *Organizers*
S. Neretina, D. Qin, *Organizers, Presiding*

8:30 COLL 483. Supramolecular, chemistry-based, reversible surface charge reversal. **L. Liz Marzan**

9:00 COLL 484. Competing role of surface chemistry on nanostar stability and SERS activity. **A.J. Haes**, W. Xi

9:30 COLL 485. Understanding the protein corona one molecule and one nanoparticle at a time. **S. Link**

10:00 Intermission.

10:15 COLL 486. Efficient plasmon-induced hot electron transfer at metal/semiconductor junctions. **T. Lian**

10:45 COLL 487. Direct Optical Lithography of Functional Inorganic Nanomaterials (DOLFIN) enabled by novel nanocrystal surface chemistry. Y. Wang, J. Pan, H. Cho, **D. Talapin**

11:15 COLL 488. Optimization of the surface, ligands, and structure of semiconductor nanocrystal quantum dots (QDs) for photocatalytic charge transfer reactions. **K. McClelland**, E. Weiss

Applied Materials for New Frontiers: Ten Years of ACS Applied Materials & Interfaces

Sponsored by MPPG, Cosponsored by COLL[‡], INOR[‡], PMSE[‡] and POLY[‡]

Engineered Lignocellulosic Materials & Multiphase Systems: Anselme Payen Award Symposium in Honor of Orlando Rojas

Sustainable Materials in High Performance Applications

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Exploring the Frontiers of Chemistry through NASA Research

Getting There: Advanced Materials for Space Travel

Sponsored by COMSCI, Cosponsored by ANYL, BIOL, BIOT, CELL, COLL, ENFL, I&EC, INOR, NUCL, PHYS, PMSE and POLY

Interdisciplinary Chemistry for New Frontiers in Biology and Medicine

Structure, Imaging & Sensing



TECHNICAL PROGRAM

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GSSPC: Artificial Molecular Machines & the Next Generation of Molecular Control

Sponsored by CHED, Cosponsored by COLL, I&EC, ORGN[‡], PHYS, POLY and PRES

Light-Driven Chemistry: Photoelectrochemistry & Photocatalysis

Sponsored by CATL, Cosponsored by COLL, ENFL, I&EC, INOR and PHYS

TUESDAY AFTERNOON

Section A

Orange County Convention Center
Room W230D

ACS Awards Lectures

Cosponsored by PROF
R. Nagarajan, *Organizer*
L. Tribe, *Presiding*

2:00 Introductory Remarks.

2:10 COLL 489. Award Address (ACS Award in Colloid Chemistry sponsored by the Colgate-Palmolive Company).
Tunable plasmonic nanoparticles: New materials and new applications. **N.J. Halas**

3:00 Introductory Remarks.

3:10 COLL 490. Award Address (ACS Award in Surface Chemistry sponsored by the Procter & Gamble Company)
Models for heterogeneous catalysts: Complex materials at the atomic level. **H. Freund**

Section B

Orange County Convention Center
West Hall B4 - Theater 2

Basic Research in Colloids, Surfactants & Interfaces

Nanomaterials

R. Nagarajan, *Organizer*
T. Guo, *Presiding*



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- 2:00 COLL 491.** Fabrication and flow characteristics of monodisperse bullet-shaped microparticles with controllable structures. **Q. Cai**, X. Ju, C. Chen, Y. Faraj, Z. Jia, J. Hu, R. Xie, W. Wang, Z. Liu, L. Chu
- 2:20 COLL 492.** New insights to optical properties of fluorescent quantum dots by polarized resonance synchronous spectroscopy. **J. Xu**, Y. Yuan, O. Chen, D. Zhang
- 2:40 COLL 493.** Theoretical study of X-ray-Induced Energy Transfer (XIET) from nanomaterial donors to nanomaterial acceptors. **T. Guo**
- 3:10 COLL 494.** *In-situ* analysis of nucleation and growth of transition metal oxalate precursor particles via time evolution of solution composition and particle size distribution. **H. Dong**, A. Wang, G. Smart, D. Johnson, G. Koenig
- 3:30 COLL 495.** Colloidal semiconductor CdSe magic-size clusters with 415 nm bandgap. **K. Yu**
- 3:50 COLL 496.** Applying charge equilibration methods to CdSe quantum dots to gain atomistic insight into the magic-size phenomenon. **K.C. Tvrdy**, N. Weeks
- 4:10 COLL 497.** Effects of branch morphology and crystallinity of Au-Co nanoparticles for enhanced oxygen evolution catalysis. **M. Myekhlai**, L. Gloag, T. Benedetti, R. Tilley, J. Gooding
- 4:30 COLL 498.** Latent fingerprint development and imaging with NIR(980nm)-to-NIR(800nm) upconversion nanocrystals. **A. Baride**, G. Sigdel, P. May

Section C

Orange County Convention Center
West Hall B4 - Theater 3

Basic Research in Colloids, Surfactants & Interfaces

Colloidal Systems

R. Nagarajan, *Organizer*
A. Chervanyov, *Presiding*

- 2:00 COLL 499.** Novel clustered state of colloidal dispersions: Transport properties of concentrated dispersions of particles with competing interactions validated against measurements of lysozyme with application to biopharmaceuticals. **N.J. Wagner**, G. Naegele, J. Bergenholtz
- 2:30 COLL 500.** Strategies of optimizing CO₂-responsive assemblies by understanding their switching behaviors and feasibility in application. **Y. Lu**, Y. Zhu, D. Sun, Q. Liu, Z. Xu
- 2:50 COLL 501.** Polymer mediated interaction between colloids and their effect on thermodynamic properties of filled polymer melts and blends. **A. Chervanyov**
- 3:20 COLL 502.** How do surfactants control the agglomeration of clathrate hydrates? **P.M. Naullage**, A.A. Bertolazzo, V. Molinero



TECHNICAL PROGRAM

3:40 COLL 503. Effects of antifreeze proteins and their hyperactive mutants on calcite crystallization. **A. Kishishita**, J.J. Lugo, J.O. Castellon, F. Rojas, X. Wen

4:00 COLL 504. Controllable fabrication of ultra-thin capsules encapsulated with smart nanogels for simple detection of lead(II) ions. **L. Wenying**, X. Ju, R. Xie, W. Wang, Z. Liu, L. Chu

4:20 COLL 505. Rheological properties of hard-sphere suspensions in biaxial shear flow. **R. Tao**, Z. Tsinas, L. Guerrero, A. Forster

4:40 COLL 506. Stabilization of nano-HMX suspensions with PVP to improve the milling process. **M. Doukkali**, E. Gauthier, r. patel, V. Stepanov, H. Hadim

5:00 COLL 507. Effect of electrolyte type and concentration on the electrokinetic behaviour of clay- polyelectrolyte dispersions. **M. Nasser**, S. Shaikh, A. Benamor

Section D

Orange County Convention Center
West Hall B4 - Theater 4

Novel Functionalization Methods for Textiles & Fibers

N. Pomerantz, M. Richards, *Organizer, Presiding*

2:00 COLL 508. Nanocellulose coatings on cellulose non-woven fabrics: High flux affinity membranes for water purification. **B. Jalvo**, A. Aguilar, A. Mathew

2:25 COLL 509. Garment-integrated thermoelectric devices. **T.L. Andrew**

2:50 COLL 510. Electrochemical properties of 3-dimensional flexible substrates with iridium oxide nanoparticles for use as a supercapacitor. **S. McGraw**, D. Wickramasinghe, K. Chow, M. Craps, R. Czerw, K. Senecal

3:15 COLL 511. Textile functionalization by porous protein crystal conjugation and guest molecule loading. L. Hartje, D. Andales, L. Gintner, L. Johnson, Y. Li, **C. Snow**

3:40 COLL 512. Inorganic nanocoating technology for functional textile. **A. Abbas**

4:05 COLL 513. Directed evolution of tandem repeat protein fibers. **M.C. Demirel**, H. Jung

4:30 COLL 514. Colloidal chemistry of NFC based sustainable textile dyeing technology and factors affecting dye performance. **A. Liyanapathirana Dona**, S. Sharma, S. Minko

4:55 COLL 515. Fabric modification with nanocellulosic fibers as functional carriers. **S. Seyedi Ghezghapan**, M. Savchak, A. Liyanapathirana Dona, S. Sharma, S. Minko, I.A. Luzinov

Section E



TECHNICAL PROGRAM

Orange County Convention Center
West Hall B4 - Theater 5

Understanding the Inorganic-Organic Interface in Colloidal Nanomaterials

Characterization of the Ligand Coating on Nanocrystal Surfaces

H. M. Mattoussi, V. M. Rotello, *Organizers*
J. Vela, E. A. Weiss, *Presiding*

2:00 COLL 516. Fluorinated quantum dots. K. Perez, B. Nagasing, **E.A. Weiss**

2:30 COLL 517. What calorimetry can teach us about quantum dots: A tale of ITC. L. Hicks, Z.B. Di Giusto, **J.D. Keene**

2:50 COLL 518. Design of histone-mimic nanoparticles for DNA and RNA compaction using molecular modeling. M. Manning, J.A. Nash, **Y.G. Yingling**

3:20 COLL 519. Spatially controlled bioorthogonal catalysis for imaging and drug delivery. **R. Das**, A. Gupta, G.Y. Tonga, R.F. Landis, T. Mizuhara, V.M. Rotello

3:40 Intermission.

4:00 COLL 520. Atomistic modeling of nanoparticles self-assembly with complex coupling. **P. Kral**

4:30 COLL 521. Unveiling the surface chemistry of colloidal NaPnE_2 nanocrystals ($\text{Pn} = \text{Sb, Bi}$; $\text{E} = \text{S, Se}$). **J. Vela**

Section F

Orange County Convention Center
West Hall B4 - Theater 6

Basic Research in Colloids, Surfactants & Interfaces

Emulsions, Foams & Dispersions

R. Nagarajan, *Organizer*
M. Lisunova, *Presiding*

2:00 COLL 522. Structure and collective dynamics of boehmite-oriented aggregation. **E. Nakouzi**, J.A. Soltis, B.A. Legg, G.K. Schenter, X. Zhang, T.R. Graham, K. Rosso, L. Anovitz, J. Chun, J. De Yoreo

2:20 COLL 523. Enhancement of anaerobic digestion sludge dewatering performance using *in-situ* crystallization in combination with cationic organic polymers flocculation. **P. Yang**

2:40 COLL 524. Chemical fusion of the soft matter under the mechanical stirring. **M. Lisunova**



TECHNICAL PROGRAM

3:10 COLL 525. Entry, bridging and spreading of *n*-hexane at the air/zwitterionic surfactant solution interface in presence of salts with respect to foamability and foam stability. **S. Varade**

3:30 COLL 526. Synthesis of magnetically responsive Janus particles using biodegradable natural chemicals for functional magnetic emulsions. **X. He**, C. Liang, Q. Liu, Z. Xu

3:50 COLL 527. Reversible sol-gel phase-changing electro-responsive smart particles-dispersed colloidal suspensions. **T. Do**, U. Choi

4:10 COLL 528. Improving BFFT of waterborne polyurethane coating by building encapsulated polyisocyanate emulsion with hydrophobic inter-facial agent. **R. Wang**, Z. Jiang, Z. Wang, M. Zhao, J. Zhang, J. Li

4:30 COLL 529. Structure-property relationship of commercial surfactants and bilgewater emulsions stability. **M.R. Willner**, J.K. Church, J. Lundin, D. Diaz, W. Lee, D.M. Paynter

Section G

Orange County Convention Center
West Hall B4 - Theater 7

Basic Research in Colloids, Surfactants & Interfaces

Colloids, Ions & Interactions

R. Nagarajan, *Organizer*
A. Karmakar, *Presiding*

2:00 COLL 530. Multicomponent self-assembled gels: Compositional effects on rheological and tribological responses. **B.V. Farias**, S.A. Khan

2:20 COLL 531. Combined supramolecular and mesoscale modelling of liquid–liquid extraction of rare earth salts. **A. Karmakar**

2:50 COLL 532. Studies of caffeine interactions with cations and osmolytes. **Y. Zhang**, T.S. Thompson, W.T. Price, N. Johnson, A.P. Allsbrook, J. Skubal, G. MacDonald

3:10 COLL 533. Mineralization in balanced salt solutions. **M.V. Phelps**

3:30 COLL 534. Effect of electrolyte type and concentration on the electrokinetic behaviour of clay-polyelectrolyte dispersions. **M. Nasser**, A. Benamor

3:50 COLL 535. Unprecedented volume exclusion co-ion effect in self-assembly of macroions. **J. Chen**, K. Qian, K. Xiao, J. Luo, H. Li, M. Tsige, T. Liu

4:10 COLL 536. Reverse binding affinities of metal cations in nanoconfined cavity. **J. Luo**, S. Ye, T. Li, E. Sarnello, H. Li, T. Liu

4:30 COLL 537. Simple method for visual detection of lead (II) based on smart polymeric materials. **Y. Liu**, X. Ju, R. Xie, W. Wang, Z. Liu, L. Chu



TECHNICAL PROGRAM

Section H

Orange County Convention Center
West Hall B4 - Theater 8

Basic Research in Colloids, Surfactants & Interfaces

Carbon Materials

R. Nagarajan, *Organizer*
S. Srivastava, *Presiding*

2:00 COLL 538. Colloidal and chemical properties of graphene oxide and step wisely reduced graphene oxide. **S. Azizighannad**, S. Mitra

2:20 COLL 539. Exploring the role of induced defects in carbon nanotubes through a novel camphor-mediated combustion approach in electromagnetic interference shielding application. **S. Srivastava**, K. Manna

2:50 COLL 540. Ionic strength dependence of short DNA conformations at carbon nanotubes: Free energy landscape study. **A.A. Alizadehmojarad**, L. Vukovic

3:10 COLL 541. Effect of the metal substrate on interlayer interactions in bilayer graphene. **M. Christian**, E.R. Johnson

3:30 COLL 542. Examining charge carrier mobility in graphene oxide-titanium oxide thin films. **E. Barrios**, L. Zhai

3:50 COLL 543. Anchoring Ti^{4+}/WO_3 onto functionalized graphene oxide: Enhanced adsorption capacity and photocatalytic activity. **Q. Zhang**, J. Pu

4:10 COLL 544. Structure-dependent Fluorescence Resonance Energy Transfer (FRET) in aqueous, carbon, quantum-dots-embedded PC60-PC₆₁BM colloids. **Y. Kim**, P. Guo, R. Schaller

4:30 COLL 545. Melt-rheology and morphology of multi-walled carbon nanotube-based polypropylene composites: Assessing the state of nanotube dispersion. **A. Bhattacharyya**, D. Parija

4:50 COLL 546. Carbon nanodots (CNDs): Fundamentals of the optoelectronic properties and antioxidation. **J. Wei**, W. Zhang, Z. Ji, Z. Zeng, A.T. Sheardy, D. Arvapalli

Section I

Orange County Convention Center
West Hall B4 - Theater 9

Basic Research in Colloids, Surfactants & Interfaces

Lipids, Peptides, Proteins

R. Nagarajan, *Organizer*
T. Wei, *Presiding*



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

2:00 COLL 547. Confocal Raman microscopy investigation of small-molecule partitioning in hybrid supported bilayers. **M. Zare**, J.P. Kitt, J.M. Harris

2:20 COLL 548. Surface chemistry and spectroscopic study of α -synuclein and its NAC part. **C. Wang**

2:40 COLL 549. Interactions of gold nanoparticles with phospholipid bilayer studied with coarse-grained molecular dynamics simulations. **T. Wei**

3:10 COLL 550. Novel route to designing radiofrequency and near-infrared responsive multifunctional nanostructures using lipid templates for cancer theranostics. **G.D. Bothun**, A. Pan, S. Meenach, J. Mdgolam

3:40 COLL 551. Vitamin K analog, menaquinone-2, adopts a folded conformation in solution and at a model membrane interface. **J.T. Koehn**, E. Magallanes, B.J. Peters, D.C. Crick, D.C. Crans

4:00 COLL 552. Understanding the role of interfacial and bulk interactions between novel cellulose ethers and bile salts to modulate lipid digestion. J. Zornjak, J. Liu, A. Esker, D. Novo, K.J. Edgar, **C. Fernandez Fraguas**

4:20 COLL 553. Interaction of surfactant with model lipid membranes: Influence of surfactant hydrophobic chain fluidity. **Y. Chen**, j. webster, p. li

Applied Materials for New Frontiers: Ten Years of ACS Applied Materials & Interfaces

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Lignocellulosic Materials & Multiphase Systems

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TECHNICAL PROGRAM

Light-Driven Chemistry: Photoelectrochemistry & Photocatalysis

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WEDNESDAY MORNING

Section A

Orange County Convention Center
West Hall B4 - Theater 1

Understanding the Inorganic-Organic Interface in Colloidal Nanomaterials

Chemistry & Physics of Colloidal Nanocrystals

H. M. Mattoussi, V. M. Rotello, *Organizers*
M. Kovalenko, D. Talapin, *Presiding*

8:30 COLL 554. Ligand density and conformation on gold nanoparticles inferred by NMR. **C.J. Murphy**

9:00 COLL 555. Improving the stability of CsPbX₃ (X=Cl, Br, I) perovskite quantum dots via ligand design. **S. Wang, L. Du, H.M. Mattoussi**

9:20 COLL 556. Small angle x-ray scattering for sizing of semi-conducting colloidal nanoparticles. **B. Abecassis, J. Maes, N. Castro, Z. Hens**

9:50 Intermission.

10:10 COLL 557. Colloidal atomic layer deposition. W. Cho, A. Hazarika, K. Mulloy, J. Portner, **D. Talapin**

10:40 COLL 558. Surface chemistry of colloidal Cu_{2-x}S and CuInS₂-based nanocrystals. **C. de Mello Donega**

11:10 COLL 559. Interrogating, J, spectral overlap in terbium(III) doped nano-spinels as green emitters for solid-state lighting. **D.A. Hardy, R.A. Tigaa, G.F. Strouse**

Section B

Orange County Convention Center
West Hall B4 - Theater 2

Basic Research in Colloids, Surfactants & Interfaces

Drops, Wetting & Interface Dynamics



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

R. Nagarajan, *Organizer*
R. M. Espinosa-Marzal, *Presiding*

8:30 COLL 560. Understanding uniform, fast and scalable buoyancy-driven macro-sized drop generations. **J. Youngkyun**, T. Do, U. Choi, S. Choi

8:50 COLL 561. Mechanistic modeling of wetting behaviors of complex rock/oil/water systems for estimating rupture disjoining pressure: A comparison of experimentally-estimated values with published, theoretically derived values. **D. Saini**

9:10 COLL 562. Spontaneous displacement of high viscosity micron-size oil droplets from a curved solid in aqueous solutions. **R. LI**, R. Manica, A. Yeung, Z. Xu

9:30 COLL 563. Structural and dynamic properties of Ionic liquid-solid interfaces. M. Han, **R.M. Espinosa-Marzal**

10:00 COLL 564. Spreading of wetting liquids on surfaces with irregular roughness. **M. Varady**, E. Emmons, A. Tripathi, D. Boyne, T. Pearl, B.A. Mantooth

10:20 COLL 565. Droplets sliding down a vertical surface under increasing horizontal forces. **S. Tang**, Y. Valkya Reddy Bhimavarapu, S. Gulec, R. DAS, R. de la Madrid, R. Tadmor

10:40 COLL 566. Interactions at submerged liquid-repellent surfaces: Gas meniscus formation and development. **M. Eriksson**, M. Järn, M. Tuominen, V. Wallqvist, P. Claesson, H. Teisala, D. Vollmer, M. Kappl, H. Butt, P. Gane, J. Schoelkopf, A. Swerin

11:00 COLL 567. Dynamic surfactant behaviour and interface coverage during single droplet formation in microfluidics. **I. Kiratzis**, D. Vigolo, M. Simmons

11:20 COLL 568. Porous liquid infused surfaces in microfluidics: Pressure and heat transfer measurements. **R.L. Goodwin**, A. Shiave, R.V. Mohan, J.R. Alston

Section C

Orange County Convention Center
West Hall B4 - Theater 3

Basic Research in Colloids, Surfactants & Interfaces

Biosensing, Bioimaging & Drug Delivery

R. Nagarajan, *Organizer*
M. Richards, *Presiding*

8:30 COLL 569. Microscale droplets of thermotropic liquid crystals that respond to rhamnolipids and amphiphiles involved in the regulation of bacterial quorum sensing. **B.J. Ortiz**, M.E. Boursier, D. Manson, H.E. Blackwell, D.M. Lynn

8:50 COLL 570. Design of chiral gold nanoparticles for biosensing. **H. Jang**, N. Kotov



TECHNICAL PROGRAM

9:10 COLL 571. Shaping magnetic fields for effective drug transport across liposome membranes. **V. Chikan**

9:40 COLL 572. Aqueous 0D, 1D, and 2D semiconductor nanocrystals: Single nanoparticle analysis and bioimaging applications. **J. Geng**, L. Ma, S. Lim, S. Sarkar, A. Smith

10:00 COLL 573. Antimicrobial-peptide-conjugated MoS₂-based nanoplatform for multimodal synergistic inactivation of superbugs. **P.C. Ray**

10:20 COLL 574. Surface-supportive Fe-Mil88B thin films for drug delivery. **A. Bui**, J. Dinh, F. Tian

10:40 COLL 575. Physicochemical characterisation of PAMAM dendrimer as multifunctional nanocarriers. **B. Jachimska**

11:00 COLL 576. Dynamic liquid colloids: A new sensing material for the rapid detection of food-borne pathogens. **L. Zeininger**, T.M. Swager

11:20 COLL 577. Surface chemistry and spectroscopic studies of β -galactosidase-carbon dots conjugate: Its use in biosensing. **S.K. Sharma**, S. Paudyal, K.J. Mintz, Y. Zhou, E.M. Zaharan, R.M. Leblanc

Section D

Orange County Convention Center
West Hall B4 - Theater 4

New Frontiers in Hybrid Nanosized Metallic & Semiconductor Materials

B. P. Chauhan, *Organizer, Presiding*

8:30 COLL 578. Electronic and optical properties of (4,8) boron-group V nanosheets. P.A. Brown, **K.L. Shuford**

9:00 COLL 579. Submicron surface-plasmon-polariton perovskite laser. **S. Cho**, Y. Yang, M. Soljacic, S. Yun

9:25 COLL 580. Hybrid nanocluster-catalyzed, one-pot, mild, and unprecedented stereoselective synthetic route to functional silanes and germanes. **B.P. Chauhan**, T. Hopkins, A. Sarkar

9:55 Intermission.

10:15 COLL 581. Self-Assembled Monolayer Field-Effect Transistors (SAMFETs) and their application in organic integrated circuits. **B. Zhao**, B. Gothe, M. Halik

10:40 COLL 582. Bulk assembly of metal halide clusters and their tunable photophysical properties. **C. Zhou**, H. Lin, M. Worku, J. Neu, Y. Zhou, Y. Tian, S. Lee, P.I. Djurovich, T. Siegrist, B. Ma

11:05 COLL 583. Engineering supraparticle assemblies. **N.S. Ramesar**, G. Silveira, T. D. Nguyen, J. Bahng, S.C. Glotzer, N. Kotov

Section E



TECHNICAL PROGRAM

Orange County Convention Center
West Hall B4 - Theater 5

Nanomaterials

Surface Chemistry in Biology & Nanomedicine

J. A. Hollingsworth, R. Nagarajan, *Organizers*
M. A. Firestone, *Presiding*

8:30 COLL 584. Surface modification of core/shell quantum dots enables dynamic visualization of neuronal membrane proteins implicated in mental illness. **S.J. Rosenthal**

9:00 COLL 585. Assessment of binding avidity and adhesion forces by multivalent dendrimer nanoprobos. S. Tang, J. Cannon, **S. Choi**

9:30 COLL 586. Zwitterionic multidentate polymer coating for non-fouling quantum dots. **Z. Han**, A. Smith

9:50 COLL 587. Short-wave infrared quantum dots with compact sizes for microscopic molecular imaging in cells and tissues. **S. Sarkar**, P. Le, J. Geng, Y. Liu, Z. Han, M.U. Zahid, A. Smith

10:10 COLL 588. Ring DNA-carbon nanotube conjugates. **A.A. Alizadehmojarad**, A.G. Beyene, P. Kral, M. Landry, L. Vukovic

10:30 COLL 589. Computational design of nanoparticles with tunable water-mediated interactions. B.C. Dallin, **R. Van Lehn**

10:50 COLL 590. Lipase-catalyzed enzymatic biodegradation of carbon dots follow sequential oxidation pathways. **I. Srivastava**, D. Sar, P. Mukherjee, A. Schwartz-Duval, Z. Huang, R. Bhargava, D. Pan

11:10 COLL 591. Engineering of safe nanocapsules for targeted antibacterial applications. **K. Ivanova**, E. Ramon, A. Ivanova, T. Tzanov

11:30 COLL 592. Functionalization of gold nanoparticles for generation of drug and nucleic acid delivery nanoplatfoms. A. Shabana, U.K. Mondal, A. Kizewski, **M.A. Ilies**

Section F

Orange County Convention Center
West Hall B4 - Theater 6

Surface Chemistry

Biomaterials & Membranes

S. L. Tait, *Organizer*
N. Jiang, S. Youm, *Presiding*



TECHNICAL PROGRAM

8:30 COLL 593. Chemically resolving metal-supported regioisomeric assemblies at nanoscale by ultra-high vacuum, tip-enhanced Raman spectroscopy: Conformation & interaction. S. Mahapatra, J. Schultz, L. Li, **N. Jiang**

8:50 COLL 594. Amusements with salt-water oscillator. **A.K. Das**

9:10 COLL 595. Changes in protein's secondary structure as a result of its interaction with a gold surface. **P. Komorek**, E. Martin, M. Walek, I. Brand, B. Jachimaska

9:30 COLL 596. Genomic DNA functionalized 3D printed architected materials for drug capture. **D. Yee**, S. Krishnamoorthy, R.H. Grubbs, S. Hetts, J.R. Greer

9:50 COLL 597. Substituent effects on the organization of methacrylate monomers and existing intermolecular interactions at air-liquid interface using sum frequency generation spectroscopy. **U.I. Premadasa**, K.A. Cimatu

10:10 Intermission.

10:20 COLL 598. Parallel orientation to the interface: Surface chemistry and spectroscopic study of α -synuclein and the NAC part. **C. Wang**

10:40 COLL 599. Semiconducting block copolymer thin films via surface-initiated polymerization. **S. Youm**, E.E. Nesterov

11:00 COLL 600. 3D structure fabrication using 2D controlled wetting surfaces. **T. Shimosaka**, T.J. McCarthy

11:20 COLL 601. *Operando* PM-IRAS+Raman spectroscopy for elucidating surface poisoning mechanisms of Pd-based hydrogen separation membranes in complex reaction mixtures. **C. O'Brien**

11:40 COLL 602. SuFEx-based hydrolysis strategy for the preparation of sulfate cation exchange resins. **L. Chen**, A. Kassick, S. Averick, J.J. Locklin

12:00 COLL 603. Facile grafting of zwitterions on membrane surface using bio-inspired polydopamine. **H. Lin**

Section G

Orange County Convention Center
West Hall B4 - Theater 7

Colloidal Nanoparticle Synthesis & Assembly

F. Bai, O. Chen, H. Fan, *Organizers*
T. Li, *Organizer, Presiding*
Y. Jiang, *Presiding*

8:30 COLL 604. Janus-type MnOx-AgI nanoparticles as self-sensitized oxygen-evolving catalysts. L. Zhang, L. Jin, Y. Yang, P. Kerns, X. Su, M. Meng, B. Liu, **J. He**

9:00 COLL 605. High-pressure nanocrystals: New structures and new optical properties. **B. Zou**

9:30 COLL 606. Sub-50nm ultra-thin hybrid ED membrane made by colloidal self-assembly and plasma-defined atomic layer deposition. **Y. Jiang**, T. Zhang, C. Fan, S.L. Rempe



TECHNICAL PROGRAM

10:00 Intermission.

10:10 COLL 607. Architecting nanomaterials for naval applications. **A. Smith**

10:40 COLL 608. Crystal structure of Au₃₆(SPhCH₃)₂₄ gold nanomolecules. **V. Ganesh Raj**, A. Antonyamy

11:00 COLL 609. Self-assembly of non-spherical nanoparticles into functional supercrystals. **Z. Quan**

11:20 COLL 610. Electric field-driven assembly of silver nanocrystal superlattices. Y. Yu, D. Yu, **C. Orme**

11:40 COLL 611. Pressure response to the structure and optical properties of metal halide perovskite nanocrystals. **G. Xiao**

Section H

Orange County Convention Center
West Hall B4 - Theater 8

Biomembrane Synthesis, Structure, Mechanics & Dynamics

J. Katsaras, S. Muralidharan, M. Nieh, A. N. Parikh, *Organizers*
K. Gawrisch, M. Nagao, *Presiding*

8:30 COLL 612. Measuring the transverse lipid diffusion of peptidolipidic systems using a novel SANS approach. **M.H. Nguyen**, D. Marquardt, M. DiPasquale, B. Rickeard

8:50 COLL 613. Self-assembly/disassembly of giant double-hydrophilic polymersomes at biologically-relevant pH. **W. Paxton**, S. Shin, P. Mcaninch, I.M. Henderson, A. Gomez, A.C. Greene

9:15 COLL 614. Effect of cholesterol on DOPC lipid membranes. **R. Ashkar**, M. Doktorova, F. Heberle, H.L. Scott, E.G. Kelley, M. Nagao, R. Usery, F.N. Barrera, J. Katsaras, G.W. Feigenson, G. Khelashvili

9:40 COLL 615. Imaging membrane viscosity through nonlinear light scattering. **H. Dai**, M. Wilhelm, M. Sharifian

10:05 COLL 616. Determination of biomembrane elastic properties via analysis of thermal fluctuations of lipid orientation in molecular simulations. **F.L. Brown**

10:30 COLL 617. Interrogating cell membrane organization with secondary ion mass spectrometry. **M.L. Kraft**, A.N. Yeager, P. Weber, J. Zimmerberg

10:55 COLL 618. Transverse lipid organization dictates bending fluctuations in model plasma membranes. B. Rickeard, M.H. Nguyen, M. DiPasquale, E.G. Kelley, M. Nagao, **D. Marquardt**

11:20 COLL 619. Correlated membrane bound protein conformational transitions and lipid dynamics provides new insights into leakage kinetics by pore forming toxins. I. I. P., R. Cheerla, **G.K. Ayappa**, J. Basu

Section I



TECHNICAL PROGRAM

Orange County Convention Center
West Hall B4 - Theater 9

Surface Chemistry of Colloidal Nanocrystals

J. Chen, X. Xia, *Organizers*
S. Neretina, D. Qin, *Organizers, Presiding*

8:30 COLL 620. Impact of surface potential on plasmonic and electronic properties of metal oxide nanocrystals. **D.J. Milliron**

9:00 COLL 621. Surface matters: Interface effects on optoelectronic behavior of semiconductor nanocrystals and hybrid semiconductor-metal nanoparticles. **U. Banin**

9:30 COLL 622. Cooperative action of hot carrier and surfactant in SPR-driven growth of Au nanostars. **W. Wei**

10:00 Intermission.

10:15 COLL 623. Surface chemistry effects on the ultrafast dynamics of propagating surface plasmon polaritons in metal nanostructures. **G.V. Hartland**

10:45 COLL 624. Computational prediction of activation energy without transition state calculation. M. Liu, **S. Zou**

11:15 COLL 625. Plasmonic hot-carrier-mediated tunable photochemical reactions. **Y. Zhang**, T. Nelson, H. Guo, S. Tretiak, G.C. Schatz

Producing Equilibrium Amorphous Packings

Vapor Deposited Glasses

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Producing Equilibrium Amorphous Packings

Vapor Deposited Glasses

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Nanoparticles in Nature: Detection, Characterization, Origin & Formation Mechanisms

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TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

Environmental Interfaces under Nano-scale Confinement

Sponsored by GEOC, Cosponsored by COLL

Bio-Based Gels & Porous Materials

3D printing & Rheology of Cellulose & Nanocellulose

Sponsored by CELL, Cosponsored by ANYL, BIOL and COLL

Light-Driven Chemistry: Photoelectrochemistry & Photocatalysis

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WEDNESDAY AFTERNOON

Section A

Orange County Convention Center
West Hall B4 - Theater 1

Understanding the Inorganic-Organic Interface in Colloidal Nanomaterials

Energy & Charge Transfer Interactions in Nanoparticle Complexes

V. M. Rotello, *Organizer*
H. M. Mattoussi, *Organizer, Presiding*
B. E. Cohen, *Presiding*

2:00 COLL 626. Challenging the polymer barricades around quantum dots: keeping copper ions away from the surface during click reactions. **B.E. Cohen**, V. Mann, A. Powers

2:30 COLL 627. Energy transfer controlled by the semiconductor nanocrystal to ligand interface. **E. Raulerson**

2:50 COLL 628. Understanding charge transfer from semiconductor nanocrystals to organics following LSPR excitation. **M. Blemker**

3:10 COLL 629. Investigating the energy transfer between organic and inorganic semiconductor two-dimensional material. **M.A. Mahmoud**

3:30 Intermission.



TECHNICAL PROGRAM

3:50 COLL 630. Characterizing the Brownian diffusion of nanocolloid and molecular solutions: Diffusion ordered NMR spectroscopy versus dynamic light scattering. C. Zhang, Z. Jin, G. Palui, **H.M. Mattoussi**

4:20 COLL 631. Point of anchor: Charge transfer between acetylenyl ligands and nanoparticles. **Y. Peng**, B. Lu, S. Chen

4:40 COLL 632. Dendrimer-stabilized gold nanoflowers embedded with ultrasmall iron oxide nanoparticles for multimode tumor theranostics. S. Lu, X. Li, J. Zhang, C. Peng, M. Shen, **X. Shi**

Section B

Orange County Convention Center
West Hall B4 - Theater 2

Biomaterials & Biointerfaces

Bacteria at Interfaces & Antibacterial Materials

Y. Lapitsky, R. Wylie, *Organizers, Presiding*

2:00 COLL 633. Role of shape, chemical heterogeneity, and modulus on bacterial adhesion. M. Shave, **M.M. Santore**

2:30 COLL 634. Biofilm bridge formation of *Staphylococcus aureus* biofilms, a gram positive bacteria, on slippery, lubricant-infused porous surface. **H. Valquier-Flynn**, W. Lei, J. Bruchmann, P. Levkin, T. Schwartz, C. Wilson, A.E. Holmes

2:50 COLL 635. Novel microbe-resistant hybrid membranes for healing burns, wounds, and scars. **K. Mukhopadhyay**, K. Crawford

3:10 COLL 636. Single-cell optical trapping technique for real-time antibacterial characterization of novel wound management materials. T.J. Beckmann, D. Danhausen, W. Chura, **J.J. Keleher**

3:30 COLL 637. Multiphoton, FRET-based, theranostic nanoplatfrom for two-photon bioimaging and two-photon excited photodynamic therapy of multiple drug-resistant bacteria. **P.C. Ray**

3:50 COLL 638. Metal-protein nanocomposites with bactericidal and antibiofilm efficacies. **G. Ferreres Cabanes**, K. Ivanova, A. Bassegoda, J. Torrent-Burgués, T. Tzanov

4:10 COLL 639. Nano-forest chitosan-gelatin films: An implant coating model for enhanced bone regeneration. **S. Altuntas**, H. Dhaliwal, N. Bassous, A.E. Radwan, P. Alparslan, T. Webster, F. Buyukserin, M. Amiji

4:30 COLL 640. Lectin-conjugated nanocarriers to treat chronic oral diseases. **S. Wijetunge**, Y. Sun

4:50 COLL 641. Ag-Cu alloy nanoparticle synthesis and targeting infection in osteoblast cells. **S.M. Qadri**, T. Abdulrehman, Y. Haik

5:10 COLL 642. Antibacterial polyurethane foam with incorporated lignin-capped silver nanoparticles for chronic wound treatment. **A.G. Morena**, I.S. Stefanov, T. Tzanov

Section C



TECHNICAL PROGRAM

Orange County Convention Center
West Hall B4 - Theater 3

Basic Research in Colloids, Surfactants & Interfaces

Nanocolloids: Applications

R. Nagarajan, *Organizer*
S. Menegatti, *Presiding*

2:00 COLL 643. Microfluidic synthesis of hollow nanoparticles by using flow-induced interfacial self-assembly of polystyrene-block-poly(ethylene glycol). **X. Nguyen**, H. Jeon, D. Park, J. Huh, J. Go

2:20 COLL 644. Sealable spherical mesoporous silica shell nanoreactors as fiducial nanoscale probes for x-rays. **T. Guo**

2:50 COLL 645. Tuning the surface chemistry of graphene oxide nanoparticles for controlling drug release: modeling and experiments. J.D. Schneible, K. Shi, E.E. Santiso, K.E. Gubbins, **S. Menegatti**

3:20 COLL 646. Development of magnetic surfactants for low energy separations: Effect of surfactant stability on magnetic response. **A.E. Smith**, P. Scovazzo, A.W. Fortenberry, D.M. Reed

3:40 COLL 647. Controlled assembly and reduction of graphene oxide networks for conductive composites. **M. Meloni**, S. Víctor-Román, A. King, G. Fratta, E. Istif, M. Large, M. Peláez Fernández, S. Ogilvie, R. Arenal, A. Benito, W. Maser, A. Dalton

4:00 COLL 648. Microfluidic based chips for SERS ultrasensitive detection. **S. Gómez**, D. García-Lojo, I. Pastoriza-Santos, J. Perez-Juste

4:20 COLL 649. Building random alloy surfaces from intermetallic seeds as a general route to strain-engineered electrocatalysts. **J.T. Gamler**, H. Ashberry, X. Sang, R. Unocic, S.E. Skrabalak

4:40 COLL 650. Janus liposomes: Gel-assisted formation and functionalization. **Z. Liu**

Section D

Orange County Convention Center
West Hall B4 - Theater 4

Basic Research in Colloids, Surfactants & Interfaces

Nanoparticles Synthesis & Assembly

R. Nagarajan, *Organizer*
M. Cotlet, *Presiding*

2:00 COLL 651. Formation of 2D semiconductors with mesoporosity. T. Hsieh, **Y. Liu**



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

2:20 COLL 652. Layer-dependent charge transfer kinetics in atomically thin MoS₂: PbS/CdS quantum dot hybrids. **M. Cotlet**

2:50 COLL 653. Switchable surfactants for the preparation of monodisperse, sinter-resistant, supported nanoparticle catalysts. **K.N. Bryant**, S.R. Saunders

3:10 COLL 654. Time evolution of CsPbBr₃ nanocrystal synthesis: Cesium-bromine complexation dictates growth. **J. Wen**, B. Roman, F. Rodriguez Ortiz, N. Mireles Villegas, N. Porcellino, M. Sheldon

3:30 COLL 655. Upconversion luminescence enhancement using patterned reflective surfaces with applications in security printing. A. Baride, M.Y. Hossan, A. Schaum, D. Lewis, M.T. Berry, **P.S. May**

3:50 COLL 656. Role of gold oxidation state in the synthesis of Au-CsPbX₃ heterostructure nanoparticles. **F. Rodriguez Ortiz**, B. Roman, N. Mireles Villegas, J. Wen, M. Sheldon

4:10 COLL 657. Light-assisted cation exchange in CsPbX₃ nanocrystals. **T. Qiao**, D.H. Son

4:30 COLL 658. Deposition of graphene stabilized droplets for conductive surfaces. **F. Chen**, I. George, D.H. Adamson, D. Varghese

Section E

Orange County Convention Center
West Hall B4 - Theater 5

Nanomaterials

Hierarchical & Controlled Nanomaterial Assembly: Strategies & Functionality

J. A. Hollingsworth, R. Nagarajan, *Organizers*
N. B. Shustova, *Presiding*

2:00 COLL 659. Directing nanoscale self-assembly through valence control. **O. Gang**

2:30 COLL 660. Synthetic approaches for preparation of binary, heterogeneous nanoparticle composites for solid-state photonics. **M.A. Firestone**, A. Singh, J.A. Hollingsworth, P. Welch

3:00 COLL 661. Properties of three-dimensional flow-through electrodes made from solution-synthesized metal nanowires. M. Kim, **B.J. Wiley**

3:30 COLL 662. Synthesis and characterization of stimuli responsive poly(N-vinylcaprolactum-co-itaconic acid) microgel containing silver nanoparticles with tunable optical and catalytic properties. **M. Ajmal**

3:50 COLL 663. Molecular spacing of nanostructured carbon materials for energy storage: Synthesis and characterization. **W. Hixson**, J. Zuczek, N. Elathram, N. Zelenka, M. Bonfield, J.C. Poler

4:10 COLL 664. Nanostructured graphite-based materials for hydrogen energy storage. **Y. Zhang**



TECHNICAL PROGRAM

4:30 COLL 665. Atomistic simulations of carbon nanotube deposition on functionalized silicon substrates. **Z. Shen**, R. Van Lehn, J. Dwyer, P. Gopalan

4:50 COLL 666. 3-Dimensional templates from self-assembled 2-dimensional graphene. D. Varghese, C.D. Liyanage, A.V. Dobrynin, **D.H. Adamson**

5:10 COLL 667. Optical behavior of lipid bilayer encapsulated black phosphorous. **J.A. Maurer**, S.F. Bartolucci

Section F

Orange County Convention Center
West Hall B4 - Theater 6

Surface Chemistry

Self-Assembled Monolayers & Surface Functionalization

S. L. Tait, *Organizer*

R. F. Farias Perez, E. Nakouzi, *Presiding*

2:00 COLL 668. Vapor-phase plotting of organosilane chemical gradients. **J. Bautista-Gomez**, A.V. Forzano, J.M. Austin, M.M. Collinson, D.A. Higgins

2:20 COLL 669. Optimized surface functionalization with self-assembled monolayers for enhanced alpha detection from uranium hexafluoride (UF_6). **K. Knight**, K. Charbonnet, W.A. Alexander

2:40 COLL 670. Enantiospecific interactions between chiral molecules and magnetic surfaces. **F. Tassinari**, K. Banerjee-Gosh, R. Naaman, Y. Paltiel

3:00 COLL 671. Structure and reactivity of NO_2 -functionalized N-heterocyclic carbene monolayers on Au (111) surface. **E. Gross**

3:20 COLL 672. Patterned alkylsilane self-assembled monolayers for *in vitro* study of cardiac and neurodegenerative diseases. **A. Goswami**, C. Long, J.J. Hickman

3:40 Intermission.

3:50 COLL 673. Modification of inorganic oxides with poly(hydridomethyl)siloxanes as an approach to mixed functional surfaces. R. Perez, G. Fardella, **J.W. Krumpfer**

4:10 COLL 674. Visualizing mineral-solution interfaces using 3D atomic force microscopy. **E. Nakouzi**, B.A. Legg, S. Zhang, G.K. Schenter, J. Chun, C.J. Mundy, M.D. Baer, S.N. Kerisit, J. De Yoreo

4:30 COLL 675. Robust and transparent zwitterionic polymer with antifogging and self-cleaning properties under UV irradiation. **Q. Liu**, J.J. Locklin

4:50 COLL 676. Suitable characteristics for surfactants substituent of antifoam silicon oil. **R.F. Farias Perez**, C.R. Mansur



TECHNICAL PROGRAM

5:10 COLL 677. Surface reactivity of sodium silicate glasses in aqueous environment and its effects on mechanochemical wear: a ReaxFF molecular dynamics study. **S. Hahn**, A.C. Van Duin

5:30 COLL 678. Pre-treatment of dentin with chondroitin sulfate modulates dentinal tubule occlusion by toothpaste components. **S. Saeedi**, G. Sereda

Section G

Orange County Convention Center
West Hall B4 - Theater 7

Colloidal Nanoparticle Synthesis & Assembly

O. Chen, H. Fan, T. Li, *Organizers*
F. Bai, *Organizer, Presiding*
Y. Jiang, *Presiding*

2:00 COLL 679. Evidence of stratification in binary colloidal films using microbeam small-angle X-ray scattering. **A.J. Carr**, W. Liu, K. Yager, A.F. Routh, S. Bhatia

2:20 COLL 680. Independent control of diameter and length of silver nanowires, assembly in the form of percolative networks for transparent electrodes and advanced optoelectrical characterizations in functional devices. **J. Simonato**, C. Celle, D. Toybou, D. Bellet, T. Sannicolo

2:40 COLL 681. DNA-programmed nanoparticle crystallization at interfaces. **R. Macfarlane**

3:00 COLL 682. Synthesis of Janus gold nanoprisms and high yield gold nanoprism dimers in solution. **M. Chowdhury**, C.A. Grapperhaus, M. O'Toole

3:20 COLL 683. Template-confined DNA-mediated nanoparticle assembly on surfaces. **W. Zhou**, C.A. Mirkin

3:40 Intermission.

3:50 COLL 684. Microfluidic studies of colloidal perovskite quantum dots. **M. Abolhasani**

4:10 COLL 685. Monte Carlo simulation of gold nanowire self-assembly driven by van der Waals forces. **O. Jahanmahin**, D. Kirby, C.D. Keating, K.A. Fichthorn

4:30 COLL 686. Synthesis and applications of chiral Au nanoparticles. **N. Shukla**, A. Pradhan, Y. Han, A.J. Gellman

4:50 COLL 687. Controllable synthesis and shape-directed self-assembly of gold nanoarrows. **L. Qi**

5:10 COLL 688. Effect of crystal quality on the brilliance of structural color from self-assembled colloidal crystals. **T. Liu**, B. Vansaders, S.C. Glotzer, M.J. Solomon

Section H

Orange County Convention Center
West Hall B4 - Theater 8



TECHNICAL PROGRAM

Biomembrane Synthesis, Structure, Mechanics & Dynamics

S. Muralidharan, M. Nieh, A. N. Parikh, *Organizers*
J. Katsaras, *Organizer, Presiding*
R. Tero, *Presiding*

2:00 COLL 689. Interfacial behavior between lipid films and soluble saccharides: A cooperative adsorption model. **K. Link**, G.N. Spurzem, R.A. Walker

2:20 COLL 690. Lipid-lipid interactions in *Escherichia coli* mimetic inner membrane. **J. Hoyo**, J. Torrent-Burgués, T. Tzanov

2:45 COLL 691. Quantification of weak and ultraweak carbohydrate-carbohydrate interactions in cellular recognition. **A. Janshoff**

3:10 COLL 692. Design of polymer-based asymmetric membranes and compartmentalized vesicles. L. Beaute, E. Ibarboure, J. Le Meins, O. Sandre, N. McClenaghan, **S. Lecommandoux**

3:35 COLL 693. Connecting cell plasma membrane lipid oxidation to cell dysfunction in oxygen toxicity. **K. Ren**, N. Malmstadt

4:00 COLL 694. α -Synuclein disrupts inter-membrane interactions. **P. Chung**, Z. Qingteng, H. Hwang, A. Leong, P. Maj, R. Szczygiel, E. Dufresne, S. Narayanan, E. Adams, K.C. Lee

4:25 COLL 695. Morphogenesis of lipid domains in the presence of melatonin. **D. Bolmatov**, M. Lavrentovich, J. Katsaras

4:50 COLL 696. Probing the translational dynamics of MAC-derived lipid bilayers as a component of synthetic cells. **A. Smith**, L. Keranen Burden, S. Virolainen, T. Larsen, D. Burden

Section I

Orange County Convention Center
West Hall B4 - Theater 9

Surface Chemistry of Colloidal Nanocrystals

S. Neretina, X. Xia, *Organizers*
J. Chen, D. Qin, *Organizers, Presiding*

2:00 COLL 697. Interface synthesis and machine learning for controlling stability and energy alignment of nanoparticles. **Y. Wu**

2:30 COLL 698. Collapsed polymer-protected synthesis of complex nanocrystals and their arrays. **Z. Nie**

3:00 COLL 699. Bio-inspired approaches for the generation of multifunctional inorganic nanoparticles via responsive and reactive peptide ligands. **M.R. Knecht**

3:30 Intermission.



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

3:45 COLL 700. Ion-mediated ligand exchanges in semiconductor nanocrystals. **M. Zamkov**

4:15 COLL 701. Synthesis of trimetallic nanorods and nanoframes as electrocatalysts. X. Wang, Y. Wang, **J. Zhao**

4:45 COLL 702. Synthesis and characterization of highly branched ruthenium nanoparticles for oxygen evolution reaction. **A.R. Poerwoprajitno**, L. Gloag, T. Benedetti, S. Cheong, J.D. Watt, D. Huber, J. Gooding, R. Tilley

Producing Equilibrium Amorphous Packings

Making & Transforming Stable Glasses

Sponsored by PHYS, Cosponsored by COLL and PMSE‡

Light-Driven Chemistry: Photoelectrochemistry & Photocatalysis

Sponsored by CATL, Cosponsored by COLL, ENFL, I&EC, INOR and PHYS

Bio-Based Gels & Porous Materials

Gels in Medical Applications

Sponsored by CELL, Cosponsored by ANYL, BIOL and COLL

WEDNESDAY EVENING

Hydrocarbon/Water/Mineral Interactions in the Subsurface

Sponsored by GEOC, Cosponsored by COLL

Molecular Processes at Mineral-Water Interfaces: Predictions via Linking Theory & Experiments

Sponsored by GEOC, Cosponsored by COLL

THURSDAY MORNING

Section A



TECHNICAL PROGRAM

Orange County Convention Center
West Hall B4 - Theater 1

Basic Research in Colloids, Surfactants & Interfaces

Interface Science

R. Nagarajan, *Organizer*
L. Zarzar, *Presiding*

8:30 COLL 703. Multilayering of α -alkyl ester sulfonate at the air-water interface. **P. Li**, J. Penfold, R.K. Thomas

8:50 COLL 704. Structural coloration by cascading total internal reflection and interference at microscale concave interfaces. A. Goodling, S. Nagelberg, B. Kaehr, C. Meredith, S. Cheon, A. Saunders, M. Kolle, **L.D. Zarzar**

9:20 COLL 705. Potential-induced reorganization of redox-active self-assembled monolayers in the presence of anionic surfactants. **f. ben amara**, K. Tu, A. Storelli, I. Burgess, A. Badia

9:40 COLL 706. Formation of surface multilayers at the air-water interface from sodium polyethylene glycol monoalkyl ether sulfate/AlCl₃ solutions. **J. Webster**, P. Li, J. Penfold, R.K. Thomas

10:00 COLL 707. AFM colloidal probe measurements implicate capillary condensation in punch-particle surface interactions during tableting. M. Badal Tejedor, **N. Nordgren**, M. Schueleit, A. Millqvist-Fureby, M.W. Rutland

10:20 COLL 708. Static friction of hydrogel interfaces. T. Shoaib, **R.M. Espinosa-Marzal**

10:50 COLL 709. Mapping surface wetting with trifunctional organosilanes bound at the vapor/solid interface. **J.C. Garano**, N. Kuruppu Arachchige

11:10 COLL 710. Exploration of surface cleaning and surface interactions via atomic force microscopy. **M. Belioka**, M.S. Reid, T. Pettersson

11:30 COLL 711. Probing the surface structure of fluorinated bottlebrush polymers with vibrational sum frequency generation spectroscopy and molecular dynamics simulations. **A. Chowdhury**, D. Chang, J.Y. Carrillo, Y. Ma, S.T. Retterer, K. Hong, B. Doughty

11:50 COLL 712. Development of microscopy systems for the visualization of Langmuir monolayer films. **B. Allen**, S. Croslow, A. Sostarecz

Section B

Orange County Convention Center
West Hall B4 - Theater 2

Basic Research in Colloids, Surfactants & Interfaces

Surfactant Science



TECHNICAL PROGRAM

R. Nagarajan, *Organizer*
K. Sakurai, *Presiding*

8:30 COLL 713. Multiscale approach to study molecular and interfacial characteristics of vesicles. X. Yu, **M. Dutt**

9:00 COLL 714. Structures and kinetics of monodisperse platonic micelles: Part 5. **K. Sakurai**

9:30 COLL 715. Self-assembly, rheology, and surface properties of biosurfactant-surfactant mixtures. **S. Amin**, L. Xu, Y. Zhou

9:50 COLL 716. Synergistic interaction in mixed surfactant system in presence of oil and various counter-ions: Effects on foam stability and emulsification. **S. Varade**

10:10 COLL 717. Tunable surfactant phase transition in the presence of additives: a deposition study. **R.A. Gonçalves**, B. Lindman, M.G. Miguel, T. Iwata, Y.M. Lam

10:30 COLL 718. Study of temperature-induced coacervate-to-vesicle transition of globular fusion proteins towards engineered protein vesicles. **Y. Jang**, M. Hsieh, M. Grover, J. Champion

10:50 COLL 719. Developing a data set of experimental results to support model development for simulations of the CnEm nonionic surfactants. **W.C. Swope**, M. Johnston, A. Duff, J. McDonagh, R. Anderson, G. Alva, A. Tek

11:10 COLL 720. Heads up: Molecular interactions between surfactant head groups at an oil-water interface. **R. Ciszewski**, G. Richmond

11:30 COLL 721. Poly: Gone! Desorption of polymer upon formation of bulk micelles. **B. Schabes**, E. Hopkins, G. Richmond

Section C

Orange County Convention Center
West Hall B4 - Theater 3

Basic Research in Colloids, Surfactants & Interfaces

Colloids Functionalized with Soft Matter

R. Nagarajan, *Organizer*
J. E. Smith, *Presiding*

8:30 COLL 722. Antimicrobial peptide-modified transition metal dichalcogenide nanosheets for the optical sensing of bacteria. **T. Kang**, L. Sin, I. Hwang, S. Jeon, C. Choi, J. Kim

8:50 COLL 723. Controlled fabrication of multifunctional clay/calixarene nanocomposite through ultra-fast photoinduced thiol-yne addition for an efficient heavy metal removal from industrial waste water. **K. Jlassi**, K. Eid, M. H. Sliem, A. Abdullah



TECHNICAL PROGRAM

9:10 COLL 724. Digital microfluidic applications of polymer-encapsulated quantum dot nanofluids. **N.P. Godman**, U.N. Tohgha, E.L. Alvino, S.T. Iacono

9:30 COLL 725. Structured DNA and aptamer interactions with gold nanoparticle surfaces. **J.E. Smith**

10:00 COLL 726. Shape-control, fluorescence functionality, and interfacial assemblies of polymer nanoparticles. **N.R. Visaveliya**

10:20 COLL 727. Phase transferable polymer encapsulated metallic nanoparticles. **M. Confer**, S. Street

10:40 COLL 728. Antifouling zwitterionic quantum dot surface chemistry: Impact on intracellular diffusion. **M. Debayle**, E. Balloul, F. Dembele, X. Xu, M. Hanafi, C. Monzel, M. Copepy, M. Dahan, A. Fragola, T. Pons, N. Lequeux

11:00 COLL 729. Polymeric coating of individual lead halide perovskite microcrystals in polar solvents. **S. Cho**, S. Yun

Section D

Orange County Convention Center
West Hall B4 - Theater 4

Basic Research in Colloids, Surfactants & Interfaces

Molecular & Colloidal Assemblies

R. Nagarajan, *Organizer*
J. J. Richardson, *Presiding*

8:30 COLL 730. Low temperature, polarization resolved, magneto-photoluminescence spectroscopy of individual colloidal lead salt quantum dots. **Y. Kim**, Z. Hu, A. Singh, S. Goupalov, J.A. Hollingsworth, H. Htoon

8:50 COLL 731. Formation and controlled growth of imine-linked covalent organic framework nanoparticles. **R.L. Li**, N. Flanders, A.M. Evans, W. Ji, I. Castano, N.C. Gianneschi, L.X. Chen, W.R. Dichtel

9:10 COLL 732. Nano-bionics: Assembly of functional metal-organic nanomaterials inside plants. **J.J. Richardson**, K. Liang

9:40 COLL 733. Zwitterion/thiol copolymers for antifouling. **S. Lteif**, J.B. Schlenoff

10:00 COLL 734. Probing synthesis, bandgaps and stability of a family of Cs₂AgMX₆ lead-free double perovskite nanocrystals (M = Sb, Bi, In; X = Cl, Br). **J. Dahl**, E. Chan, P. Alivisatos

10:20 COLL 735. Quantitative understanding of aggregation-induced emission with polarized resonance synchronous spectroscopy and polarized stokes'-shifted fluorescence spectroscopy. **J. Xu**, D. Zhang

10:40 COLL 736. Nonphotochemical laser-induced nucleation of a "dense liquid droplet" of aqueous glycine formed by optical gradient forces. **O. Gowayed**, J.J. Fuentes Rivera, T. Tasnim, J. Aber, B.A. Garetz

11:00 COLL 737. Iron sulfide supraparticles as artificial viruses for gene and gene editing therapies. **E.S. Turali-Emre**, A.E. Emre, N. Kotov



TECHNICAL PROGRAM

11:20 COLL 738. Self-recognition introduced by host-guest complexation in charge regulated self-assembly of gamma-cyclodextrin derivative. **J. Chen, J. Luo, T. Liu**

Section E

Orange County Convention Center
West Hall B4 - Theater 5

Nanomaterials

Metallic & Semiconducting Nanomaterials: Synthesis & Properties

J. A. Hollingsworth, R. Nagarajan, *Organizers*
Y. Kim, *Presiding*

8:30 COLL 739. One-dimensional carrier confinement in excitonic nanoshells. **L. Royo Romero, M. Zamkov**

8:50 COLL 740. Biexciton dynamics in CdS/CdSe/CdS nanoshell quantum dots. **D. Porotnikov, P. Moroz, M. Zamkov**

9:10 COLL 741. Metal amidinate precursors for general solution-phase synthesis of intermetallic nanocrystals. **A. McGrath, F. Ronning, S. Ivanov**

9:30 COLL 742. Intrinsic exciton photophysics of PbS nanocrystals revealed by low-temperature single dot spectroscopy. **Z. Hu, Y. Kim, S. Krishnamurthy, J.R. McBride, S.J. Rosenthal, J.A. Hollingsworth, H. Htoon**

9:50 COLL 743. Structural transformations of functional nanoparticles. **Z. Quan**

10:10 COLL 744. Crystal structure and optical properties of the smallest piece of metallic gold: Faradaurate-279. **N. Sakthivel, S. Theivendran, V. Ganeshraj, M. Stener, L. Sementa, A. Fortunelli, R. Guda, A.G. Oliver, A. Antonysamy**

10:30 COLL 745. Optical spectroscopy of plasmonic aerosols. **J. Geldmeier, P. Johns, N. Greybush, J. Naciri, J. Fontana**

Section F

Orange County Convention Center
West Hall B4 - Theater 6

Surface Chemistry

Nanomaterials

S. L. Tait, *Organizer*
M. Ganguly, I. Schweigert, *Presiding*

8:30 COLL 746. Controlled intra-particulate surface cross-linking synthesis of multi-color carbon dots from a single source. **I. Srivastava, T. Kampert, H. Rezvani, P. Fathi, D. Pan**



TECHNICAL PROGRAM

8:50 COLL 747. Single-step hybrid nanocoating on contact lenses to face associated conditions and discomfort. **J. Hoyo**, K. Ivanova, E. Guaus, T. Tzanov

9:10 COLL 748. Direct thermodynamic investigation of CdSe quantum dots & their ligand exchange interactions using isothermal titration calorimetry. **M.Y. Gee**, A.B. Greytak

9:30 COLL 749. Iron-oxide nanocomposites for ice nucleation and environmental remediation. **M. Ganguly**, P.A. Ariya

9:50 Intermission.

10:00 COLL 750. Use of oleophilic magnetite nanoparticles as efficient sorbent for water contaminants. **M. Sarcletti**, D. Vivod, T. Luchs, T. Rejek, L. Portilla, A. Hirsch, D. Zahn, M. Halik

10:20 COLL 751. Potent method of extracting glyphosate from water using superparamagnetic nanoparticles. **H. Park**, M. Sarcletti, M. Halik

10:40 COLL 752. Preparation of pure and decorated metal oxide materials for energy-environmental applications using novel physical deposition methods and their characterization. **D. Paradiso**, J.Z. Larese

11:00 COLL 753. Surface reactions of atmospheric species on amorphous zirconium hydroxide and hydroxylated titanium oxide from cluster models. **I. Schweigert**

Section G

Orange County Convention Center
West Hall B4 - Theater 7

Colloidal Nanoparticle Synthesis & Assembly

O. Chen, H. Fan, T. Li, *Organizers*
F. Bai, *Organizer, Presiding*
Y. Jiang, *Presiding*

8:30 COLL 754. Orientation of CdSe nanoplatelets for advanced magneto-optical characterization. **A. Brumberg**, S. Harvey, B. Diroll, B. Lee, S. Crooker, R. Schaller

8:50 COLL 755. High-temperature crystallization of nanocrystals into three-dimensional superlattices. **L. Wu**, M. Cargnello, C. Tassone

9:10 COLL 756. Self-assembling of neutral and charged nanoparticles into core-shell nanohybrids with size control. **K. Hussain**, P. Yi

9:30 COLL 757. Probing crystal growth of gibbsite and boehmite nanocrystals. **X. Zhang**, Y. Chen, J. Hu, N. Washton, C. Pearce, K. Page, Z. Wang, J.J. De Yoreo, S.B. Clark, K. Rosso

9:50 COLL 758. Reversible aggregation of covalently cross-linked gold nanocrystals by linker oxidation. **Z. Luan**, A. Abelson, M. Law

10:10 Intermission.



TECHNICAL PROGRAM

10:20 COLL 759. Base side of noble-metal clusters: An efficient route to exceptional captamine-protected gold, $Au_n(\text{DMAET})_p$, $n = 25 - 144$. **M. Hoque**, D.M. Black, K. Mayer, R.L. Whetten

10:40 COLL 760. Coupling radio- and photo-luminescent emitters in crystalline colloidal arrays. M. Burdette, I. Bandera, G. Gray, **S.H. Foulger**

11:00 COLL 761. Towards precise control of colloidal plasmonic nanoparticles: Synthesis and surface engineering. **G. Chen**, R. Gallagher, X. Zhang

11:20 COLL 762. Effect of pH on the synthesis of monodispersed gold bipyramids with finely tunable LSPR peaks. **X. Zhang**, R. Gallagher, D. Lawrence, G. Chen

11:40 COLL 763. Circularly polarized light-driven assembly of gold nanostructures and their chirality measure. **J. Kim**, J. Yeom, H. Calcaterra, G. Zhao, P. Zhang, N. Kotov

Section H

Orange County Convention Center
West Hall B4 - Theater 8

Biomembrane Synthesis, Structure, Mechanics & Dynamics

J. Katsaras, M. Nieh, A. N. Parikh, *Organizers*
S. Muralidharan, *Organizer, Presiding*

8:30 COLL 764. Investigating the physical presence of vitamin E in lipid membranes. **M. DiPasquale**, M.H. Nguyen, B. Rickeard, D. Marquardt

8:50 COLL 765. Hybrid polymer/lipid vesicles made from amphiphilic block copolymer poly(dimethylsiloxane)-b-poly(ethylene oxide) as cell-membrane-mimic: Formation, structure, and membrane properties. **M. Fauquignon**, E. Ibarboure, M. Schmutz, A. Brulet, J. Le Meins

9:10 COLL 766. Molecular thermodynamics of receptor competition for uptake by endocytosis. **A. DeGroot**, C. Zhao, C. Hayden, S. Mihelic, M. LaMonica, J. Stachowiak

9:30 COLL 767. Compartments and crowding: Biophysical features of living cells. **W. Su**, D.L. Gettel, M. Chabanon, P. Rangamani, A.N. Parikh

9:50 COLL 768. Activation of the EphA2 receptor tyrosine kinase by a conditional transmembrane peptide. **F.N. Barrera**

10:15 COLL 769. Direct cytosolic delivery of macromolecules via connectosomes. **C. Zhao**, A. Meriwether, H. Ali, M. Wu, J. Stachowiak

10:35 COLL 770. Supported lipid bilayers of *Escherichia coli* extracted lipids and their substrate and calcium dependence. **Y. Kakimoto**, R. Tero

10:55 COLL 771. Lipids alter rhodopsin function via solvent-like and ligand-like interactions. **L. Salas**, N. Leioatts, A. Grossfield



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

11:15 COLL 772. Cholesterol-induced microdomains formation in completely miscible lipid bilayers which promotes the fusion of proteoliposome. **M.W. Goh**, A. Hirano-Iwata, M. Niwano, R. Tero

11:35 COLL 773. Investigating interactions and stability of bacteriorhodopsin upon entrapment in sol-gel derived porous materials. **S. Gakhar**, K. Johnson, C. Tan, S. Risbud, M.L. Longo

11:55 COLL 774. Sizes and yields of giant unilamellar vesicles using cellulose paper and cotton fabric. **J. Pazzi**, M. Xu, A. Subramaniam

Section I

Orange County Convention Center
West Hall B4 - Theater 9

Surface Chemistry of Colloidal Nanocrystals

J. Chen, S. Neretina, *Organizers*
D. Qin, X. Xia, *Organizers, Presiding*

8:30 COLL 775. Multi-coordinating polymer ligand for the functionalization of semiconductor, metal, and metal-oxide nanoparticles. **L. Du**, W. Wang, C. Zhang, Z. Jin, G. Palui, H.M. Mattoussi

8:50 COLL 776. Interchange of L-, Z-, and bound-ion-pair X-type ligation on cadmium selenide quantum belts. **Y. Yao**, W.E. Buhro

9:10 COLL 777. Controlled synthesis of single and binary alkanethiolate-capped Pd nanoparticle catalysts for understanding the isolated effects of surface ligands. **Y. Shon**

9:30 COLL 778. Molecular dynamics simulations of metastable peptide crystals: A cross beta transformation and selective adsorption of charged gold nanoparticles. **P. Rehak**, P. Kral

9:50 Intermission.

10:05 COLL 779. Ligand exchange on ternary sodium bismuth dichalcogenide using multidentate ligands. **A.M. Medina-Gonzalez**, B.A. Rosales, J. Vela

10:25 COLL 780. Ligand design for direct optical (254nm, 365nm and 405 nm) and e-beam lithography of functional all-inorganic nanomaterials. **Y. Wang**, J. Pan, D. Talapin

10:45 COLL 781. Photoligation with lipoic acid ligands is an effective strategy for preparing biocompatible gold colloids. **Z. Jin**, Y. Sugiyama, C. Zhang, L. Du, H.M. Mattoussi

11:05 COLL 782. Basal plane functionalization of group V and VI layered transition metal dichalcogenides. **A. Jawaid**, R.A. Vaia

Producing Equilibrium Amorphous Packings



TECHNICAL PROGRAM

Hard Spheres & Jammed Systems

Sponsored by PHYS, Cosponsored by COLL and PMSE†

Bio-Based Gels & Porous Materials

Nanostructuration of Gels & Aerogels & their Use as Sensors

Sponsored by CELL, Cosponsored by ANYL, BIOL and COLL

THURSDAY AFTERNOON

Producing Equilibrium Amorphous Packings

Glass Transition in Bulk & in Thin Films

Sponsored by PHYS, Cosponsored by COLL and PMSE

Bio-Based Gels & Porous Materials

Gels, Aerogels & Carbogels

Sponsored by CELL, Cosponsored by ANYL, BIOL and COLL

COMP

Division of Computers in Chemistry

H. Woodcock and J. Shen, *Program Chairs*

SUNDAY MORNING

Section A

Orange County Convention Center
West Hall B4 - Theater 21

Electron-Molecule & Molecule-Molecule Interactions



TECHNICAL PROGRAM

Cosponsored by PHYS†
R. Kumar, J. P. Simons, *Organizers*
F. Wang, *Organizer, Presiding*
K. B. Bravaya, M. F. Falcetta, *Presiding*

8:30 COMP 1. Model Hamiltonians for characterizing non-valence correlation-bound anions of molecules and clusters. **K.D. Jordan**, T. Choi

9:00 COMP 2. How Ken Jordan enhanced my life and scholarly career. **J.P. Simons**

9:30 COMP 3. Rydberg anions, solvated-electron precursors, and their Dyson orbitals. **J.V. Ortiz**

10:00 COMP 4. Prediction and characterization of a non-valence temporary anion shape resonance for a model (H₂O)₄ system. **M.F. Falcetta**, D.N. Maienshein, M.C. Fair, A. Kairalapova, K.D. Jordan

10:30 Intermission.

10:50 COMP 5. Chemistry driven by electrons: Metastable electronic states and spin-forbidden processes. **K.B. Bravaya**

11:20 COMP 6. Predicting the electron binding energies of dipole-bound anions via quantum Monte Carlo. **B.M. Rubenstein**, H. Hao, J. Shee, S. Upadhyay, C. Ataca, K.D. Jordan

11:50 COMP 7. Ring-opening attachment: How electron-attachment at energies substantially above threshold can produce long-lived anions. **T. Sommerfeld**

Section B

Orange County Convention Center
West Hall B4 - Theater 22

Computational Modeling in Two-Dimensional Materials & Heterostructures

E. Durgun, T. Low, *Organizers*
O. Ozelik, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 COMP 8. Electronic and thermal transport in two-dimensional materials from first-principles. **N. Marzari**

9:00 COMP 9. First-principles simulations of excited electronic states: Optical properties, particle radiation, and heterojunctions. **A. Schleife**

9:25 COMP 10. Structural and electronic phases of 2D transition metal dichalcogenides. **O.V. Yazyev**

9:50 COMP 11. Silicene, germanene, and stanene: Novel elemental 2D artificial allotropes of Si, Ge and Sn. **G. Le Lay**

10:15 Intermission.



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

10:35 **COMP 12.** Electronic properties of excitons in gapped chiral fermion systems. **D. Xiao**

11:00 **COMP 13.** Control of electronic properties of two-dimensional materials: Bilayer graphene, porous crystalline 2D materials, and heterostructures. **J.L. Mendoza-Cortes**

11:25 **COMP 14.** First-principles modeling of electron dynamics and transport in disordered two-dimensional materials. **K. Kaasbjerg**

11:50 **COMP 15.** Advances in *ab initio* calculations of light-matter interaction in two-dimensional transition metal dichalcogenides. **M. Bernardi**

Section C

Orange County Convention Center
Room W308B

Machine Learning in Chemistry

C. M. Aikens, *Organizer*
A. E. Roitberg, S. Varma, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 **COMP 16.** Towards efficient, accurate, scalable, and transferable quantum machine learning with AM-ons: The DNA of chemistry. **B. Huang**, A. von Lilienfeld

9:05 **COMP 17.** Machine learning of electron densities, energies, and free energies: Bypassing the Schrödinger equation and costly phase-space integrals. **M.E. Tuckerman**

9:35 **COMP 18.** Deep learning of quantum chemical Hamiltonians. **D. Yaron**, H. Li, C. Collins

10:05 Intermission.

10:20 **COMP 19.** Predicting new molecular properties with multimodal learning. **O. Isayev**

10:50 **COMP 20.** All-in-one general purpose ML potential with long-range physics. **J.S. Smith**, B.T. Nebgen, N. Lubbers, O. Isayev, A.E. Roitberg, K. Barros, S. Tretiak

11:20 **COMP 21.** Accelerating *ab initio* simulation using surrogate machine learning models. **J.A. Garrido Torres**, P.C. Jennings, M.H. Hansen, T. Bligaard

11:40 **COMP 22.** Speeding up atomistic structural search with machine learning. **B. Hammer**

Section D

Orange County Convention Center
West Hall B4 - Theater 23



TECHNICAL PROGRAM

Drug Design

QSAR

M. R. Landon, Y. Tseng, *Organizers*
N. Giddings, *Presiding*

8:30 COMP 23. Protein interaction atlas for prediction of genetic variations involved in drug interactions and disease development. **D. Janezic**, J. Konc

8:50 COMP 24. *N*- and *S*-oxidation model of the flavin-containing monooxygenases. **P.J. Walton**, M. Öeren, P.A. Hunt, M.D. Segall

9:10 COMP 25. Matched molecular pairs analysis for the prediction of cytosol-mediated metabolic liabilities. **V. Siramshetty**, P. Shah, D. Nguyen, A. Zakharov, N. Southall

9:30 Intermission.

9:45 COMP 26. *In silico* approach on designing bisindole derivatives as carbonic anhydrase II inhibitor. **N. Misral**, **N. Arasid**, S. Hasbullah

10:05 COMP 27. Crystallization inhibition properties of cellulose esters and ethers for a group of chemically diverse drugs: Experimental and computational insight. L.I. Mosquera-Giraldo, **C.H. Borca**, A.S. Parker, Y. Dong, K.J. Edgar, S.P. Beaudoin, L.V. Slipchenko, L. Taylor

10:25 COMP 28. AI-driven QSAR modeling of P450-mediated drug metabolism. **A. Zakharov**, E. Gonzalez, P. Shah, D. Nguyen, N. Southall, N. Torimoto-Katori, S. Sakamuru, M. Xia, T. Zhao, R. Obach, C.E. Hop, A. Simeonov, X. Xu

10:45 COMP 29. Affinity and selectivity determinants of bitropic ligands targeting D2 and D3 dopamine receptors. **H.S. Hayatshahi**, R. Luedtke, J. Liu

11:05 COMP 30. Anticipating human metabolites *in silico*: An antimalarial case study. **R.D. Clark**

Section E

Orange County Convention Center
West Hall B4 - Theater 24

Molecular Mechanics

J. Shen, *Organizer*
C. Devereux, *Presiding*

8:30 COMP 31. Kirkwood-Buff derived force field for peptides and proteins. S. Karunaweera, E.A. Ploetz, **P.E. Smith**

9:00 COMP 32. Contributions to the isothermal compressibility of globular proteins provided by a fluctuation solution theory analysis of molecular dynamics simulations. **E.A. Ploetz**, N.L. Kariyawasam Manachchige, P.E. Smith



TECHNICAL PROGRAM

9:15 **COMP 33.** Coarse-grained simulation of cation interactions with lipid bilayers. **R.D. Hills**

9:45 **COMP 34.** Atomistic approach toward modelling additive machining. **J.J. Karnes**, T. Weisgraber, J.S. Oakdale, J. Biener

10:00 **COMP 35.** Markov state model analysis of the protein binding interactions of the Barnase-Barstar complex. **Z. He**, F. Paul, B. Roux

10:15 Intermission.

10:30 **COMP 36.** Polarizable coarse grain force field for metallic systems: A discrete interacting multipole model. **Z. Rinkevicius**, P. Palevicius, M. Kaminskas, K. Bockute, M. Ragulskis, G. Laukaitis

11:00 **COMP 37.** Ion-hydroxyl interactions: From high-level quantum benchmarks to transferable polarizable force fields. **V. Wineman-Fisher**, Y. Al-Hamdani, I. Adduo, A. Tkatchenko, S. Varma

11:15 **COMP 38.** No more histograms: Variational and Bayesian approaches to estimating potentials of mean force. **M.R. Shirts**, A. Ferguson

11:45 **COMP 39.** REVO: Resampling of Ensembles by Variance Optimization. **N. Donyapour**, A. Dickson

12:00 **COMP 40.** Calculating free-energy differences by conveyor belt thermodynamic integration. **D. Hahn**, P. Hunenberger

12:15 **COMP 41.** Conformational free-energy surface of cyclooctane in the collective variables space from autoencoder neural network. **M. Lee**, B. Seo, S. Kim, Y. Lee, W. Lee

Section F

Orange County Convention Center
West Hall B4 - Theater 25

Sampling Conformations & Pathways in Biomolecular Systems: Recent Developments & Applications

A. Ma, P. Tiwary, W. Yang, *Organizers*
G. A. Voth, *Presiding*

8:30 **COMP 42.** Equilibrium and nonequilibrium modeling of biomolecular machines. **R. Elber**

9:00 **COMP 43.** Quantitative characterization of mechanism using pathway histograms. **D.M. Zuckerman**, E. Suarez, J. Copperman

9:30 **COMP 44.** Protein-protein binding pathways and calculations of rate constants using fully continuous explicit solvent simulations. **L.T. Chong**

10:00 Intermission.

10:45 **COMP 45.** Mapping the ligand-binding landscape. **A. Dickson**



TECHNICAL PROGRAM

11:15 COMP 46. Exact construction of probability landscapes and global flow maps of discrete flux of stochastic networks without Monte Carlo sampling or Fokker-Planck approximations. **J. Liang**

11:45 COMP 47. Free energy, kinetics, and reaction coordinates of biomolecular processes from transition path sampling simulations. **P. Bolhuis**

Advances in Data Collection & Analysis of Biomolecular Structures

Sponsored by PHYS, Cosponsored by COMP

Computational Methods in Lanthanide & Actinide Chemistry

Sponsored by NUCL, Cosponsored by COMP and INOR

Carbon Dioxide Conversion & Utilization

CO₂ Hydrogenation to Fuels & Chemicals

Sponsored by ENFL, Cosponsored by CATL, COMP and GEOC

Data Science for Catalysis Research

Sponsored by CATL, Cosponsored by CINF, COMP and ENFL

Quantum Embedding Electronic Structure Methods

Sponsored by PHYS, Cosponsored by COMP

Computational Electrocatalysis

Sponsored by CATL, Cosponsored by COMP and ENFL

Sustainable Software for Computational Molecular Science



TECHNICAL PROGRAM

Interoperability & Reproducibility in the Computational Molecular Sciences

Sponsored by PHYS, Cosponsored by COMP

Advances in Methods for Comparing Molecular & Supramolecular Simulations to Experiments

Sponsored by CATL, Cosponsored by CINF, COMP and PHYS

SUNDAY AFTERNOON

Section A

Orange County Convention Center
West Hall B4 - Theater 21

Electron-Molecule & Molecule-Molecule Interactions

Cosponsored by PHYS†
J. P. Simons, F. Wang, *Organizers*
R. Kumar, *Organizer, Presiding*
D. D. Sherrill, V. K. Voora, *Presiding*

1:30 COMP 48. Adventures with ions: Insights in the spectral signatures of large amplitude vibrations in ion/water complexes. **A.B. McCoy**, R.J. DiRisio, M. Boyer, M.J. Joyner

2:00 COMP 49. Variational random phase approximation method for accurate ionization potentials and interaction energies. **V.K. Voora**, S. Balasubramani, F.U. Furché

2:30 COMP 50. Equation of motion coupled-cluster theory: Adventures beyond the CCSD level. **J. Stanton**

3:00 COMP 51. Trapping and characterization of reaction intermediates in proton coupled electron transfer and CO₂ activation with cryogenic ion chemistry and spectroscopy. **M.A. Johnson**

3:30 Intermission.

3:50 COMP 52. Systematic studies of non-covalent interactions in clusters and condensed phases. **D.D. Sherrill**

4:20 COMP 53. Improving the accuracy of diffusion Monte Carlo nodal surfaces through multi-determinant trial wavefunctions for molecules and solids. K. Gasperich, T. Applencourt, A. Scemama, E. Giner, K.D. Jordan, M. Caffarel, **A. Benali**

4:50 COMP 54. Dissociative electron attachment in microhydrated molecules. **J. Fedor**

Section B

Orange County Convention Center
West Hall B4 - Theater 22



TECHNICAL PROGRAM

Computational Modeling in Two-Dimensional Materials & Heterostructures

T. Low, O. Ozcelik, *Organizers*
E. Durgun, *Organizer, Presiding*

1:30 COMP 55. Topics of two-dimensional materials and their heterostructures. **M. Chou**

1:55 COMP 56. Tuning the electronic and optical properties of phosphorene. **F. Peeters**

2:20 COMP 57. Exploring MXenes/graphene heterostructures for ion battery applications from first-principles. I. Demiroglu, Y. Aierken, F. Peeters, D. Cakir, C. Sevik, **O. Gulseren**

2:45 COMP 58. Modeling 2D materials with electron correlations and randomly distributed defects. **D. Gunlycke**

3:10 Intermission.

3:25 COMP 59. Nanophononic devices based on two-dimensional materials: Multiscale modeling. **D. Donadio**, S. Chen, C.A. Sievers, G. Barbalinardo

3:50 COMP 60. Exploring $PtX_nY_{(2-n)}$ ($X, Y = S, Se$ and Te ; $0 \leq n \leq 2$) monolayers: Is Janus $PtXY$ the most favorable one? F. Ersan, **C. Ataca**

4:15 COMP 61. Structural and electronic properties of monolayer group III monochalcogenides. S. Demirci, N. Avazli, E. Durgun, **S. Jahangirov**

4:40 COMP 62. Tackling electrons in two-dimensional materials for electronic and energy applications. **Y. Liu**

5:05 COMP 63. Wave function engineering of van der Waals heterostructures: Structural and electronic properties. **O. Ozcelik**, A. Chaves, J. Azadani, M. Fathi, T. Low

Section C

Orange County Convention Center
Room W308B

Machine Learning in Chemistry

C. M. Aikens, *Organizer*
A. E. Roitberg, S. Varma, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 COMP 64. Deep and generative learning for structure-based drug design. **D. Koes**

2:05 COMP 65. Recurrent neural network modeling of molecular data sequentialized in time and space. **J. Sunseri**, D. Koes



TECHNICAL PROGRAM

2:25 **COMP 66.** Distance-based Boolean applicability domain for category QSAR. **F. Berenger**, Y. Yamanishi

2:45 **COMP 67.** Mindfulness and care of the foundation of AI. **T.R. Stouch**

3:05 **COMP 68.** Comparison of random forest and deep learning approaches for ADMET endpoint prediction. E.N. Feinberg, V.S. Pande, **A.C. Cheng**

3:35 Intermission.

3:50 **COMP 69.** Machine learning methods to evaluate correlations and causalities in allosteric signaling in proteins. **S. Varma**

4:20 **COMP 70.** Machine learning to predict molecular interactions. **J. Cheoh**

4:40 **COMP 71.** PotentialNet for molecular property prediction. **E.N. Feinberg**, V.S. Pande

5:00 **COMP 72.** Learning molecular models from microscopic simulation and experimental data. **C. Clementi**

Section D

Orange County Convention Center
West Hall B4 - Theater 23

Undergraduate Research Roundtable & Career Panel

M. C. Nagan, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 **COMP 73.** Modeling Fe(II)-based chromophores for solar energy conversion with quantum mechanical calculations. **E. Jakubikova**

2:25 **COMP 74.** Delineating function from protein conformational ensembles. **D. Hamelberg**

3:15 Discussion.

4:05 Intermission.

4:20 Panel Discussion.

5:10 Concluding Remarks.

Section E

Orange County Convention Center
West Hall B4 - Theater 24

Molecular Mechanics: Computational Studies of Transmembrane Proteins



TECHNICAL PROGRAM

J. Shen, *Organizer*
F. Samarjeet, *Presiding*

1:30 COMP 75. Multimodal control of membrane protein function by biological membranes. **E. Tajkhorshid**

2:00 COMP 76. Interfacial activation of lipolytic enzymes by cellular membranes. **V. Mouchlis**, D. Hayashi, J.A. McCammon, E.A. Dennis

2:15 COMP 77. Molecular dynamics of potassium channel permeation, selectivity, and gating. **B.L. de Groot**

2:45 COMP 78. Activation of Hv1 by constant pH molecular dynamics. **J. Henderson**, R. Harris, Y. Huang, J. Shen

3:00 COMP 79. Elucidating mechanisms of substrate transport via membrane transporters. **D. Shukla**

3:30 Intermission.

3:45 COMP 80. Molecular mechanism of GPCR-mediated arrestin activation. **R.O. Dror**

4:15 COMP 81. Structure, dynamics, and activation of the CGRP receptor, a medically important class B GPCR. **C.A. Reynolds**

4:45 COMP 82. Impact of lipid interactions and receptor conformation on GPCR dynamics revealed by MD simulations in *in-vivo* mimetic membranes. **W. Song**, M.S. Sansom

5:00 COMP 83. Extended eighth-shell method for periodic boundary conditions with rotations. **F. Samarjeet**, B. Brooks, A.C. Simmonett

5:15 COMP 84. Simulations of hydrophobic gating in an ion channel: TMEM175. **C.I. Lynch**, S. Rao, G. Klesse, M.S. Sansom

Section F

Orange County Convention Center
West Hall B4 - Theater 25

Sampling Conformations & Pathways in Biomolecular Systems: Recent Developments & Applications

A. Ma, P. Tiwary, *Organizers*
W. Yang, *Organizer, Presiding*

1:30 COMP 85. Recent advances in systematic bottom-up coarse-graining. **G.A. Voth**

2:00 COMP 86. Free energy landscapes and mechanistic pathways of catalytic reactions of serine hydroxymethyltransferase in aqueous medium. **A. Chandra**, K. Soniya

2:30 COMP 87. Structural studies of peptide/surface interactions using a high-dimensional enhanced sampling scheme. **J. Pfaendtner**



TECHNICAL PROGRAM

3:00 Intermission.

3:45 **COMP 88.** Recent developments and applications of variationally enhanced sampling. **O. Valsson**

4:15 **COMP 89.** Free-energy simulations in explicit and implicit solvent models on GPUs. E. King, R. Qi, **R. Luo**

4:45 **COMP 90.** Quantifying protein-ligand recognition pathways. N. Ahalawat, **J. Mondal**

Advances in Data Collection & Analysis of Biomolecular Structures

Sponsored by PHYS, Cosponsored by COMP

Computational Methods in Lanthanide & Actinide Chemistry

Sponsored by NUCL, Cosponsored by COMP and INOR

Carbon Dioxide Conversion & Utilization

CO₂ Conversion to Carbonates

Sponsored by ENFL, Cosponsored by CATL, COMP and GEOC

Data Science for Catalysis Research

Sponsored by CATL, Cosponsored by CINF, COMP and ENFL

Modeling Dynamics in Dense Manifolds of Electronic States

Electronic Structure

Sponsored by PHYS, Cosponsored by COMP[†]

Quantum Embedding Electronic Structure Methods

Sponsored by PHYS, Cosponsored by COMP



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

Computational Electrocatalysis

Sponsored by CATL, Cosponsored by COMP and ENFL

Advances in Methods for Comparing Molecular & Supramolecular Simulations to Experiments

Sponsored by CATL, Cosponsored by CINF, COMP and PHYS

Sustainable Software for Computational Molecular Science

Workflows

Sponsored by PHYS, Cosponsored by COMP

MONDAY MORNING

Section A

Orange County Convention Center
West Hall B4 - Theater 21

Electron-Molecule & Molecule-Molecule Interactions

Cosponsored by PHYS[‡]
R. Kumar, F. Wang, *Organizers*
J. P. Simons, *Organizer, Presiding*
J. A. Piquemal, K. Szalewicz, *Presiding*

8:30 COMP 91. Some recent developments in energy decomposition analysis of electronic structure calculations. **M.P. Head-Gordon**

9:00 COMP 92. Nuclear dynamics with accurate force fields from quantum mechanics. **K. Szalewicz**

9:30 COMP 93. Energy decomposition analysis of molecular properties. **D. Lambrecht**

10:00 Intermission.

10:20 COMP 94. Energy landscapes and molecule-molecule interactions. **D. Wales**

10:50 COMP 95. Accurate and scalable polarizable force fields for molecular simulation: The road ahead. **J.A. Piquemal**

11:20 COMP 96. Advanced force fields with anisotropic atomic polarizability and charge transfer and solved with SCF-less methods. **T.L. Head-Gordon**



TECHNICAL PROGRAM

Section B

Orange County Convention Center
West Hall B4 - Theater 22

Drug Design in the 21st Century: Where Computational Methods Are & Are Not Useful

K. P. Cusack, M. Z. Hoemann, *Organizers*
T. Vargo, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 COMP 97. From genome variations to drug targets. **O. Lichtarge**

9:05 COMP 98. Recent advances in Rosetta protein structure prediction methods. **H. Park**, D. Baker

9:35 COMP 99. Case studies in computational drug discovery. **D. Koes**

10:05 COMP 100. Finding new chemical matter using electrostatic and shape-based approaches: Successes and failures.
T. Cheeseright, M.D. Mackey

10:30 Intermission.

10:35 COMP 101. Predicting CYP-mediated metabolism, drug-drug interaction, and toxicity. **N. Moitessier**

11:05 COMP 102. Structural analysis of ROR γ inverse agonists. **M. Argiriadi**, W. Qiu, A. Korepanova, J. Amaudrut, P. Bodelle, E. Breinlinger, K.P. Cusack, P. Masson, O. Poupardin, D. Potin, M.E. Kort

11:30 COMP 103. Atomistic modeling of protein-ligand binding: Successes, limitations, and opportunities. **R. Abel**, L. Wang, E. Harder, S. Bhat, K. Konze, K. Leswing, P. Bos, M. Dahlgren, H. Yu, G. Ross

11:55 COMP 104. Leveraging design and synthesis concepts and project tractability. **S. Van Epps**

Section C

Orange County Convention Center
Room W308B

Machine Learning in Chemistry

C. M. Aikens, *Organizer*
A. E. Roitberg, S. Varma, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 COMP 105. ANAKIN-ME: Using deep learning to develop a fully-transferable and chemically accurate GPU-accelerated potential. **A.E. Roitberg**



TECHNICAL PROGRAM

9:05 **COMP 106.** Machine learning architectures to enhance chemical functional group predictions. **J. Fine**, A.A. Rajasekar, **G. Chopra**

9:25 **COMP 107.** Travelling through levels of resolution with machine-learning methods. **T. Lemke**, S. Hunkler, O. Kukhareenko, C. Peter

9:55 **COMP 108.** Active search for organic functional materials with artificial intelligence. **D.P. Tabor**

10:25 Intermission.

10:40 **COMP 109.** Data-driven, many-body molecular models with chemical and spectroscopy accuracy. **F. Paesani**

11:10 **COMP 110.** Towards exact molecular dynamics simulations with machine-learned force fields. **S. Chmiela**, H. Sauceda, K. Müller, A. Tkatchenko

11:40 **COMP 111.** Thermal stability of 2D materials: Descriptor realization from machine learning. **G.R. Schleder**, **A. Fazio**

12:00 **COMP 112.** Machine learning for molecular properties. **S. Tretiak**

Section D

Orange County Convention Center
West Hall B4 - Theater 23

Probing Reactive Intermediates through Chemical Computations

S. Kim, R. S. Paton, S. Vyas, *Organizers, Presiding*

8:30 Introductory Remarks.

8:40 **COMP 113.** Dynamic effects on fates of reactive intermediates. **D.J. Tantillo**

9:10 **COMP 114.** Dynamics of entropic intermediates and nonclassical carbocations. **K.N. Houk**, T. Benton, C. Jamieson, X. Xue

9:40 **COMP 115.** DFT analysis of organotin catalytic mechanisms in polymeric reactions. **J.A. Clark**, E.E. Santiso

10:00 Intermission.

10:15 **COMP 116.** Transition metal catalyzed reactions: From mechanistic studies to computational predictions. **O. Wiest**, B. Tutkowski, P. Helquist, P. Norrby

10:45 **COMP 117.** Discovering and breaking design rules in single-site catalysis with new computational tools. **H.J. Kulik**

11:15 **COMP 118.** Understanding the steric and electronic effects in nucleophilic additions to 3-phosphonyl arynes. **J. Scanlon**, P. Willoughby, J. Lilly, G. Mraz



TECHNICAL PROGRAM

11:35 Concluding Remarks.

Section E

Orange County Convention Center
West Hall B4 - Theater 24

Simulation of Protein-Membrane Interfaces

A. Gorfe Abebe, *Organizer*
M. Buck, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 **COMP 119.** New membrane burial potential used in force-induced unfolding simulations of membrane proteins. Z. Wang, J.M. Jumper, K.F. Freed, **T.R. Sosnick**

9:05 **COMP 120.** Understanding molecular mechanisms in oncogenic proteins through high-throughput mutagenesis: Application to Ras. **J. Kuriyan**

9:35 **COMP 121.** Visualizing molecular mechanisms of lipid modulation of protein function with advanced simulation techniques. **E. Tajkhorshid**

10:05 **COMP 122.** Conformational coupling across domains of the serotonin-bound full length 5HT_{3A} receptor revealed by Cryo-EM. **Y. Gicheru**, S. Basak, S. Rao, M.S. Sansom, S. Chakrapani

10:20 Intermission.

10:35 **COMP 123.** Activation dependent G-protein-coupled receptor-membrane interactions. **Y. Miao**, A. Bhattarai, J. Wang

10:50 **COMP 124.** Membrane pore formation by antimicrobial, lytic, and designed peptides. **T. Lazaridis**

11:20 **COMP 125.** Exploring the mechanism of the antifungal lipopeptide fengycin using molecular simulations. S. Sur, **A. Grossfield**

11:50 **COMP 126.** Studies of a peripheral membrane protein in yeast (Osh4) and its peptide that senses lipid packing. **J.B. Klauda**

Section F

Orange County Convention Center
West Hall B4 - Theater 25

Sampling Conformations & Pathways in Biomolecular Systems: Recent Developments & Applications

A. Ma, P. Tiwary, W. Yang, *Organizers*
P. Bolhuis, *Presiding*



TECHNICAL PROGRAM

8:30 COMP 127. Using long-timescale molecular dynamics simulations to benchmark enhanced sampling methods. **A.C. Pan**

9:00 COMP 128. Enhanced sampling, free energy calculations, and drug discovery. **L. Wang**, E. Harder, R. Abel, Y. Wu, Y. Deng, J. Kaus

9:30 COMP 129. Sampling conformational changes and ligand binding pathways in kinases and GPCRs with enhanced-sampling algorithms. **F. Gervasio**

10:00 Intermission.

10:45 COMP 130. Free-energy landscapes of protein-ligand binding by generalized REST. **Y. Sugita**

11:15 COMP 131. Adaptive dynamic reporting: A novel enhanced sampling method. **K. Corbett**, L. Zheng, D. Wu, W. Yang

11:45 COMP 132. Gaussian accelerated molecular dynamics (GaMD): Enhanced sampling of ligand binding and protein-protein interactions. **Y. Miao**, A. Bhattarai, J. Wang

Advances in Data Collection & Analysis of Biomolecular Structures

Sponsored by PHYS, Cosponsored by COMP

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Sponsored by PROF, Cosponsored by AGFD, ANYL, BIOL, BIOT, CARB, CELL, CHED, CMA, COLL, COMP, ENVR, GEOC, I&EC, MEDI, MPPG, NUCL, ORGN, PHYS, PMSE, POLY, PRES, WCC and YCC

Carbon Dioxide Conversion & Utilization

CO2 Capture & Separation

Sponsored by ENFL, Cosponsored by CATL, COMP and GEOC

Data Science for Catalysis Research

Sponsored by CATL, Cosponsored by CINF, COMP and ENFL

Modeling Dynamics in Dense Manifolds of Electronic States



TECHNICAL PROGRAM

Light-Matter Interaction

Sponsored by PHYS, Cosponsored by COMP

Quantum Embedding Electronic Structure Methods

Sponsored by PHYS, Cosponsored by COMP

Computational Electrocatalysis

Sponsored by CATL, Cosponsored by COMP and ENFL

Sustainable Software for Computational Molecular Science

Experiences & Challenges Developing Open & Modular Software

Sponsored by PHYS, Cosponsored by COMP

MONDAY AFTERNOON

Section A

Orange County Convention Center
West Hall B4 - Theater 21

Electron-Molecule & Molecule-Molecule Interactions

Cosponsored by PHYS†

R. Kumar, J. P. Simons, *Organizers*

F. Wang, *Organizer, Presiding*

S. S. Iyengar, J. A. Steckel, *Presiding*

1:30 COMP 133. Natural representation of molecular polarizability for efficient QM/MM simulations. K. Wolinski, **P. Pulay**

2:00 COMP 134. Non-covalent interactions in synthetic foldamers and peptide ions: When intramolecular looks like intermolecular. K.N. Blodgett, C.P. Harrilal, **T.S. Zwier**, J.L. Fischer

2:30 COMP 135. Adiabatic, sudden, and non-adiabatic processes in photoelectron spectroscopies involving samarium rich homo- and hetero-lanthanide oxides. **S.S. Iyengar**, C. Jarrold

3:00 COMP 136. Electron-molecule reactions probed by 2D and time-resolved photoelectron imaging. **J.R. Verlet**

3:30 Intermission.



TECHNICAL PROGRAM

3:50 COMP 137. Honoring Ken Jordan: Water, water everywhere! **G.C. Shields**

4:20 COMP 138. High-throughput calculations of metal organic frameworks: Mixed matrix membranes for carbon capture. **J.A. Steckel**, S. Budhathoki, P. Boone, C.E. Wilmer

4:50 COMP 139. Dispersion. **M.S. Gordon**

Section B

Orange County Convention Center
West Hall B4 - Theater 22

ACS Award for Research at an Undergraduate Institution: Symposium in Honor of Carol A. Parish

Cosponsored by PROF
H. L. Woodcock, *Organizer*
B. Miller, *Organizer, Presiding*

1:30 COMP 140. Honoring Carol Parish: MERCURY, mentoring, and undergraduate research. **G.C. Shields**

2:00 COMP 141. Development of OPLS-AA force field parameters for deep eutectic solvent simulations. **B. Doherty**, O. Acevedo

2:20 COMP 142. Janus: An open-source python library for the use and implementation of adaptive QM/MM methods. **B. Zhang**, D. Altarawy, T. Barnes, J. Turney, H.F. Schaefer

2:40 COMP 143. Combined selected configuration interaction and many-body treatment of static and dynamical correlation in oligoacenes. **J.B. Schriber**, K.P. Hannon, C. Li, F.A. Evangelista

3:00 Intermission.

3:15 COMP 144. Carbon-based nanomaterials: From graphene sheets to carbon nanodots, and high-level theoretical studies. **H. Lischka**

3:45 COMP 145. Combining spin-flip and IP/EA approaches for handling spin and spatial degeneracies: Application to double exchange systems. **S. Houck**, N. Mayhall

4:05 COMP 146. Diradical pyrazine isomer characterization and analytical gradients for state-averaged MC-PDFT. **T. Scott**, R. Nieman, H. Lischka, A. Sand, L. Gagliardi, D.G. Truhlar, C.A. Parish

4:25 COMP 147. Computational beginnings and managing chemical careers in a sea of entropy. **R. Hindman**

Section C

Orange County Convention Center
Room W308B

Machine Learning in Chemistry



TECHNICAL PROGRAM

C. M. Aikens, *Organizer*
A. E. Roitberg, S. Varma, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 **COMP 148.** Accelerating discovery in inorganic chemistry with machine learning. **H.J. Kulik**

2:05 **COMP 149.** Physics-based machine learning for materials and molecules. **M. Ceriotti**, E. Engel, M.J. Willatt

2:35 **COMP 150.** Impact of chemical descriptors in machine learning on methane adsorption prediction for porous materials at varying pressures. **M. Pardakhti**, E. Moharrerri, S.L. Suib, R. Srivastava

2:55 **COMP 151.** Forward and inverse discovery of solid-state materials using data-driven models. **Y. Jung**

3:25 Intermission.

3:40 **COMP 152.** Large-scale atomistic simulations of materials using SNAP potentials. **A.P. Thompson**

4:10 **COMP 153.** Material discovery by accelerated and universal learning for novel catalysis. **B. Yeo**

4:30 **COMP 154.** Polymer genome: A data-powered polymer informatics platform for property predictions. **R. Ramprasad**

Section D

Orange County Convention Center
West Hall B4 - Theater 23

Probing Reactive Intermediates through Chemical Computations

S. Kim, R. S. Paton, S. Vyas, *Organizers, Presiding*

1:30 Introductory Remarks.

1:40 **COMP 155.** Using DFT calculations to understand the unique photoreactivity of corannulene azide. **A.D. Gudmundsdottir**, M. Chakraborty

2:10 **COMP 156.** Combining theory and experiment to develop sustainable strategies for C-C bond formation. **O. Gutierrez**

2:40 **COMP 157.** Using N-heterocyclic carbene ligands to control cross coupling selectivity. **S.R. Neufeldt**

3:10 Intermission.

3:25 **COMP 158.** Molecular simulations in the study of reactive intermediates towards discovery of novel materials. **V. Glezakou**, R. Rousseau



TECHNICAL PROGRAM

3:55 COMP 159. Simulation of reactivity of organic molecules in beyond Li-ion energy storage systems. **R. Surendran Assary**

4:25 COMP 160. Accelerated design of catalysts for the selective oxidation of methane to methanol. **T. Yang, A. Nandy, H.J. Kulik**

4:45 Concluding Remarks.

Section E

Orange County Convention Center
West Hall B4 - Theater 24

Simulation of Protein-Membrane Interfaces

M. Buck, A. Gorfe Abebe, *Organizers*
K. A. Hristova, *Presiding*

1:30 COMP 161. Joining neutron scattering and simulations for complex biomembranes. **X. Cheng**

2:00 COMP 162. Membrane-associated signaling proteins: The role of the lipid anchor in membrane partitioning processes. **R. Winter**

2:30 COMP 163. Membrane remodeling by proteins: Challenges for multiscale computer simulation. **G.A. Voth**

3:00 COMP 164. Coarse-grained simulations of transmembrane domain interactions in the semaphorin-plexin-neuropilin signal system. **Z. Meng, Z. Li, M. Buck**

3:15 Intermission.

3:30 COMP 165. Gramicidin increases lipid flip-flop in symmetric and asymmetric lipid vesicles. **M.N. Doktorova, F.A. Heberle, D. Marquardt, R. Rusinova, L. Sanford, T. Peyear, J. Katsaras, G.W. Feigenson, H. Weinstein, O.S. Andersen**

3:45 COMP 166. Soft interfaces in membrane protein-lipid interactions. **M.F. Brown**

4:15 COMP 167. Conformational states along the gating pathway of ionotropic glutamate receptors: computation meets electrophysiology. **H. Zhou**

4:45 COMP 168. Influence of pH on membrane protein structure and function. **C.L. Brooks**

5:15 COMP 169. Phosphoinositide lipid interaction studies between TRPM8 and PIRT membrane proteins suggest a lipid shuttling-sequestering regulatory mechanism. **W.D. Van Horn**

Section F

Orange County Convention Center
West Hall B4 - Theater 25



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

Sampling Conformations & Pathways in Biomolecular Systems: Recent Developments & Applications

A. Ma, P. Tiwary, W. Yang, *Organizers*
O. Valsson, *Presiding*

1:30 COMP 170. Combined force-field sampling problem in simulations of disordered amyloid- β peptides. **T.L. Head-Gordon**

2:00 COMP 171. Probing the rules governing domain formation and protein partitioning in membrane. **J.E. Straub**, A. Bandara, G.A. Pantelopulos

2:30 COMP 172. Efficient sampling of reaction pathways by temperature-accelerated sliced sampling simulations. R. Javed, **N. Nair**

3:00 Intermission.

3:45 COMP 173. Approaches to probe pathways, thermodynamics, and reactive flux in biomolecular systems. **H. Vashisth**

4:15 COMP 174. Blind protein structure prediction with physics and ambiguous data: CASP and CASP-NMR. **A. Perez**, C. Liu, E. Brini, J. Robertson, R. Nassar, K. Dill

4:45 COMP 175. Protein structure refinement requires sampling on rough energy landscapes. **M. Feig**

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Sponsored by PROF, Cosponsored by AGFD, ANYL, BIOL, BIOT, CARB, CELL, CHED, CMA, COLL, COMP, ENVR, GEOC, I&EC, MEDI, MPPG, NUCL, ORGN, PHYS, PMSE, POLY, PRES, WCC and YCC

Advances in Data Collection & Analysis of Biomolecular Structures

Sponsored by PHYS, Cosponsored by COMP

Carbon Dioxide Conversion & Utilization

CO₂ as an Oxidant

Sponsored by ENFL, Cosponsored by CATL, COMP and GEOC

Modeling Dynamics in Dense Manifolds of Electronic States



TECHNICAL PROGRAM

Dense Manifolds in Molecules

Sponsored by PHYS, Cosponsored by COMP

Computational Electrocatalysis

Sponsored by CATL, Cosponsored by COMP and ENFL

Sustainable Software for Computational Molecular Science

Best Practices in Software Development from CMS Communities & Beyond

Sponsored by PHYS, Cosponsored by COMP

Undergraduate Research Posters

Computational Chemistry

Sponsored by CHED, Cosponsored by COMP and SOCED

TUESDAY MORNING

Section A

Orange County Convention Center
West Hall B4 - Theater 21

ACS Award for Computers in Chemical & Pharmaceutical Research in Honor of Arnie Hagler

Cosponsored by PROF
M. K. Gilson, *Organizer, Presiding*
T. R. Stouch, *Presiding*

8:30 Introductory Remarks.

8:40 COMP 176. Physics-based force fields for next-generation accuracy and transferability in molecular simulations. **J.R. Schmidt**

9:30 Discussion.

9:50 COMP 177. Development of polarizable, multipole-based AMOEBA+ force field. **P. Ren, C. Liu**

10:40 Discussion.



TECHNICAL PROGRAM

11:00 Intermission.

11:15 **COMP 178.** Introducing the Open Force Field Initiative: Better force fields through open, data-driven science. **M.R. Shirts**, D.L. Mobley, J.D. Chodera, M.K. Gilson, L. Wang

12:05 Discussion.

Section B

Orange County Convention Center
West Hall B4 - Theater 22

ACS Award for Research at an Undergraduate Institution: Symposium in Honor of Carol A. Parish

Cosponsored by PROF
B. Miller, H. L. Woodcock, *Organizers*
B. Zhang, *Presiding*

8:30 **COMP 179.** Modeling excellence: Dr. Carol Parish's impact and influence on undergraduate research. **B. Miller**

9:00 **COMP 180.** Exploring the role for the third active-site metal ion in DNA polymerase ϵ with QM/MM free-energy simulations. **D. Stevens**, S. Hammes-Schiffer

9:20 **COMP 181.** Studies of monoamine transporter interactions with MDPV, a component of illicit "bath salts". **T.W. Steele**

9:40 Intermission.

9:55 **COMP 182.** Biosynthesis to biocatalysis: New targets and new processes. **R.A. Splain**

10:15 **COMP 183.** Total synthesis of *ent*-laurendecumallene B. **C.A. Taylor**, Y. Zhang, S.A. Snyder

10:35 **COMP 184.** Modulation of MEMO1: Virtual screening, biochemical validation, and inhibition of cancer cell migration. **J.A. Pollock**

11:05 Intermission.

11:20 **COMP 185.** Thermal decomposition of sulfur species. **A. Vasiliou**, C.A. Parish, S. Dutton, M. Phillips, H. Hu

11:50 **COMP 186.** Applying nitrogen vacancy centers in diamond for improving magnetic resonance technologies. **A. Parker**

12:10 **COMP 187.** From DNA damage to next-gen sequencing: How a strong foundation translates into success. **M. Zimmerley**

Section C

Orange County Convention Center
West Hall B4 - Theater 25



TECHNICAL PROGRAM

Quantum Mechanics: Strong Electron Correlation

A. E. DePrince, H. P. Hratchian, *Organizers*
E. N. Brothers, *Presiding*

8:30 COMP 188. Automatic algorithms for the active space selection. **E. Sayfutyarova**

9:05 COMP 189. Model wavefunctions for strongly-correlated electrons. **P. Johnson**

9:30 COMP 190. General framework for developing wavefunctions. **T.D. Kim**, R.A. Miranda Quintana, P. Ayers

9:55 Intermission.

10:15 COMP 191. Mapping the interacting electronic problem onto a seniority-zero one in density-matrix functional theory. B. Senjean, N. Nakatani, **E. Fromager**

10:50 COMP 192. Minimally parametrized exchange–correlation functional for static, dynamic, and strong correlation, including dispersion corrections. E. Proynov, J. Kong, **R. Peverati**

11:15 COMP 193. Accuracy of the finite basis electron densities: A lesson from Levy's constrained search. **M. Mostafanejad**, A.E. DePrince

11:40 COMP 194. Unified treatment of derivative discontinuity, delocalization, and static correlation effects in DFT: The LDA plus Density Matrix Minimization (LDA+DMM) method. **F. Zhou**, V. Ozolins

Section D

Orange County Convention Center
West Hall B4 - Theater 23

Probing Reactive Intermediates through Chemical Computations

S. Kim, R. S. Paton, S. Vyas, *Organizers, Presiding*

8:30 Introductory Remarks.

8:40 COMP 195. Active vanadia-titania sites for oxidation of lignin model compounds. **V. Vorotnikov**, A. Robinson, G. Beckham

9:10 COMP 196. Advancing tools for probing reactive intermediates in the chemistry of heavy elements. **W. Dejong**

9:40 COMP 197. Multireference computations elucidate the mechanism of a photochemical cascade reaction towards fluoropolyacetylene. H. Corzo, B. Boswell, N.Z. Burns, **S.A. Lopez**

10:10 Intermission.



TECHNICAL PROGRAM

10:25 COMP 198. Density functional theory investigations of water splitting mechanisms and nanoparticle growth mechanisms. **C.M. Aikens**

10:55 COMP 199. Modeling catalytic reactions with multireference electronic structure theories. S. Stoneburner, C.A. Gaggioli, **L. Gagliardi**

11:25 COMP 200. Determining the reaction mechanism of a plastic-degrading aromatic polyestherase via transition path sampling. **B.C. Pollard**, B. Knott, H.L. Woodcock, G. Beckham

11:45 Concluding Remarks.

Section E

Orange County Convention Center
West Hall B4 - Theater 24

Simulation of Protein-Membrane Interfaces

M. Buck, A. Gorfe Abebe, *Organizers*
S. Khalid, *Presiding*

8:30 COMP 201. Comparative study between membrane interactions of signal proteins Plexin-B1, EphA2 and the K-Ras Ras: Raf complex. **Z. Li**, M. Buck

9:00 COMP 202. When the membrane is both the medium and the substrate: The functional mechanism of TMEM16 scramblases. **H. Weinstein**

9:30 COMP 203. Mechanism of action of pH-triggered membrane active peptides. S.Y. Kim, A. Pittman, G. King, W.C. Wimley, **K.A. Hristova**

10:00 COMP 204. Molecular dynamics of light-harvesting complex II trimers in thylakoid membrane. **S. Thallmair**, S. Marrink

10:15 Intermission.

10:30 COMP 205. Membrane curvature sensing by lipid anchored K-Ras small GTPase. **Y. Zhou**

10:45 COMP 206. Conformational dynamics of full length Ras on the millisecond timescale. **C. Neale**, **A.E. Garcia**

11:15 COMP 207. Membrane protein interactions with lipids: GPCRs and ion channels. W. Song, G. Hedger, a. Duncan, Q. Wang, **M.S. Sansom**

11:45 COMP 208. Anionic lipid binding to peripheral membrane proteins, what can fluorescence spectroscopy tell us? D.P. Mallory, X. Li, X. Shi, **A.W. Smith**

Section F

Orange County Convention Center
West Hall B4 - Theater 20



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

Sampling Conformations & Pathways in Biomolecular Systems: Recent Developments & Applications

A. Ma, P. Tiwary, W. Yang, *Organizers*
A. Dickson, *Presiding*

8:30 COMP 209. Immunotherapy modeling: Molecular Interaction and recognition of MHC/peptide/TCR complexes. **R. Zhou**

9:00 COMP 210. Design of enzymes to create promoting vibrations: What can we learn from artificial enzymes, laboratory evolution, and chosen mutagenesis? **S.D. Schwartz**

9:30 COMP 211. Exploring free energy and fitness landscapes of proteins for allostery and binding. **R.M. Levy**

10:00 Intermission.

10:45 COMP 212. How magnesium remodels the free energy landscapes of RNA: integrated experimental and computational studies. S. Roy, S. Hennelly, H. Lammert, J.N. Onuchic, **K. Sanbonmatsu**

11:15 COMP 213. Accelerated computation of *ab initio* QM/MM-quality enzymatic reaction free energy profile using re-parameterized semi-empirical QM/MM reference potentials. X. Pan, P. Li, J. Pu, Y. Mei, **Y. Shao**

11:45 COMP 214. Quantitative comparison of adaptive sampling methods for protein dynamics. **C. Clementi**

Advances in Data Collection & Analysis of Biomolecular Structures

Sponsored by PHYS, Cosponsored by COMP

Deep Learning

Sponsored by CINF, Cosponsored by COMP

Carbon Dioxide Conversion & Utilization

Electrocatalysis

Sponsored by ENFL, Cosponsored by CATL, COMP and GEOC

Modeling Dynamics in Dense Manifolds of Electronic States

Materials & Surfaces



TECHNICAL PROGRAM

Sponsored by PHYS, Cosponsored by COMP

Quantum Embedding Electronic Structure Methods

Sponsored by PHYS, Cosponsored by COMP

Sustainable Software for Computational Molecular Science

High-Performance & Massively-Parallel Chemistry

Sponsored by PHYS, Cosponsored by COMP

TUESDAY AFTERNOON

Section A

Orange County Convention Center
West Hall B4 - Theater 21

ACS Award for Computers in Chemical & Pharmaceutical Research in Honor of Arnie Hagler

Cosponsored by PROF
M. K. Gilson, *Organizer*
M. R. Shirts, *Presiding*

1:30 COMP 215. Can the rules of quantum chemistry be learned? A perfect force field without a functional form. **A.E. Roitberg**

2:20 Discussion.

2:40 COMP 216. Evaluating and improving force field accuracy for computer-aided drug design. **M.K. Gilson**, J. Yin, S. Kantonen, N.M. Henriksen, H. Muddana, D. Slochower, K. Kellett

3:30 Intermission.

3:45 COMP 217. Award Address (ACS Award for Computers in Chemical and Pharmaceutical Research sponsored by the ACS Division of Computers in Chemistry). Biomolecular force fields: Where have we been, where are we now, where do we need to go, and how do we get there? **A. Hagler**

4:35 Discussion.

4:55 Concluding Remarks.

Section B



TECHNICAL PROGRAM

Orange County Convention Center
West Hall B4 - Theater 22

ACS Award for Research at an Undergraduate Institution: Symposium in Honor of Carol A. Parish

Cosponsored by PROF
B. Miller, H. L. Woodcock, *Organizers*
C. A. Taylor, *Presiding*

1:30 COMP 218. Potential roles for sigma hole interactions in M-H bond activation and elsewhere. **K. Donald**

2:00 COMP 219. Gaia: A new era of the Milky Way. **A. Beane**, M. Ness, M. Bedell, M. Mac Low, R. Sanderson, D. Anglés-Alcázar

2:20 COMP 220. Solving tough problems with computers. **J. Mancini**

2:40 Intermission.

2:55 COMP 221. Connectivity map: Beyond the first one million gene expression profiles. **M. Macaluso**

3:15 COMP 222. Cochlear implants: A tale of how computers can become our ears. **E.X. Vivas**

3:35 COMP 223. Award Address (ACS Award for Research at an Undergraduate Institution sponsored by the Research Corporation for Science Advancement). It's the right chemistry! Research with undergraduates in the Parish laboratory. **C.A. Parish**

Section C

Orange County Convention Center
West Hall B4 - Theater 25

Quantum Mechanics: Strong Electron Correlation

H. P. Hratchian, *Organizer*
A. E. DePrince, *Organizer, Presiding*

1:30 COMP 224. Recent developments in adaptive methods for strongly correlated electrons. **F.A. Evangelista**, J.B. Schriber, C. Li

2:05 COMP 225. Adiabatic-connection analysis of RPA correlation in the asymmetric Hubbard dimer. E. Vaughan, **J.E. Bates**

2:30 COMP 226. Dynamic correlation model for variational two-electron reduced density matrix driven complete active space self-consistent field methods. **E. Maradzike**, A.E. DePrince

2:55 Intermission.

3:15 COMP 227. New paradigms for molecular conductivity and excited spectra via variational 2-RDM theory. **D.A. Mazziotti**



TECHNICAL PROGRAM

3:50 COMP 228. Relativistic quantum chemistry with reduced-density-matrices: The effect of angular momentum constraints. **R. Li**

4:15 COMP 229. Towards full configuration interaction for metal complexes. **A.E. Rask**, P.M. Zimmerman

Section D

Orange County Convention Center
West Hall B4 - Theater 23

Probing Reactive Intermediates through Chemical Computations

S. Kim, R. S. Paton, S. Vyas, *Organizers, Presiding*

1:30 Introductory Remarks.

1:40 COMP 230. Hydration-dehydration transitions and ion-carbon interactions control the selective anion transport through a synthetic cage embedded in lipid membrane. **J. Park**, M. Baik, K. Kim

2:10 COMP 231. Time-resolved mechanism of enzyme SpnF-catalyzed Cope rearrangement: Timing of bond formation and entropic intermediate. **Z. Yang**, X. Xue, K.N. Houk

2:30 COMP 232. Towards realistic, *in-situ* modeling of the electrolysis of water: Ensemble and solvation effects. **M. Ha**, S.M. Alia, B.S. Pivovar, R.E. Larsen

2:50 COMP 233. Quantum nature of proton transfer for space exploration by hypergolic propellants. Y. Han, **D. Kilin**

3:20 COMP 234. Computational study of the gas phase formation of c-SiC₃ molecules in the circumstellar envelope of carbon stars. **L. Bertels**, T. Yang, B.B. Dangi, R. Kaiser, M.P. Head-Gordon

3:40 Concluding Remarks.

Section E

Orange County Convention Center
West Hall B4 - Theater 24

Simulation of Protein-Membrane Interfaces

M. Buck, A. Gorfe Abebe, *Organizers*
M. G. Kurnikova, *Presiding*

1:30 COMP 235. Simulations of crowded environments near membrane interfaces. **M. Feig**

2:00 COMP 236. How does information cross the cell membrane? An atomic-level perspective. **R.O. Dror**



TECHNICAL PROGRAM

2:30 COMP 237. Common mechanisms of catalysis in small and heterotrimeric GTPases and their respective GAPs. **K. Gerwert**, C. Kötting

3:00 COMP 238. Structural determinants of protein partitioning into ordered membrane domains: insights from experiment and simulations. **I. Levental**, X. Lin, A. Gorfe Abebe

3:15 Intermission.

3:30 COMP 239. How does membrane modulate the function of key players in the MAPK signaling pathway? **P. Srivastava**, A. Gorfe Abebe

4:00 COMP 240. Simulation and experiment in the nuclear pore complex. **D. Cowburn**, S. Sparks, B. Raveh, R. Hayama, A. Sali, M.P. Rout

4:30 COMP 241. Role of intrinsically disordered regions of proteins in membrane mediated cell signaling. T. Travers, C. Lopez, J. Hettige, R. Mansbach, **S. Gnanakaran**

5:00 COMP 242. Proteins interacting with membrane surfaces: The case of the oncogene KRas4b. **S.G. Sligar**, M.A. McLean

Section F

Orange County Convention Center
West Hall B4 - Theater 1

Sampling Conformations & Pathways in Biomolecular Systems: Recent Developments & Applications

A. Ma, P. Tiwary, W. Yang, *Organizers*
R. M. Levy, *Presiding*

1:30 COMP 243. Automatic reaction coordinate discovery in artificial intelligence guided computer simulations. **R. Covino**, H. Jung, G. Hummer

2:00 COMP 244. Three birds with one stone: Reaction coordinate, thermodynamics, and kinetics from all-atom simulations. **P. Tiwary**

2:30 COMP 245. Targeted adversarial learning optimized sampling. **J. Zhang**, Y.I. Yang, M. Parrinello, F. Noé

3:00 Intermission.

3:45 COMP 246. Activated dynamics of biomolecules from the perspective of energy flow. **A. Ma**

4:15 COMP 247. Optimization of conformational sampling protocols using an analytic model of alchemical molecular binding. **E. Gallicchio**

4:45 COMP 248. Insights into the mechanism of the PIK3CA E545K activating mutation using MD simulations. H. Leontiadou, I. Galdadas, C. Athanasiou, **Z. Cournia**



TECHNICAL PROGRAM

Division of Physical Chemistry Award Symposium

Sponsored by PHYS, Cosponsored by COMP

Deep Learning

Sponsored by CINP, Cosponsored by COMP

Carbon Dioxide Conversion & Utilization

Photo, Electro & Plasma Catalysis

Sponsored by ENFL, Cosponsored by CATL, COMP and GEOC

TUESDAY EVENING

Section A

Orange County Convention Center
West Hall C

Chemical Computing Group Graduate Student Travel Awards

K. N. Kirschner, C. L. Simmerling, *Organizers*

6:00 - 8:00

COMP 249. GPU-accelerated constant pH and redox potential molecular dynamics with multidimensional replica exchange simulations in amber. **V.D. Cruzeiro**, A.E. Roitberg

COMP 250. Rare events in complex systems: Methods and applications. **R.S. DeFever**, S. Sarupria

COMP 251. Accurate predictions of electron binding energies of dipole-bound anions via quantum Monte Carlo methods. **H. Hao**, J. Shee, S. Upadhyay, C. Ataca, K.D. Jordan, B.M. Rubenstein

COMP 252. Open-shell coupled-cluster valence-bond theory augmented with an independent amplitude approximation for three-pair correlations: Application to a model oxygen-evolving complex and single molecular magnet. **J. Lee**, D. Small, M.P. Head-Gordon

COMP 253. Optimization of the Drude polarizable protein force field. **F. Lin**, A.D. Mackerell

Section A



TECHNICAL PROGRAM

Orange County Convention Center
West Hall C

COMP Poster Session

H. L. Woodcock, *Organizer*

6:00 - 8:00

COMP 254. Characterization and transformations of complex metal oxides: pH-dependent cation release of nanoscale LiCoO_2 . **A. Abbaspour Tamijani, J.W. Bennett, D. Jones, R.J. Hamers, S.E. Mason**

COMP 255. Computational investigation of myosin 19 structure-function. **J. Airas**, E. Modeste, Y. Ali, C.A. Parish, O.A. Quintero

COMP 256. Application of extended Huckel theory to pharmacophore modeling. **A. Ajamian**

COMP 257. Protocol for the analysis of vibrational circular dichroism spectra of small molecules using Gaussian and MOE. **A. Ajamian**

COMP 258. Assessment and preparation of crystal structures for drug design. **A. Ajamian**

COMP 259. Quasi-2D MLH perovskites: DFT modeling approach. **O.A. Allam, S. Jang**

COMP 260. Solvation dynamics from the water's perspective. **S. Ambaye**, D. Rogers

COMP 261. Measuring configurational entropy of charged amino acids. **D.B. Amirkulova**

COMP 262. Highly correlated multireference study of tetralin diradical. **C. Ancajas**, C.A. Parish

COMP 263. DFT study of the selectivity of DOPA-decarboxylase. **P. Antwine**, M.L. Cafiero, L.W. Peterson

COMP 264. Designing of biorational insecticide against diamondback moth, *Plutella xylostella* infestation on cabbage (*Brassica oleracea* var. *capitata* L.) by computer-aided pesticide design approach. **N. Arasid, N. Misral**, N. Hassan, K. Lam, M. Hassan

COMP 265. Effect of the composition on the nucleation process in CuNi system. **S. Bechelli**, B. Gonzalez, C. Desgranges, J. Delhommelle

COMP 266. Electronic energies are not enough: An ion mobility-aided, quantum chemical benchmark analysis of H^+GPGG conformers. **D. Beckett**, T.J. El-Baba, D.E. Clemmer, K. Raghavachari

COMP 267. Basis set dependence of interaction-induced dipole moments of CO_2 dimers. **R. Beil**, R.J. Hinde

COMP 268. Simulating water exchange to buried binding sites. **I. Ben-Shalom**, C. Lin, R. Walker, M.K. Gilson

COMP 269. Monte Carlo simulation of heavy metal ions in aqueous solution using Lennard-Jones 12-6 potential. **N.P. Bigham**, J. Kegerreis



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- COMP 270.** Role of water in governing multimodal ligand conformational equilibria. **C. Bilodeau**, E.Y. Lau, S.M. Cramer, S. Garde
- COMP 271.** Binding interactions between human pepsin and RT inhibitors: A MD approach. **A. Blake**, C.A. Parish
- COMP 272.** Predicting stacking interactions of salt-bridges and aromatic amino acids with heterocyclic drug fragments based on new molecular descriptors. **A.N. Bootsma**, S.E. Wheeler
- COMP 273.** Understanding DNA polymerase β fidelity mechanism using MD simulations. **S. Boutros**, S. Kirmizialtin
- COMP 274.** DFT investigations on the regioselectivity of indole addition to unsymmetrical silyloxyallyl cations. **C. Bresnahan**, A. Milet, R. Kumar, R. Kartika
- COMP 275.** Gibbs ensemble simulations probing the miscibility gap in water/hydrogen mixtures at high temperatures and pressures. **C.E. Bunner**, M.S. Minkara, J.I. Siepmann
- COMP 276.** Understanding allosteric regulation of human ribonucleotide reductase using molecular dynamic simulations. **P. Buteler**, A.E. Roitberg
- COMP 277.** Computational investigation of cancer-related single nucleotide polymorphisms in TET2. **P.J. Camacho**, E.M. Leddin, G. Cisneros
- COMP 278.** Putting NanoPutians to work: A computational exploration of anthropomorphic host-guest chemistry. **C. Chan**, M.M. Francl
- COMP 279.** *De novo* molecular design of DNA methyltransferases inhibitors. **D.E. Chávez-Ponce de León**, N. Sánchez-Cruz, J.L. Medina-Franco
- COMP 280.** Molecular simulations probing the thermophysical properties of stretched homogeneous and bubbly water systems. **J. Chen**, B. Xue, K. Mahesh, J.I. Siepmann
- COMP 281.** Charge density and structure of the complex surface of gold nanoparticles. **G. Chong**, E. Laudadio, M. Wu, C.J. Murphy, R.J. Hamers, R. Hernandez
- COMP 282.** Machine learning-based integration of proteome-scale interaction modeling and phenotypic experiments to design small molecules drugs. J. Majumder, J. Fine, E. Kischuk, D. Knapp, T.L. Ratliff, **G. Chopra**
- COMP 283.** Prevalence in the general population of missense mutations on the taste receptor genes responsible for the detection of sweet and umami taste in humans. **K. Christopher**, W.B. Floriano, K. Gagnon
- COMP 284.** DFT study of yersiniabactin-metal complexes. **N. Clement**, P.M. Todebush, C. Miller, L. Streit
- COMP 285.** Molecular modeling of 1-benzazepine analogues that bind to the ACh Protein (2PH9) using Hyperchem and AutoDock. **P.M. Colon**, A.C. Gonzalez, C. Garcia, M. Ortiz Marciales
- COMP 286.** NMR j -coupling constants and chemical shift of Pt–Pt bonded metal complexes in aqueous solution by *ab initio* molecular dynamics and localized orbital analysis. P.R. Batista, A. Marchenko, **L. Colucci Ducati**, J. Autschbach
- COMP 287.** Design of novel inhibitors for the catechol-O-methyltransferase enzyme. **E. Cook**, L.W. Peterson, M.L. Cafiero



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- COMP 288.** Symmetric and non-symmetric short iterative Lanczos integrators for time-dependent coupled-cluster theory. **B. Cooper**, A.E. DePrince
- COMP 289.** Comparison of quantum mechanical and standard molecular dynamics parameters for the C12 ligand. **S. Darancou**, S.T. Shipman
- COMP 290.** Computational investigation of binding energetics for selective lanthanide extraction. **M.Y. Darrows**, A. Perry, O. Sode
- COMP 291.** Solvation mechanism of cardiovascular drug LASSBio-294 in ionic liquids: A computational study. **S. Dasari**, B. Mallik
- COMP 292.** Dissociative N_2 chemisorption on $Fe_3O_4(001)$ surface: The emergence of new subsurface layers and surface relaxations. **G.D. Degaga**, M. Seel, T. Trought, K.A. Perrine, S. Nemsak, E.J. Crumlin, R. Pandey
- COMP 293.** Conformational coupling to asymmetric ATP hydrolysis in the transport cycle of p-glycoprotein. **S. Dehghanighahnaviyeh**, K. Kapoor, E. Tajkhorshid
- COMP 294.** Evaluation of electronic dipole moments in time-independent excited-state DFTB. **M.Y. Deshaye**, T. Kowalczyk
- COMP 295.** Computational examination of structure and reactivity in ruthenium silyl and silylene complexes. **W.Q. DeSnoo**, D.L. Kohen, M.T. Whited
- COMP 296.** Molecular molding of dipeptide micelles. **O. Devereaux**, F.H. Billiot, A. Billiot, K.F. Morris, E. Billiot, Y. Fang
- COMP 297.** Thermochemical studies with machine learning. **C. Devereux**, J.S. Smith, O. Isayev, A.E. Roitberg
- COMP 298.** Development of OPLS-AA force field parameters for ionic liquid and deep eutectic solvent simulations. **B. Doherty**, O. Acevedo
- COMP 299.** Computational study of self-assembly of polypeptoids in aqueous solution: From atomistic to coarse-grained simulations. **P. Du**, R. Kumar
- COMP 300.** Connecting the TraPPE force fields to the MoSDeF framework. **B.L. Eggimann**, K. Beardslee, C.E. Bunner, J.I. Siepmann
- COMP 301.** Computational simulation of homeomorphic isomerism in phosphine macrobicycles: Topology, spectroscopy, and stability of *in/out* isomers. **A. Ehnbohm**, L. Perez, M.B. Hall, J.A. Gladysz
- COMP 302.** Describing transition metal chemistry with the random phase approximation. **H. Eshuis**, J. Chedid, N. Ferrara
- COMP 303.** Computational treatment of the methylsulfinyl radical-ozone reaction. **M.L. Estep**, K.B. Moore, H.F. Schaefer
- COMP 304.** Molecular dynamics of MEMO1: Apo dynamics, peptide complex dynamics, small ligand binding, and analysis. **H.D. Evans**, J. Airas, Q. McKoy, C.A. Taylor, K.J. Rubenstein, J.A. Pollock, C.A. Parish
- COMP 305.** Survey of quantum chemical methods for computing interaction energies in organometallic systems. **R. Evans**, L.W. Peterson, M.L. Cafiero



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- COMP 306.** Molecular dynamics and metadynamics based studies of Brg1/DNA interaction. **s. evoli**, J. Wereszczynski
- COMP 307.** PotentialNet: Step-change improvement in ADME-Tox prediction with deep featurization. **E.N. Feinberg**, V.S. Pande, A.C. Cheng
- COMP 308.** Do cyclotides aggregate with lipid bilayers? Experimental and computational characterization of the interaction between cyclotide, cyclotide mimetics, and lipid bilayers. **N.Y. Forlemu**, A.V. Mallia, S.M. Mwangela
- COMP 309.** The Good, the Bad, and the Ugly: "Hipen," a new dataset for validating (S)QM/MM free energy simulations. **L. Warrensford**, F.L. Kearns, H.L. Woodcock
- COMP 310.** Elucidating the stability of 14-3-3 and Raf using protein simulations. **T. Harris**, C. Neale, A.E. Garcia
- COMP 311.** Towards a more complete understanding of non-covalent interactions in base pair stacking. **D.P. Harding**, S.E. Wheeler
- COMP 312.** Improving the prediction of loop conformations and drug binding in GPCR structure models. **B. Arora**, K. Venkatesh, P. Sexton
- COMP 313.** Hyper-predictive MD-QSAR models of kinase-inhibitor interactions using deep-learning and molecular-dynamics trajectories. **D. Fourches**
- COMP 314.** Measuring the desolvation energy of the active-site of enzymes within the dopamingeric metabolic pathway. **C. Frost**, L.W. Peterson, M.L. Cafiero
- COMP 315.** Kirkwood-Buff derived force field for glycerophospholipids. **S. Gajaweera**, P.E. Smith
- COMP 316.** Next-generation of protein-structure prediction powered by deep-learning. **M. Gao**, H. Zhou, J. Skolnick
- COMP 317.** Multi-determinant trial wavefunctions for solids. **K. Gasperich**, T. Applencourt, A. Scemama, K.D. Jordan, A. Benali
- COMP 318.** Effect of mutations on the binding of ligands in phenylalanine hydroxylase. **R.M. Giampapa**, L.W. Peterson, M.L. Cafiero
- COMP 319.** Characterization of stabilization effects in N-aminated peptide derivatives. **N. Giddings**, M.P. Sarnowski, K.P. Pedretty, J.R. Del Valle, H.L. Woodcock
- COMP 320.** Control of diverse emission features in functionalized single-walled carbon nanotubes. **B.J. Gifford**, S.K. Doorn, S. Tretiak
- COMP 321.** Topologically intriguing ribbons and hoops from oligomeric ferrocene. **A. Goldberg**, M.M. Francl
- COMP 322.** Autochemistry: A new research paradigm based on artificial intelligence and big data. **T. Gressling**
- COMP 323.** Coarse-grained model for simulating the boiling point of asphaltenes. **S. Groven**, C. Desgranges, J. Delhommelle
- COMP 324.** Machine learning for molecular property predictions, and the software ecosystem that enables it. **J. Hachmann**



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- COMP 325.** Unravelling the composition dependent anomalies of pair hydrophobicity and protein structure in water-ethanol binary mixture. **R. Halder**, B. Jana
- COMP 326.** Development of general alkane parameters for the MASTIFF intermolecular force field. **A. Hansel**, M. Van Vleet
- COMP 327.** Computational molecular dynamics study of heteroepitaxial growth patterns comparing Cu/Ni and Pt/Ni on Ni(111) and Ni(100). **K. Haug**, P. Ly, P. Weiss
- COMP 328.** Study of the binding interactions between human pepsin and HIV-1 protease inhibitors. **A. Henderson**, C.A. Parish
- COMP 329.** Predicting human liver microsomal stability. **T. Shieh**, B. Su, Y. Tseng
- COMP 330.** Predicting synthesizable functional edge reconstructions in 2D monolayers. **G. Hu**, P. Ganesh
- COMP 331.** Molecular simulation study of the interaction between nucleobases with graphene. **H. Hwang**, D. Oh, V. Vasudevan, S. Jang
- COMP 332.** Density functional theoretical study on the repeat units of benzothiadiazole and fluorinated phenylene-based wide band gap copolymers. **S. Hwang**, H. Woo
- COMP 333.** QSAR model to predict properties of amphiphilic polymeric micells. **K. Iduoku**, O. Antypenko, B. Rasulev
- COMP 334.** Supercharging computational chemistry with machine learning and AI. **O. Isayev**
- COMP 335.** Surveying the potential energy surface of the carbon dioxide/water dimer. **O. Isbell**
- COMP 336.** Supramolecular peptide amphiphile-polymeric hybrid hydrogels for photo-actuation: Modeling and simulation. **A. Iscen**, G.C. Schatz
- COMP 337.** Gauging the flexibility of the active site in Soybean Lipoxygenase1 (SLO-1) through an Atom-centered Density Matrix Propagation (ADMP) treatment that facilitates the sampling of rare events. **S.S. Iyengar**
- COMP 338.** Non-valence correlation-bound anions. **A. Kairalapova**, K.D. Jordan
- COMP 339.** Simulation study of non-conserved mutations in the *lac* repressor protein. **N.L. Kariyawasam Manachchige**, L. Swint-Kruse, P.E. Smith
- COMP 340.** Elucidating the crowding effect on protein-ligand binding process. **K. Kasahara**, H. Oshima, G. Nawrocki, I. Yu, S. RE, M. Feig, Y. Sugita
- COMP 341.** Applying structure-based descriptors to predict potential energy and atomic forces with machine learning techniques. **H. Kim**, S. Lee, J. Im, T. Ko, S. Kim, Y. Kim, Y. Hyon, H. Chang
- COMP 342.** Halogen bonding as a mechanism for aromatic and non-aromatic explosive detection. **M. Kitimet**
- COMP 343.** Clean and simple wave function interpretation with intrinsic bond orbitals: From [F-H-F]⁻ to proton coupled electron transfer in enzymes. **G. Knizia**



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- COMP 344.** DREAMing of big data and scalable machine learning: Predicting kinase binding with matrix factorization. **D. Koes**, J. King, P. Francoeur, A. Kowalczyk, S. Rajashekar, C. Chennubhotla
- COMP 345.** Nature of non-commensurate variables in grand canonical Monte Carlo simulations. **L. Laratelli**, A. Hogan, M. Mulcair, B. Space
- COMP 346.** Computational study of the thermodynamic process of the binding and folding of pHLIP. **J. Layton**, A. Clark, C. Gupta, B. Mertz
- COMP 347.** Predicting quasi-two-dimensional electronic structure in Sb₂Te₃-based alloys. **N.Q. Le**, A.A. Podpirka, C.D. Stiles
- COMP 348.** Computational investigation of TET2 activity on RNA-containing substrates. **E.M. Leddin**, J.E. DeNizio, M.Y. Liu, R.M. Kohli, G.A. Cisneros
- COMP 349.** Molecular dynamics study for the ion-channel opening of NMDAR. **J. Lee**
- COMP 350.** Influence of PTFE-binder content on coverage of Pt/C electrode in a high-temperature polymer-electrolyte membrane fuel cells. S. Kwon, J. Lee, S. Lee, H. Kim, **S. Lee**
- COMP 351.** Relative binding affinity of an inhibitor to two human carbonic anhydrase isozymes. **S. Lenka**, A.E. Roitberg
- COMP 352.** Dynamic topographical mapping. **H. Li**
- COMP 353.** Nonadiabatic photodynamics of the retinal protonated Schiff base in channelrhodopsin 2. **R. Liang**, F. Liu, T.J. Martinez
- COMP 354.** Regioselectivity of reactions of phosphonyl arynes. **J. Lilly**, **G. Mraz**, P. Willoughby, J. Scanlon
- COMP 355.** Computational screening of zeolites for effective removal of problematic compounds in the International Space Station. **S. Lin**, Y. Zhao, A.J. Hernandez, Z. Chen
- COMP 356.** Studying solvation effect using time-dependent, complete active space configuration interaction coupled with polarizable force-field. **H. Liu**, X. Li
- COMP 357.** Graph based neural network model for predicting aqueous solubility. **H. Liu**, B. Su, T. Cho, Y. Tien, Y. Tseng
- COMP 358.** Predicting molecular energy using force-field optimized geometries and atomic vector representations learned from improved deep tensor neural networks. **J. Lu**, C. Wang, Y. Zhang
- COMP 359.** Density functional theory investigation of brown carbon species in aqueous aerosol mimics. **E. Lugos**, D. Grace, R. Holappa, J.L. Woo, M.M. Galloway, **H.P. Hendrickson**
- COMP 360.** Influence of chemical composition on the relaxation rates of charge carriers in PbX/CdX, X = S or Se, core/shell quantum dots. **L. Lystrom**, S. Kilina, P.K. Tamukong
- COMP 361.** Design of novel inhibitors for the aldehyde dehydrogenases. **C. Magee**, L. Peterson, M.L. Cafiero
- COMP 362.** Mechanistic analysis and catalyst design for sustainable polymer production. **M. Mandal**, A.M. Luke, J.A. Macaranas, D.E. Stasiw, B. Dereli, T.M. Reineke, W.B. Tolman, C.J. Cramer



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- COMP 363.** TD-DFT study of enantioenrichment of BINOL derivatives. **J. Marshall**
- COMP 364.** Aqueous solvation of alkaline earth metal ions using combined explicit and continuum solvent. **M. Martin**, M. Provorse Long
- COMP 365.** Optical and electrical properties of functionalized $Ti_3C_2T_2$ by first principles calculations. **F. Mehmood**, R. Pachter, G.R. Neher, J. Heckler, D.B. Lioi, A.R. Sharits, R.A. Vaia, D. Nepal, W. Kennedy
- COMP 366.** Exploring the thermodynamics of plant growth hormone signal transduction. **A. Moffett**, D. Shukla
- COMP 367.** DFT study of the selectivity of tyrosinase. **E. Moix**, D. Wilson, L.W. Peterson, M.L. Cafiero
- COMP 368.** Computational study of halogen bonding in nitrogen containing rings. T.L. Ellington, **J. Mosely**, G.S. Tschumper
- COMP 369.** Tales of strong correlation narrated by multiconfigurational pair-density functional theory. **M. Mostafanejad**
- COMP 370.** Centroid path integral investigation of zero-point motion and its effects in solid helium. **P.S. Mott**, R.J. Hinde
- COMP 371.** Identifying the effect of membrane depolarization on a model binary bilayer using molecular dynamics simulations. **V.V. Nair**, A. Gorfe Abebe
- COMP 372.** Probing pathological RNA aggregation with GPU-based coarse-grained simulations. **H. Nguyen**, D. Thirumalai
- COMP 373.** Cation behavior within zeolites. **A. Nijhawan**, D.L. Kohen, B. Lynch
- COMP 374.** Adsorption of deoxyribonucleosides on graphene: Molecular dynamics simulation approach. **D. Oh**, H. Hwang, V. Vasudevan, G. McPherson, S. Jang
- COMP 375.** Tamiflu: Analysis of drug binding and resistance. **L. Oliver**, J. Lu, Y. Zhang
- COMP 376.** Non-equilibrium alchemical molecular dynamics simulations of protein-ligand binding. **R. Pal**, E. Gallicchio
- COMP 377.** Theoretical study of nonadiabatic relaxation dynamics in $[Au_{25}(SeCH_3)_{18}]^-$ and $[Au_{13}(P_2H_4C_2H_4)_5Cl_2]^{3+}$. **P. Pandeya**, C.M. Aikens
- COMP 378.** Microscopic characterization of membrane binding and lipid-protein interactions in pH domain using advanced simulations techniques. **S. Pant**, E. Tajkhorshid
- COMP 379.** Computational studies of kinetic and dynamic resolution of polysubstituted olefins activated by amine bases bearing alkali metals. **J. Park**, H. Ryu, P. Evans, M. Baik
- COMP 380.** Computational study for understanding the action of nickle acireductone dioxygenase (Ni-ARD) through a biomimetic structural modeling. **R. Parveen**, t.R. Cundari, s.t. carrion
- COMP 381.** Random forest refinement of the KECSA2 knowledge-based scoring function for protein decoy detection. **J. Pei**, Z. Zheng, K.M. Merz



TECHNICAL PROGRAM

COMP 382. Effects of deprotonation on the binding selectivity of the phenylalanine hydroxylase active site. **M.C. Perchik**, M.L. Cafiero, L.W. Peterson

COMP 383. Computational discovery of novel bright emitters featuring thermally activated delayed fluorescence. **A. Pershin**, D. Beljonne, Y. Olivier

COMP 384. Metallophthalocyanine functionalized graphene quantum dot as a high-efficiency non-precious electrocatalyst for PEMFC: A DFT+U approach. **N.T. Pham**, S. Kang, S. Lee

COMP 385. DFT study of ligand binding in biogenic amine transporters. **A. Polzin**, L.W. Peterson, M.L. Cafiero

COMP 386. DFT study of the binding of ligands in SULT1A3 active site. **K. Puzdrakiewicz**, L. Peterson, M.L. Cafiero

COMP 387. Elucidating the phosphate binding mode of phosphate-binding protein: The critical effect of buffer solution. **R. Qi**

COMP 388. Efficient exploration of the conformational space for PEGylated proteins through biased coarse-grained molecular dynamics. **F. Ramezanghorbani**, P. Lin, C.M. Colina

COMP 389. Transference of knowledge in deep learning for chemically accurate organic reaction profiles. **K.D. Ranasinghe**, J.S. Smith, O. Isayev, A.E. Roitberg

COMP 390. Mouse liver microsomal stability prediction model based on graph convolutional neural networks. **A. Renn**, B. Su, H. Liu, Y. Tseng

COMP 391. Improving the prediction of protein-ligand binding affinity using deep learning models. **M. Rezaei**, Y. Li, X. Li, C. Li

COMP 392. Computational screening and machine learning for the design of heterogeneous oxygen reduction catalysts. **N. Ricke**, K. Chen, T. Marshall-Roth, T.A. Van Voorhis

COMP 393. Making higher-order coupled cluster methods affordable: Through tensor decomposition techniques, massively parallel implementation, and use of modified virtual orbitals. **V. Rishi**, K. Pierce, E.F. Valeev

COMP 394. Optical and charge transport properties of gold-nanocluster complexes: Single-molecule nanowires. **J.I. Rodriguez-Hernandez**, U.A. Vergara-Beltran, D.M. Resendiz-Serrano, J. Autschbach

COMP 395. Functionally relevant clustering of the arsenate reductase (ArsC) superfamily. **M. Rosen**, J.B. Leuthaeuser, C.A. Taylor, J.S. Fetrow, C.A. Parish

COMP 396. Molecular dynamics like approach to simulate a suspension of hard spheres in a Newtonian fluid. **E.J. Rosenbaum**, K. Dayal, M. Massoudi

COMP 397. Computing with molecules: Storage and machine learning using mixtures of small organic molecules. **B.M. Rubenstein**

COMP 398. Cosolvent dynamics: A tool for expanding the druggable human proteome. **F. Sabanés**, J. de Souza Cunha, A.K. Bronowska



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- COMP 399.** Understanding STAT3's DNA binding mechanism and activity changing mutations through Umbrella Sampling simulations. **F. Sabanés**, J. de Souza Cunha, R. Estrada Tejedor, A.K. Bronowska
- COMP 400.** Predicting the binding of fatty acid amide hydrolase inhibitors by free-energy perturbation. **A. Saha**, A. Shih, T. Mirzadegan, M.J. Seierstad
- COMP 401.** Molecular insights on conformational ensembles and free-energy landscape of intrinsically disordered SNAP-25. **N. Saikia**, H. Sanabria, K.R. Weninger, T. Smirnova, F. Ding
- COMP 402.** Osmotic pressure calculations in the systems with the highly concentrated DNA and polyethylen glycol polymers solutions using all-atoms molecular dynamic simulations as a way to understand biophysical processes of DNA extraction from bacteriophages. **O. Samoylova**
- COMP 403.** DFT analysis of water clusters, dopaminergic derivatives, and their desolvation energies. **E. Sanders**, M. Morris, L.W. Peterson, M.L. Cafiero
- COMP 404.** pH-Dependent properties of ionizable residues in the hydrophobic interior of a protein. **A. Sarkar**, A.E. Roitberg
- COMP 405.** Rationalization of sampling space for searching favorable binding modes. **H. Sato**, Y. Tanida, A. Matsuura
- COMP 406.** Elucidating double proton transfer mechanism in the Slr1694 BLUF photoreceptor using automated multireference calculations. **E. Sayfutyarova**, S. Hammes-Schiffer
- COMP 407.** Simulating the chelate effect. **A. Sengupta**, K.M. Merz
- COMP 408.** Real-space finite-difference implementation of orbital-free density functional theory. **X. Shao**, W. Mi, Q. Xu, S. Wang, Y. Wang, Y. Ma
- COMP 409.** Reaction mechanism of glycerophosphodiesterase (gpdq) and its synthetic analogues. **G. Sharma**, V. Jayasinghe-Arachchige, Q. Hu, T.J. Paul, R. Prabhakar
- COMP 410.** *In silico* evaluation of the resistance of the protein kinase B: Mechanistic insights from molecular dynamics simulation analysis. **S. Shubham**, R. Malik
- COMP 411.** DFT study of the selectivity of the β -1 adrenergic receptor. **M. Simons**, L.W. Peterson, M.L. Cafiero
- COMP 412.** Angle-dependent strong-field molecular ionization yields with tuned range-separated time-dependent density functional theory. **A. Sissay**, P. Sandor, F. Mauger, P. Abanador, M. Gaarde, K. Schafer, R. Jones, K. Lopata
- COMP 413.** Azide and alkyne CHARMM parameterization with Unnatural Amino Acid (uAA) protein simulation. **A. Smith**, T. Knotts
- COMP 414.** Evaluating the binding of a novel POSS-based HIV protease inhibitor drug. **Y.C. Solis**, J. Airas, C.A. Parish
- COMP 415.** How compressible are full configuration interaction wave functions for strongly correlated hydrogen systems? **N. Stair**, F.A. Evangelista
- COMP 416.** Reactions of deprotonated sPEEK fuel cell membrane model conformers with H radicals. Z. Smith, N. Ognanovich, A. Piatkowski, K. Utterbeck, **J.E. Stevens**



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- COMP 417.** Molecular dynamics simulations of melting under confinement. **E.M. Sullivan, K.E. Anderson,** J.I. Siepmann
- COMP 418.** Integrated screening for beta-lactamases inhibitors. **T.J. Sullivan,** B.J. Alper, J.H. Audie, B. Cingolani, J. Cutrone, D. Bocach, B. Lakkireddy
- COMP 419.** Slow convergence on alchemical free-energy calculation: XAV939/tankyrase-2 complex. **Y. Tanida**
- COMP 420.** Characterizing the folding of the amyloid precursor protein-C42. **J.E. Tate,** C.A. Parish, C.A. Taylor
- COMP 421.** Directing product specificity of type-III PRMT7 to type-I/II. **A. Thakur,** B. Caceres, J.M. Hevel, O. Acevedo
- COMP 422.** DFT study of novel siderophore- metal complexes. **P.M. Todebush,** C. Miller, L. Streit
- COMP 423.** Effect of pressure on mesoscopic structural changes in pyrrolidinium-based ionic liquids from molecular dynamics simulations. **D. Thummuru,** B. Mallik
- COMP 424.** New *de novo* design method of medium size cyclic peptides as inhibitors. **A. Ueda,** H. Sugiyama, A. Tomonaga
- COMP 425.** Quantum mechanics study of polyaromatic diradical formation through domino cyclization. **K. Ulep,** C.A. Parish
- COMP 426.** Determining the viability of calpain inhibitors as drugs for Alzheimer's disease. **S. Vera,** B.R. Miller
- COMP 427.** Dynamical electron correlation from an adiabatic connection formalism for doubly-occupied configuration interaction wavefunctions and related methods. **N. Vu,** A.E. DePrince
- COMP 428.** Spin-flip characterization of the Bergman cyclization of the hepta-1,6-diyne system. **S.G. Wairegi,** A. Luxon, C.A. Parish
- COMP 429.** Small Molecule *Ab-initio* for Representing Torsions (SMART) database. **B. Walker**
- COMP 430.** GPU parallelizing atomic energy calculations using explicitly correlated Gaussian functions. **Z. Wall,** M.L. Cafiero
- COMP 431.** Computational kinetics in supercritical CO₂ environment: Ethane dissociation and recombination reactions C₂H₆ ↔ CH₃ + CH₃. **C. Wang,** S.V. Panteleev, A. Masunov, S. Vasu
- COMP 432.** PgpRules: A decision tree based P-glycoprotein inhibitor and substrate prediction server. P. Wang, Y. Tu, **Y. Tseng**
- COMP 433.** First-order properties from second-order perturbation theory based on driven similarity renormalization group. **S. Wang,** C. Li, F.A. Evangelista
- COMP 434.** Evolutionary differences in structural dynamics among prolyl-tRNA synthetases from different species: A theoretical investigation using hybrid QM/MM simulations. **M. Weinzetl,** H. Hu, K. Weeks, S. Hati, S. Bhattacharyay
- COMP 435.** Computational investigation of structure-property relationships in ferrocene-based polymer materials. **L.J. Welch,** K.G. Walter, J. Feldblyum, **H.P. Hendrickson**



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- COMP 436.** Mechanism of Ti-catalyzed oxidative nitrene transfer in [2+2+1] pyrrole synthesis from alkynes and azobenzene. **X. Wen**, Z. Davis-Gilbert, I. Tonks, J. Goodpaster
- COMP 437.** Program to construct biologically relevant atomic resolution models of chondroitin sulfate biopolymers. **E. Whitmore**, G. Vesenka, H. Sihler, O. Guvench
- COMP 438.** Examining physical properties of thienyl pyridazine and oxazine structures. **S. Wild**, N.C. Tice, J.L. Jenkins
- COMP 439.** Practical approach for selecting a virtual screening model. S. Liu, M. Alnammi, S. Ericksen, F.M. Hoffmann, **S.A. Wildman**, A. Gitter
- COMP 440.** Compound informer sets derived from chemogenomic data predict kinase inhibitors. H. Zhang, C. Lee, S. Ericksen, J.C. Mitchell, S.J. Wright, R.D. Nowak, A. Gitter, F.M. Hoffmann, M.A. Newton, **S.A. Wildman**
- COMP 441.** Investigation of amyloid β biflavonoid inhibitors in Alzheimer's disease. **P.K. Windsor**, S.P. Plassmeyer, D.S. Mattock, B. Han, B. Miller
- COMP 442.** Pseudo Jahn Teller investigation into the symmetric forms of cyclobutane and malonaldehyde. **J.N. Woodford**
- COMP 443.** DFT study of the selectivity of monoamine oxidase B (MAOB). **A. Woody**, S. Jelinek, L.W. Peterson, M.L. Cafiero
- COMP 444.** Approaching temporal structure and stability of protein-water interactions by using local correlations: The local correlation analysis method. **T. Wulsdorf**, G. Klebe
- COMP 445.** ARES: An efficient real-space electronic structure calculation package. **Q. Xu**, S. Wang, X. Shao, y. Wang, Y. Ma
- COMP 446.** Role of alkyl chain length in maintaining the honeycomb structure of tricarbazo triazolophane macrocycles on the graphite surface understood via atom-resolved molecular dynamics. **J. Yang**, H.D. Castillo, S. Debnath, J. Dobscha, S.L. Tait, K. Raghavachari, A.H. Flood, P. Ortoleva
- COMP 447.** DFT exploration of halide exchange between $\text{CpRu}(\text{PPh}_3)_2\text{Cl}$ and MeI . **M. Yang**, R. Kirss
- COMP 448.** Matched pocket-fragment analysis of protein-protein interactions. **Y. Yang**, Y. Zhang
- COMP 449.** Modeling voltage-sensitive fluorescing membrane-bound probes using GAAMP parameterization to investigate their properties. **R. Youngworth**, B. Roux
- COMP 450.** Machine learning for understanding compatibility of organic-inorganic hybrid perovskite with post-treating amines. **Y. Yu**, X. Tan, Y. Wu
- COMP 451.** *Ab initio* molecular dynamics simulations of imidazolium-based ionic liquids. **K. Yue**, O. Acevedo
- COMP 452.** Development of a QM/MM simulation-based screening tool for quinone oxidoreductase inhibitors. S. Bhattacharyay, **J. Zajac**, C. Reinhardt
- COMP 453.** Pyparam: A Python-based tool for force field parameterization and optimization. **Q. Zeng**



TECHNICAL PROGRAM

COMP 454. Improving the efficiency of the multireference driven similarity renormalization group theory via sequential transformation, density fitting, and non-interacting virtual orbital approximation. **T. Zhang**, C. Li, F.A. Evangelista

COMP 455. Extraction of cluster free energy from small-N simulations of micelle formations. **X. Zhang**, J. Kindt

COMP 456. Machine learning software for automated force field parameterization. **X. Zhong**

Section A

Orange County Convention Center
West Hall C

NVIDIA GPU Award

M. E. Berger, C. L. Simmerling, *Organizers*

6:00 - 8:00

COMP 457. Highly accurate GPU-accelerated pKa prediction tool arrives in amber. **R. Harris**, J. Shen

COMP 458. Unraveling the quantum mechanical catalytic action of methyltransferases with GPU-accelerated large-scale electronic structure. **Z. Yang**, R. Rehmoor, H.J. Kulik

COMP 459. Versatile grid-based molecular input library optimized for machine learning. **J. Sunseri**, D. Koes

Section A

Orange County Convention Center
West Hall C

OpenEye Outstanding Junior Faculty Award

C. L. Simmerling, *Organizer*

6:00 - 8:00

COMP 460. Computational protein structure prediction guided by covalent labeling and SID mass spectrometry data. M. Aprahamian, J. Seffernick, S. Harvey, V.H. Wysocki, L. Jones, **S. Lindert**

COMP 461. Quantifying protein allostery upon external perturbation. **P. Tao**

COMP 462. Characterization of the optical rotation in molecules and extended 1D systems. **M. Caricato**

COMP 463. Advancing computational methods for spectroscopy, catalysis, and design. **S. Luber**, R. Han, J. Mattiat, K. Rempfer, M. Schilling, T. Zimmermann

Section A



TECHNICAL PROGRAM

Orange County Convention Center
West Hall C

Wiley Computers in Chemistry Outstanding Postdoc Award

Cosponsored by PROF
M. Cavalleri, C. L. Simmerling, *Organizers*

6:00 - 8:00

COMP 464. Transferability in machine-learning for electronic structure via the molecular orbital basis. **M. Welborn**, L. Cheng, T.F. Miller

COMP 465. Computational studies on bipyridine synthesis by contractive C–C coupling via P(V) intermediates. **J. Alegre Requena**, R.S. Paton

WEDNESDAY MORNING

Section A

Orange County Convention Center
West Hall B4 - Theater 21

Molecular Mechanics: Recent Advances in Simulations of Nucleic Acids

J. Shen, *Organizer*
C. Tian, *Presiding*

8:30 COMP 466. Advances and limitations of MD simulations of nucleic acids: Tuning the non-bonded force-field terms. **J. Sponer**

9:00 COMP 467. Convergence and reproducibility in the simulation of nucleic acids: Influence of salt, force fields and water models. **T.E. Cheatham**, R. Galindo

9:30 COMP 468. Optimization of Amber force field for nucleic acid bases. **V. Anisimov**, V. Poltev, T.E. Cheatham, J. Bernholc

10:00 Intermission.

10:15 COMP 469. Insights into DNA and RNA G-quadruplexes from polarizable molecular dynamics simulations. **J.A. Lemkul**

10:45 COMP 470. AMOEBA polarizable force field for DNA, RNA and modified nucleic acids. **Z. Jing**, R. Qi, P. Ren

11:00 COMP 471. Computational investigations on target-site searching and recognition mechanism by thymine DNA glycosylase during DNA repair process. **L. Da**



TECHNICAL PROGRAM

11:30 COMP 472. Unveiling the full binding pathway of TF-DNA complexes using MELD-accelerated molecular dynamics. **A. Bauzá, A. Perez**

Section B

Orange County Convention Center
West Hall B4 - Theater 22

Material Science

3D & 2D Materials

C. M. Aikens, *Organizer*
D. B. Amirkulova, *Presiding*

8:30 COMP 473. Mapping polaronic distortions across the metal-insulator transition of nanoscale β^1 - $\text{Cu}_x\text{V}_2\text{O}_5$. **A. Parija, J.L. Andrews, J.V. Handy, S. Banerjee**

8:55 COMP 474. New LaMnO_3 surface energy results obtained from density-functional theory. **Y. Mantz**

9:20 COMP 475. Map of the inorganic ternary metal nitrides. **W. Sun, C. Bartel, E. Arca, S. Bauers, B. Matthews, B. Orvananos, B. Chen, M. Toney, L. Schelhas, W. Tumas, J. Tate, A. Zakutayev, S. Lany, A. Holder, G. Ceder**

9:45 COMP 476. Tuning halide perovskite workfunctions with Cs coatings for photocathode applications. **A. Neukirch, S. Lewis, F. Liu, W. Nie, N. Moody, A. Mohite, S. Tretiak**

10:10 COMP 477. Tuning the structure and oxygen storage properties of oxide perovskites through chemical substitution. **D. Tafen, D.R. Alfonso, J.W. Lekse**

10:35 Intermission.

10:50 COMP 478. Interstitial defect configurations in alumina. A. Kononov, **A. Schleife**

11:15 COMP 479. Symmetry induced stability in alkali doped calcium-silicate-hydrate. **O. Ozcelik, N. Garg, C.E. White**

11:40 COMP 480. DFT analysis of Raman modes in the CDW states of layered 2H-TaSe_2 and 2H-TaS_2 . **S. Chowdhury, H.M. Hill, J.R. Simpson, P. Vora, A.R. Hight Walker, F. Tavazza**

12:05 COMP 481. Onset of vertical bonds in new GaN multilayers: Beyond van der Waals solids. **E. Durgun, A. Onen, D. Kecik, S. Ciraci**

Section C

Orange County Convention Center
West Hall B4 - Theater 25

Quantum Mechanics: Strong Electron Correlation



TECHNICAL PROGRAM

A. E. DePrince, H. P. Hratchian, *Organizers*
E. Maradzike, *Presiding*

8:30 COMP 482. Modeling dynamics of strongly correlated systems with graphics processing unit–accelerated time-dependent multireference methods. **B.G. Levine**, W. Peng, B. Fales, A.S. Durden

9:05 COMP 483. Automatic active space selection in multiconfigurational self consistent field methods with multi-step machine learning for calculating bond dissociation energies. **W. Jeong**, S. Stoneburner, L. Gagliardi

9:30 COMP 484. Examining electronic structure theory methods with machine learning. **K.D. Vogiatzis**

10:05 Intermission.

10:25 COMP 485. Multi-reference algebraic diagrammatic construction theory. **A. Sokolov**

11:00 COMP 486. Coupled cluster theory with valence orbital-optimized doubles: Geometries and excitation spectra of strongly correlated systems. **J. Lee**, M.P. Head-Gordon

11:25 COMP 487. Higher order singular-value decomposition for strongly correlated systems. V. Abraham, **N. Mayhall**

12:00 COMP 488. Current-constrained reduced density-matrix theory for molecular conductivity. **A. Raeber**, D.A. Mazziotti

Section D

Orange County Convention Center
West Hall B4 - Theater 23

Drug Design

AI & Machine Learning

M. R. Landon, Y. Tseng, *Organizers*
E. M. Leddin, *Presiding*

8:30 COMP 489. Towards accurate and precise binding affinity predictions: the λ -SAMS and 2D-vFEP(λ) methods. **T. Lee**, D.M. York

8:50 COMP 490. Theoretical estimation of membrane permeabilities of drugs by implicit membrane models and machine learning. **B. Dutagaci**, S.A. Brocke, A.D. Mackerell, M. Feig

9:10 COMP 491. Incorporating ligand conformation stability and explicit water molecules in machine-learning scoring functions. **J. Lu**, X. Hou, C. Wang, Y. Zhang

9:30 Intermission.

9:45 COMP 492. Designing for bias: Computational methods to drive rational design of G-protein biased agonists. **R. Torella**



TECHNICAL PROGRAM

10:05 **COMP 493.** Bayesian optimization for conformer generation. **L. Chan**, G. Hutchison, G.M. Morris

10:25 **COMP 494.** Computational reactivity scanning for designing lysine targeted covalent kinase inhibitors. **R. Liu**, J. Shen

10:45 **COMP 495.** Generation of complete active spaces of tautomers for drug discovery. **H. Yu**, M. Waston, A. Bochevarov

11:05 **COMP 496.** Leveraging cloud computing for *in-silico* drug design using the Quantum Molecular Design (QMD) framework. **S. Keinan**, E.H. Frush, W.J. Shipman

Section E

Orange County Convention Center
West Hall B4 - Theater 24

Simulation of Protein-Membrane Interfaces

M. Buck, A. Gorfe Abebe, *Organizers*
A. E. Garcia, *Presiding*

8:30 **COMP 497.** Regulatory mechanisms of Ras signaling at the membrane. **R. Nussinov**, H. Jang

9:00 **COMP 498.** Molecular choreography within the bacterial cell envelope: Insights from molecular dynamics simulations. **S. Khalid**, F. Samsudin, A. Boags, J. Shearer

9:30 **COMP 499.** Properties of polyunsaturated lipids at the lipid-protein interface: Effects on protein-protein interactions. **S. Feller**

10:00 **COMP 500.** Novel small molecule modulators of the hotspot PIK3CA mutants identified by computational and experimental approaches. **Z. Cournia**, P. Gkeka, H. Leontiadou, I. Galdadas, C. Athanasiou, V. Lazani, M. Pavlaki, B. Agianian, S. Christoforidis, A. Efstratiadis

10:15 Intermission.

10:30 **COMP 501.** PS membrane asymmetry influences the folding and insertion of a transmembrane helix. **H.L. Scott**, F.A. Heberle, J. Katsaras, F.N. Barrera

10:45 **COMP 502.** Lipid binding specificity of small GTPase membrane anchors. **J.F. Hancock**

11:15 **COMP 503.** Signaling proteins on the membrane surface. **J.T. Groves**

11:45 **COMP 504.** Fluctuating thermodynamics for biomolecular interactions. **S. Ham**

Deep Learning



TECHNICAL PROGRAM

Sponsored by CINF, Cosponsored by COMP

Carbon Dioxide Conversion & Utilization

CO₂ Capture & Conversion

Sponsored by ENFL, Cosponsored by CATL, COMP and GEOC

From Lab Book to Journal Article: Insights from Editors on the Publication Process

Sponsored by PHYS, Cosponsored by COMP[†]

Quantum Embedding Electronic Structure Methods

Sponsored by PHYS, Cosponsored by COMP

Sustainable Software for Computational Molecular Science

Data & Machine Learning

Sponsored by PHYS, Cosponsored by COMP

WEDNESDAY AFTERNOON

Section A

Orange County Convention Center
West Hall B4 - Theater 21

Molecular Mechanics: Recent Advances in Simulations of Nucleic Acids

J. Shen, *Organizer*
D. P. Harding, *Presiding*

1:00 COMP 505. Study of ion effects in group II introns. A. Wang, M. Levi, **U. Mohanty**, P. Whitford

1:30 COMP 506. Binding of transition and alkaline earth metal ions with a DNA duplex from classical molecular dynamics simulations. **M. Provorse Long**, M. Martin, C. Isborn



TECHNICAL PROGRAM

2:00 COMP 507. Free energy changes in the folding transitions of RNA driven by divalent cations. **H. Nguyen**, N. Hori, D. Thirumalai

2:15 COMP 508. Computational design of unnatural nucleotides for artificial life. **N.R. Jena**

2:45 Intermission.

3:00 COMP 509. Molecular mechanism of DNA specificity of CRISPR-Cas9. **G. Palermo**, C. Gravina Ricci, J.S. Chen, Y. Miao, M. Jinek, J.A. Doudna, J.A. McCammon

3:30 COMP 510. Binding of EMICORON to human vascular endothelial growth factor receptor-2 (vegfr-2) G-quadruplex probed by homology modeling and all-atom molecular dynamics simulations. **C. Wu**, H. Sullivan

4:00 COMP 511. Molecular architecture and functional dynamics of the human transcription initiation machinery. **I.N. Ivanov**, C. Yan, T. Dodd

4:30 COMP 512. Molecular mechanism for the role of histone tails in nucleosome repositioning. **K. Chakraborty**, M. Kang, S. Loverde

4:45 COMP 513. Critical inspection of the Varkud satellite ribozyme active site. **A. Ganguly**, D.M. York

Section B

Orange County Convention Center
West Hall B4 - Theater 22

Material Science

Nanomaterials

C. M. Aikens, *Organizer*
H. Liu, *Presiding*

1:30 COMP 514. DFT insights into brightening of II-VI quantum dots by hydride treatment. **L. Lystrom**, S. Kilina, S. Ivanov

1:55 COMP 515. Ultrafast coherent energy and charge transfer in nanosystems by fs laser pulses: A quantum dynamical study of CdSe QD dimers and of functionalized gold clusters. **F. Remacle**

2:20 COMP 516. Luminescence properties of ligand-protected gold and silver nanoclusters. **K.M. Weerawardene**, C.M. Aikens

2:45 COMP 517. Real-time density functional tight binding: A new computational approach for probing plasmonic properties of large material systems. **B.M. Wong**, N.V. Ilawe, M.B. Oviedo

3:10 COMP 518. *Ab initio* insights in the physical and chemical properties of bare and protected mono- and bimetallic nanoclusters: From small to nanoclusters systems (42 systems). **K.F. Andriani**, K.E. Batista, A.C. Da Silva, M.J. Piotrowski, J.L. Da Silva



TECHNICAL PROGRAM

3:35 Intermission.

3:50 **COMP 519.** Interplay of metals with carbon and boron nitride nanotubes. **C. Rohmann**, M. Zwolak

4:15 **COMP 520.** Quantum mechanical modeling of explicitly solvated noble metal nanoparticles. **E. Guidez**

4:40 **COMP 521.** Molecular dynamics simulations to design nanoreceptors with targeted recognition abilities. X. Sun, L. Riccardi, F.D. federico.debiasi92@gmail.com, F. Rastrelli, **M. Devivo**, F. Mancin

5:05 **COMP 522.** Cooperative communication between active sites in single-atom catalyst: A first-principle study. **G. Zhang**, Q. Li

Section C

Orange County Convention Center
West Hall B4 - Theater 25

Quantum Mechanics

A. E. DePrince, H. P. Hratchian, *Organizers*
J. Lee, *Presiding*

1:30 **COMP 523.** Exact exchange-correlation potentials from electron densities. **B. Kanungo**, V. Gavini

1:55 **COMP 524.** Half-projected σ -SCF for electronic excited states. **H. Ye**, T.A. Van Voorhis

2:20 **COMP 525.** There is a problem with some barrier height benchmarks. **E.N. Brothers**

2:45 **COMP 526.** Linear scaling excited state forces within the linear-response time dependent DFT formalism: Method and applications. **J. Aarons**, T.J. Zuehlsdorff, N. Hine

3:10 **COMP 527.** Development of reliable, regularized, orbital-optimized, second-Order Møller–Plesset perturbation theory and its application to biradicaloids and artificial spin-symmetry breaking. **J. Lee**, M.P. Head-Gordon

3:35 Intermission.

3:50 **COMP 528.** Halogen-bonding interactions: Revised benchmarks and a new assessment of exchange vs. dispersion. **B.M. Wong**, L.N. Anderson, F.W. Aquino, A.E. Raeber, X. Chen

4:15 **COMP 529.** Investigating the anharmonic vibrational structure of van der Waals systems. **O. Sode**, M. Keceli

4:40 **COMP 530.** Explicitly correlated dispersion and exchange dispersion energies in symmetry-adapted perturbation theory. **M. Kodrycka**, K. Patkowski

5:05 **COMP 531.** Spin splittings from first-order symmetry-adapted perturbation theory without the single exchange approximation. **J. Waldrop**, K. Patkowski

Section D



TECHNICAL PROGRAM

Orange County Convention Center
West Hall B4 - Theater 23

Drug Design

AI & Machine Learning

M. R. Landon, Y. Tseng, *Organizers*
M. L. Estep, *Presiding*

1:30 COMP 532. Improving the rationale for drug design by developing computational approaches. **F. Bai**, R. Nechushtai, H. Li, H. Jiang, J.N. Onuchic

1:50 COMP 533. Rational design of small molecules inhibiting amyloid beta aggregation. V. Man, X. He, **J. Wang**

2:10 COMP 534. Allosteric ligand modifications: A new addition to the drug designer's toolkit. T. Abramyan, Y. An, **D. Kireev**

2:30 Intermission.

2:45 COMP 535. Electrostatic complementarity as a fast and effective tool to optimize binding and selectivity of protein-ligand complexes. M. Bauer, **T. Cheeseright**, M.D. Mackey

3:05 COMP 536. Profiling diverse chemical space to map the druggable proteome. **H. wang**

3:25 COMP 537. AbbVie's structure based ligand design tools. **Y. Pevzner**

3:45 COMP 538. Rational selection of plants and design of new compounds for anti-dengue discovery using *in-silico* screening from Natural Product Discovery System (NADI). **H.A. Wahab**, V. Ganesh, K. Yong, R. Roslim, E. Kamarulzaman, M. Ismail

4:05 COMP 539. Neural networks incorporating entropy and machine learning improved crystal pose predictions and affinity ranking of small molecules. **J. Fine**, J. Konc, R. Samudrala, **G. Chopra**

Section E

Orange County Convention Center
West Hall B4 - Theater 24

Simulation of Protein-Membrane Interfaces

M. Buck, *Organizer*
A. Gorfe Abebe, *Organizer, Presiding*

1:30 COMP 540. From the simulation of transmembrane domain of single pass receptors to therapeutic strategies. F. Binamé, L. Pham-Van, C. Spenlé, M. Van der Heyden, **D. Bagnard**



TECHNICAL PROGRAM

2:00 COMP 541. Physical properties of membranes and membrane mimics: potential impact on membrane protein structure. **L.M. Columbus**, N. Swope, T. Caldwell

2:30 COMP 542. Probing the roles of membrane and cholesterol on A β biogenesis and toxicity. **J.E. Straub**, A. Bandara, G.A. Pantelopulos

3:00 COMP 543. Free-energy studies on human β defensin type 3 through a neutrally charged lipid membrane. **L. Zhang**

3:15 Intermission.

3:30 COMP 544. Capturing the association of transmembrane helices in molecular simulations. J. Domanski, P. Stansfeld, M.S. Sansom, **R.B. Best**

4:00 COMP 545. Molecular dynamics simulations of proteins sensing and remodeling lipid membranes in cells. **G. Hummer**, M. Gecht, M. Siggel, R. Covino, R.M. Bhaskara

4:30 COMP 546. Modeling dyphtheria toxin translocation domain pH triggered unfolding and membrane association. **M.G. Kurnikova**

5:00 COMP 547. High affinity KRAS inhibitors that disrupt effector binding. **A. Gorfe Abebe**

5:25 Concluding Remarks.

Modeling Dynamics in Dense Manifolds of Electronic States

Materials & Surfaces

Sponsored by PHYS, Cosponsored by COMP

Quantum Embedding Electronic Structure Methods

Sponsored by PHYS, Cosponsored by COMP

Sustainable Software for Computational Molecular Science

Software Tools: Molecular Mechanics

Sponsored by PHYS, Cosponsored by COMP

THURSDAY MORNING

Section A



TECHNICAL PROGRAM

Orange County Convention Center
West Hall B4 - Theater 21

Molecular Mechanics

J. Shen, *Organizer*
T. Harris, *Presiding*

8:30 COMP 548. Accurate and reliable prediction of irreversible covalent inhibitor binding kinetics. **H. Yu**, L. Wang, R. Abel

9:00 COMP 549. Molecular dynamics and umbrella sampling simulations elucidate differences in troponin C isoform and mutant hydrophobic patch exposure. J. Bowman, **S. Lindert**

9:30 COMP 550. Mesh free periodic parallel treecode for electrostatics in molecular simulations: An alternative to PME in parallel? **H.A. Boateng**

10:00 COMP 551. Graph-based representations and kernel methods for the prediction of molecular properties. **Y. Tang**, W. Dejong

10:15 Intermission.

10:30 COMP 552. Homology modelling in the twilight zone via a novel multi-template approach. **C.A. Reynolds**

11:00 COMP 553. Dynamics of biopolymers studied using statistical analysis of contacts. **T. Shen**

11:30 COMP 554. Molecular mechanisms for regulation of drought-resistance in plants. **D. Shukla**

12:00 COMP 555. Conserved long-range interaction networks, energetics and the determinants of protein topology. Z. Haratipour, J. Poutsma, **L.H. Greene**

12:15 COMP 556. Role of protein conformational changes in cellular cargo transport and calcium signaling. **P. Goyal**

Section B

Orange County Convention Center
West Hall B4 - Theater 22

Material Science

Porous Materials & Reactivity

C. M. Aikens, *Organizer*
R. Parveen, *Presiding*

8:30 COMP 557. Development of MOF-FF compatible interaction model for liquid methanol and Cl⁻ in methanol. **S. Siwaipram**, P.A. Bopp, J. Soetens, R. Schmid, S. Bureekaew



TECHNICAL PROGRAM

8:55 **COMP 558.** Computer-aided designing high-performance CO₂ solid sorbents. **Y. Duan**

9:20 **COMP 559.** Tailoring the electronic properties of Zn-BTC MOF via ligand functionalization. **G.D. Degaga**, R. Pandey, C. Gupta, L. Bharadwaj

9:45 **COMP 560.** Examining the gas adsorption properties in molecular porous materials based upon copper–adenine paddlewheel complexes. **T. Pham**, K. Forrest, M.J. Zaworotko, B. Space

10:10 Intermission.

10:25 **COMP 561.** Hexane isomers in zeolite NaY: Molecular dynamics study on the dependence of diffusion on molecular diameter. **A.M. Thomas**, Y. Subramanian

10:50 **COMP 562.** Multiscale modeling of aqueous phase methane diffusion in zeolite frameworks. P.M. Kekenus-Huskey, **T. Pace**, H. Rahmaninejad

11:15 **COMP 563.** Density functional theory investigation of mechanisms of degradation reactions of sulfonated PEEK membranes with H, OH and OOH radicals in fuel cells. **J.E. Stevens**, K. Utterbeck, Z. Smith, A. Piatkowski, N. Ognanovich

11:40 **COMP 564.** Multi-scale modeling of Li-ion battery anode materials using reactive force fields. **M. Bhati**, T. Senftle

12:05 **COMP 565.** Decomposition reactions dictate the performance of first-principles predictions of solid-stability. **C. Bartel**, A.W. Weimer, S. Lany, C. Musgrave, A. Holder

Section C

Orange County Convention Center
West Hall B4 - Theater 25

Quantum Mechanics

A. E. DePrince, H. P. Hratchian, *Organizers*
M. Mostafanejad, *Presiding*

8:30 **COMP 566.** Acylation and deacylation mechanism and kinetics of penicillin G reaction with streptomyces R61 DD-peptidase. **Q. Cheng**, N.J. Deyonker

8:50 **COMP 567.** Solvent effect on dipeptide bond formation: Glycine as a case study. **Z. Hosni**

9:10 **COMP 568.** Thermochemistry of C₁ and C₂ bromo compounds via connectivity-based reaction schemes and ab initio composite methods. **K.R. Jorgensen**

9:30 **COMP 569.** Dimensionality reduction of reaction coordinates and trajectories. **S.R. Hare**, D.R. Glowacki, B.K. Carpenter

9:50 **COMP 570.** Impact of ligand conformations on polyolefin growth. **A.L. Dewyer**, P.M. Zimmerman

10:10 Intermission.



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

10:25 COMP 571. Elucidating the role of the enzyme environment and mechanism of H₂ catalysis in FeNi hydrogenase. **M.E. McGreal**, J. Goodpaster

10:45 COMP 572. Ion mobility-aided, quantum chemical analysis of H⁺XPGG conformers: The roles of hydrogen bonds, free energies, and dispersion. **D. Beckett**, T.J. El-Baba, D.E. Clemmer, K. Raghavachari

11:05 COMP 573. Understanding the structure and energy relationship of double helical amylose fragments. **U. Schnupf**

11:25 COMP 574. Efficient estimation of formation enthalpies with local coupled-cluster methods: Extension to sulfur. E. Paulechka, **A. Kazakov**

11:45 COMP 575. Development of AMOEBA parameters for ionic liquids from density-based energy decomposition analysis (DEDA). **E.A. Vazquez Montelongo**, Q. Wu, G.A. Cisneros

Section D

Orange County Convention Center
West Hall B4 - Theater 23

Drug Design

Molecular Dynamics

M. R. Landon, Y. Tseng, *Organizers*
S. Lenka, *Presiding*

8:30 COMP 576. Drug resistance acquired by local and allosteric conformational changes in oncogenic tyrosine kinases. **M. Araki**, Y. Okuno

8:50 COMP 577. Reduced free-energy perturbation/Hamiltonian replica exchange molecular dynamics method with unbiased alchemical thermodynamic axis. **W. Jiang**

9:10 COMP 578. Ensemble-based molecular dynamics: Uncertainty quantification and enhanced sampling techniques in free-energy calculations. S. Wan, A.P. Bhati, **P.V. Coveney**

9:30 Intermission.

9:45 COMP 579. Investigation of cyclic ligands inhibiting CD2-CD58 interactions using molecular dynamics and molecular docking approaches. **D.P. Vercauteren**, A. Laurent

10:05 COMP 580. How binding site water and inhibitor protonation modulate the selectivities of beta-secretase 1 inhibitors. **J. Shen**, J. Henderson

10:25 COMP 581. Free-energy calculations to guide bromodomain inhibitor optimization. **J.P. Bluck**, L. See, A. Scora, J. Reynolds, F. Rianjongdee, G.M. Morris, S.J. Conway, P. Biggin

10:45 COMP 582. Macro-pKa predictions for drug-like molecules. **A. Bochevarov**, M. Waston, H. Yu



TECHNICAL PROGRAM

11:05 COMP 583. Structure, dynamics, and hydrolytic properties of the class C CMY-136 β -lactamase. A. Zavala, P. Retailleau, T. Naas, **B.I. Iorga**

Section E

Orange County Convention Center
West Hall B4 - Theater 24

Computational Studies of Water

Applications & Models

D. J. Sindhikara, *Organizer*
G. W. Dayhoff, *Presiding*

8:30 COMP 584. Incorporation of quantum chemical effect of solvent into molecular dynamics simulation. **H. Watanabe**

8:55 COMP 585. Development of AMOEBA+ polarizable atomic multipole water model. **C. Liu**, P. Ren

9:15 COMP 586. Protein-motion coupled hydration structure and dynamics. **S. Austin**, W. Yang, D. Wu

9:35 Intermission.

9:50 COMP 587. General purpose water model can improve atomistic simulations of intrinsically disordered proteins. **P. Seifpanahi**

10:10 COMP 588. New semi-empirical solvent functionals for structure-based drug discovery: Routes to customized solvent thermodynamics. **T. Wulsdorf**, G. Klebe

10:30 COMP 589. Tuning conformational and solvation selectivity by changing solvent polarity: A molecular-dynamics study. **I. Gladich**, J.S. Francisco

10:50 COMP 590. Artificial intelligence for catalyst design: Removal of ammonia pollution from water. **J. Freeze**, V.S. Batista

Modeling Dynamics in Dense Manifolds of Electronic States

Nonadiabatic Molecular Dynamics

Sponsored by PHYS, Cosponsored by COMP

Quantum Embedding Electronic Structure Methods

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TECHNICAL PROGRAM

Sustainable Software for Computational Molecular Science

Software Tools: Quantum Mechanics

Sponsored by PHYS, Cosponsored by COMP

THURSDAY AFTERNOON

Section A

Orange County Convention Center
West Hall B4 - Theater 21

Molecular Mechanics

J. Shen, *Organizer*
B. Pollard, *Presiding*

1:30 COMP 591. Selectivity in the activation mechanisms of inhibitor of κ B kinase- β . **M.R. Jones**, A.K. Wilson, B. Brooks

1:50 COMP 592. PETase: Characterization of a plastic-degrading enzyme. **F.L. Kearns**, B. Pollard, H. Austin, J. McGeehan, G. Beckham, H.L. Woodcock

2:10 COMP 593. Hydration and dispersion forces in hydroxypropylcellulose phase behavior. **G.W. Dayhoff**, D. Rogers

2:30 COMP 594. Machine learning-based classification model for β -Lactamase recognizing its ligand: TEM-1 and benzyl-penicillin complex. **F. Wang**, P. Tao

2:50 COMP 595. ff18SB: Amino-acid specific protein backbone parameters trained against quantum mechanics energies in solution. **C. Tian**, K.A. Belfon, L. Raguette, A.N. Miguez, Q. Wu, C.L. Simmerling

3:10 Intermission.

3:25 COMP 596. Development of force-field parameters for simulation of self-assembly processes in MOFs and metalloproteins. **A. Sengupta**, L. Song, K.M. Merz

3:45 COMP 597. Dynamic combinatorial analysis of local configurations in molecular dynamics simulation: Frequent substructure clustering and sub-conformational hierarchical hidden Markov model. **K. Ho**, D. Hamelberg

4:05 COMP 598. Modeling GPI-anchors and GPI-anchored proteins: three disparate biomolecular species in close proximity. **P. Banerjee**, R. Lipowsky, **M. Santer**

4:25 COMP 599. Methyl-induced polarization weakens biochemical interactions of N-methylated lysines. **S. Rahman**, Y. Al-Hamdani, S. Varma



TECHNICAL PROGRAM

4:45 COMP 600. Study of the pH-dependent properties for the *Escherichia coli* glycinamide ribonucleotide transformylase using theoretical methods. **P. Gupta**, A.E. Roitberg

Section B

Orange County Convention Center
West Hall B4 - Theater 22

Material Science

Carbon-Based Materials

C. M. Aikens, *Organizer*
F. Ramezanghorbani, *Presiding*

1:30 COMP 601. Computational design of high-chi block oligomers capable of forming lamellar and micellar mesophases with 1-nanometer domains. **J.I. Siepmann**, Q.P. Chen, Z.D. Shen, T.P. Lodge

1:50 COMP 602. Machine learning-enabled insights into the phase-transition of thermosensitive polymers. K. Bejagam, Y. An, S. Singh, **S.A. Deshmukh**

2:10 COMP 603. Interaction of supramolecular anticancer nanotubes with model cell membranes. **A. Manandhar**, M. Kang, K. Chakraborty, S. Loverde

2:30 COMP 604. Ultrashort peptide materials design via a hybrid computational approach. S. Mushnoori, E. Zang, K. Schmidt, **M. Dutt**

2:50 Intermission.

3:05 COMP 605. Molecular simulation study of the structure-hydration-antifouling relationship of different poly(N-hydroxymethyl acrylamide). **Y. Liu**, M. Zhang, B. REN, Y. Zhang, F. Yang, J. Zheng

3:25 COMP 606. Approaching peptide-surface adsorption free energy from macro and microscopic perspectives. **Z. Kuang**, K. Singh, C. Sullivan, P. Dennis, D. Oliver, C. Perry, R.R. Naik

3:45 COMP 607. Molecular-level insight into the interactions between drug amphiphiles and model cell membranes. **P.K. Tang**, M. Kang, K. Chakraborty, S. Loverde

4:05 COMP 608. Van der Waals effects on the optical and charge transfer properties in organic photovoltaics. **J.I. Rodriguez-Hernandez**, A.W. Goetz, D.E. Trujillo-Gonzalez, F. Castillo-Alvarado

4:25 COMP 609. Essential diabatic orbital method to calculate electronic couplings between poly-3-hexylthiophene polymer units for charge transfer dynamics simulations. **T. Yu**

4:45 COMP 610. Coarse-grain simulation study of the shear-band deformation mechanism in molecular crystals. **S. Izvekov**, P. Lafond, J. Brennan, J. Larentzos

5:05 COMP 611. Some computational experiments revealing anisotropic strain energies in C₆₀ fullerene. **P. Deshpande**



TECHNICAL PROGRAM

Section C

Orange County Convention Center
West Hall B4 - Theater 25

Quantum Mechanics

A. E. DePrince, H. P. Hratchian, *Organizers*
A. Ehnbom, *Presiding*

1:30 COMP 612. Non-Markovian dynamics: An extension of the Lindblad theory. **K. Head-Marsden**, D.A. Mazziotti

1:55 COMP 613. Perturbative triples corrections in the multireference driven similarity renormalization group. **C. Li**, F.A. Evangelista

2:20 COMP 614. Time-domain formulation of equation-of-motion coupled-cluster theory for linear response properties: Absorption and electronic circular dichroism spectra. **D. Nascimento**

2:45 COMP 615. Regularized Møller-Plesset perturbation theory: Assessment of third-order perturbation theory on thermochemistry, bond dissociation, and noncovalent interactions. **L. Bertels**, J. Lee, M.P. Head-Gordon

3:10 COMP 616. Generalized unitary coupled cluster wavefunctions for quantum computation. **J. Lee**, W. Huggins, M.P. Head-Gordon, K.B. Whaley

3:35 Intermission.

3:50 COMP 617. Simulating vibronic molecular spectra on a universal quantum computer. **N.P. Sawaya**, J. Huh

4:15 COMP 618. Rovibrational quartic force fields of scandium and titanium dicarbide. **N.J. Deyonker**, R.C. Fortenberry, Q. Cheng

4:40 COMP 619. Novel approach to compute vibrational spectra in cluster models of enzyme active sites. **S. Dasgupta**, J. Herbert

5:05 COMP 620. GPU-accelerated quantum Monte Carlo studies of adsorbed monolayers: Ar on MgO(100). **R.J. Hinde**

Section D

Orange County Convention Center
West Hall B4 - Theater 23

Drug Design

Molecular Dynamics

M. R. Landon, Y. Tseng, *Organizers*
D. Ghoreishi, *Presiding*



TECHNICAL PROGRAM

- 1:30 COMP 621.** Unbiased kinase DFG-flip revealed by continuous constant pH molecular dynamics. **C. Tsai**, Z. Yue, J. Shen
- 1:50 COMP 622.** Addressing the cross-docking problem through polarization. **C.A. Reynolds**, K.J. Smith, D. Reha
- 2:10 COMP 623.** Evaluation of Tinker-OpenMM to aid in the optimization of a MELK inhibitor. **M. Harger**, B. Walker, K. Dalby, P. Ren
- 2:30** Intermission.
- 2:45 COMP 624.** Thermodynamics of preorganization: A combined experimental and computational study on a congeneric series of thrombin ligands. **T. Wulsdorf**, A. Sandner, G. Klebe
- 3:05 COMP 625.** Targeting enzymes exhibiting 'ping-pong' kinetic mechanism: A case study with quinone oxidoreductase. **S. Bhattacharyay**
- 3:25 COMP 626.** Multidimensional optimization of the dielectric boundary for protein-ligand binding computations in implicit solvent. **N. Forouzes**, A. Mukhopadhyay, L. Watson, A.V. Onufriev
- 3:45 COMP 627.** Implementation of GPU-accelerated partial nudged elastic band method in AMBER. **D. Ghoreishi**, D.S. Cerutti, A.E. Roitberg
- 4:05 COMP 628.** Application of molecular dynamics in developing anti-inflammatory drugs. **V. Mouchlis**, C.T. Mu, J.A. McCammon, E.A. Dennis

Section E

Orange County Convention Center
West Hall B4 - Theater 24

Computational Studies of Water

Properties & Phenomena

D. J. Sindhikara, *Organizer*
L. Warrensford, *Presiding*

- 1:30 COMP 629.** Community analysis of molecular protrusions at liquid/liquid interfaces. **M. Servis**, A.E. Clark
- 1:50 COMP 630.** Calculating the entropy of fluids from molecular dynamics simulations. **E.A. Ploetz**, P.E. Smith
- 2:10 COMP 631.** Correlated dynamics and random walks in aqueous proton diffusion. **S.A. Fischer**, B.I. Dunlap, D. Gunlycke
- 2:30 COMP 632.** Aromatic molecules at ice surfaces: solvation and light absorption. **D. Donadio**, F.C. Bononi, T. Kling, T. Huller, C. Anastasio
- 2:50** Intermission.



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

3:05 COMP 633. Water as described by the random phase approximation. **H. Eshuis**, J. Chedid

3:25 COMP 634. Machine learning water: Insights into vibrational spectroscopy and aqueous proton defects. **T. Morawietz**, T. Markland

3:45 COMP 635. Development of reactive force-fields for HCl water clusters and subsequent analysis of cluster properties. **C. Bresnahan**, R. Kumar

4:05 COMP 636. *Ab initio* force fields for water: The multifaceted roles of atomic charge density anisotropy. **M. Van Vleet**, J.R. Schmidt, A. Misquitta

Modeling Dynamics in Dense Manifolds of Electronic States

Nonadiabatic Molecular Dynamics

Sponsored by PHYS, Cosponsored by COMP

Quantum Embedding Electronic Structure Methods

Sponsored by PHYS, Cosponsored by COMP

Sustainable Software for Computational Molecular Science

Methods

Sponsored by PHYS, Cosponsored by COMP

ENFL

Division of Energy and Fuels

H. Lin, *Program Chair*

SUNDAY MORNING

Section A

Orange County Convention Center
West Hall B4 - Theater 12



TECHNICAL PROGRAM

George A. Olah Award in Hydrocarbon or Petroleum Chemistry: Symposium in Honor of ChunShan Song

E. B. Fox, M. J. Janik, C. Song, U. T. Turaga, *Organizers*
X. Guo, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 ENFL 1. My research parter, Chunshan Song. **X. Guo**

9:00 ENFL 2. Overview of gaseous carbon waste streams utilization: Status and research needs. **A.M. Gaffney**

9:25 ENFL 3. Characterization of the nanoparticle and surface structure in platinum intermetallic alloy catalysts. N. LiBretto, S. Purdy, A.J. Kropf, G. Zhang, **J.T. Miller**

9:50 ENFL 4. Observing catalysts in real time with x-ray scattering and spectroscopy. **R.E. Winans**, S. Lee, S. Lee, T. Li

10:15 Intermission.

10:30 ENFL 5. Seeing the catalytically active phases/sites with *in situ* spectroscopy. **G. Zhang**, J.T. Miller, X. Guo, C. Song

10:55 ENFL 6. Preparation and characterization of ZUSY zeolites with highly catalytic cracking activity and superior hydride transfer capacity. **P. Liu, B. Shen**

11:20 ENFL 7. Catalyst design with atomic layer deposition. **C.L. Marshall**, P.C. Stair, H. Zhang, J.C. Bunquin, Z. Lu

11:45 ENFL 8. Experimental establishment of scaling relationships for processes on alloy catalysts. **A.J. Gellman**

12:10 Concluding Remarks.

Section B

Orange County Convention Center
West Hall B4 - Theater 13

Innovative Chemistry & Materials for Electrochemical Energy Storage

Li-Ion & Na-Ion

Cosponsored by CATL, INOR and PMSE
B. Gallant, W. Luo, Y. Mo, *Organizers*
H. Sun, *Organizer, Presiding*
C. Wang, *Presiding*

8:00 Introductory Remarks.

8:05 ENFL 9. Battery500 approach for long cycling, high-energy Li batteries. **J. Liu**



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

8:35 ENFL 10. Conversion chemistries for anodes, cathodes, and separators for Li-ion batteries. **G. Yushin**

9:05 ENFL 11. Material cation co-doping and superionic conductor incorporation to enhance the electrochemical performances of $\text{LiNi}_{0.5}\text{Mn}_{1.5}\text{O}_4$ cathode. X. Zheng, W. Liu, Q. Qu, **H. Zheng**

9:35 ENFL 12. Predicting surface active sites for lithium solvate interaction with metal oxides. **V. Murugesan**, K. Han, A. Andersen, N. Govind

9:55 Intermission.

10:10 ENFL 13. Li-excess cation-disordered rocksalt oxides with cationic/anionic redox for non-aqueous batteries. **N. Yabuuchi**

10:40 ENFL 14. Tailoring the charge transport in 3D electrode for efficient energy storage. **H. Sun**

11:10 ENFL 15. Distinct anionic oxygen activity in Li-rich layered oxide cathodes. **W. Tong**

11:40 ENFL 16. Niobium tungsten oxides for high-rate lithium-ion energy storage. **K.J. Griffith**, K. Wiaderek, G. Cibir, L.E. Marbella, C.P. Grey

Section C

Orange County Convention Center
West Hall B4 - Theater 14

Carbon Dioxide Conversion & Utilization

CO₂ Hydrogenation to Fuels & Chemicals

Cosponsored by CATL, COMP and GEOC
Y. H. Hu, H. Lin, R. Motkuri, *Organizers*
S. Kawi, *Organizer, Presiding*
X. Guo, Y. Sun, *Presiding*

8:25 Introductory Remarks.

8:30 ENFL 17. Direct transformation of CO₂ to chemicals and fuels. **Y. Sun**

8:55 ENFL 18. Developing efficient heterogeneous catalysts for the conversion of CO₂ to value-added products. **S. Raveendran**

9:20 ENFL 19. Direct CO₂ hydrogenation into olefins and aromatics with high selectivity. **P. Gao**, C. Yang, S. Li, Y. Sun

9:40 ENFL 20. Activation and hydrogenation of CO₂ over iron-based bimetallic catalysts: Insight from DFT. **H. Wang**, X. Nie, X. Guo, C. Song

10:00 ENFL 21. CO₂ conversion to MeOH-DME fuels: Catalytic and technological aspects. G. Bonura, C. Cannilla, A. Mezzapica, L. Frusteri, **F. Frusteri**



TECHNICAL PROGRAM

10:20 Intermission.

10:35 ENFL 22. Catalytic conversion of CO₂ into high value-added chemicals. **X. Guo**, C. Song

11:00 ENFL 23. From single atoms to clusters: Manipulating CO₂ reduction pathways on metal catalysts. Y. Zhu, J. Zheng, J. Fulton, L. Kovarik, J. Szanyi, J. Lercher, **O. Gutierrez-Tinoco**

11:20 ENFL 24. Direct conversion of CO₂ into olefin-rich higher hydrocarbons over Fe-Cu bimetallic catalyst. **W. Wang**, X. Wang, C. Song

11:40 ENFL 25. CO₂ hydrogenation to methanol over an RhPd/ZSM-5 catalyst under mild conditions in aqueous media. Z. Li, Z. He, K. Wang, **Z. Liu**

Section D

Orange County Convention Center
West Hall B4 - Theater 15

Applied Electrocatalysis for Renewable Energy & Synthesis

Redox Organic Chemistry

H. Wang, Y. Yang, *Organizers*
Y. Sun, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 ENFL 26. Electron-proton-transfer mediators in electrochemical energy conversion and chemical synthesis. **S.S. Stahl**

8:45 ENFL 27. Using electricity to amp up organic synthesis: Electrocatalytic alkene difunctionalization. **S. Lin**

9:20 ENFL 28. Electrolytic hydrogen without H₂. R.S. Sherbo, A. Kurimoto, **C.P. Berlinguette**

9:55 Intermission.

10:05 ENFL 29. Selective electrocatalytic reduction and oxidation of small organic molecules. **M. Koper**

10:45 ENFL 30. Efficient production of biorenewable monomers from paired electrocatalytic hydrogenation and oxidation of 5-Hydroxymethylfurfural (HMF). **W. Li**, X. Chadderdon, D. Chadderdon

11:20 ENFL 31. Immobilized polymeric electrocatalysts for redox organic reactions. **Y. Sun**

11:55 Concluding Remarks.

Section E



TECHNICAL PROGRAM

Orange County Convention Center
West Hall B4 - Theater 16

Bioenergy & Bioproducts

Biofuel

Cosponsored by CELL
J. Fu, A. B. Padmaperuma, J. Shao, *Organizers*
W. Li, S. Turn, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 ENFL 32. Regional supply chain analysis for alternative jet fuel production in the tropics. **S. Turn**, J. Fu, R. Ogoshi, S. Chan, S. Summers

9:05 ENFL 33. Effect of bio-derived additives on fatty acid methyl esters for improved biodiesel cold flow properties. **M. Senra**, S. McCartney, L. Soh

9:35 ENFL 34. Study of the feasibility of joint production of jet fuel and bioethanol from biomass. **X. Zhang**

9:55 ENFL 35. Selective hydroconversion of oleic acid into aviation fuel range alkanes over the ultrathin Ni/ZSM-5 nanosheets. **F. Feng**, L. Wang, X. Zhang, Q. Wang

10:15 ENFL 36. Depolymerization of kraft lignin into liquid fuel using a cobalt-doped zinc oxide flakes catalyst. **X. Dou**, W. Li

10:35 Intermission.

10:50 ENFL 37. Biorefinery to produce value chemicals and fuels from spent coffee grounds blended with microalgae. **A. Prates Pereira**, C. Chuck, P. Pienkos

11:10 ENFL 38. Enhancing the production of light olefins and aromatics from fast pyrolysis of cellulose. **J. Shao**, M. Yang, H. Yang, X. Bai, H. Chen

11:30 ENFL 39. Optimization of analytical techniques used to quantify and identify sulfur-containing impurities in fatty acid methyl esters produced from brown grease. **V.T. Wyatt**, K.C. Jones, R. Cairncross

11:50 ENFL 40. Hythane production of post-hydrothermal liquefaction wastewater generated from human faces: A comparison of two-stage fermentation and catalytic hydrothermal gasification. **B. Si**, J. Watson, A. Aierzhati, Y. Zhang, Z. Liu

Symposium in Honor of Chuck Peden's Research Career: Catalysis for Energy & the Environment

Sponsored by CATL, Cosponsored by ENFL, ENVR, I&EC and PHYS



TECHNICAL PROGRAM

Data Science for Catalysis Research

Sponsored by CATL, Cosponsored by CINP, COMP and ENFL

Elucidation of Mechanisms & Kinetics on Surfaces

Mechanisms on Surfaces: C-C Coupling, C-H & C-O Bond Manipulations

Sponsored by CATL, Cosponsored by ENFL, ENVR, INOR and PHYS

Computational Electrocatalysis

Sponsored by CATL, Cosponsored by COMP and ENFL

SUNDAY AFTERNOON

Section A

Orange County Convention Center
West Hall B4 - Theater 12

George A. Olah Award in Hydrocarbon or Petroleum Chemistry: Symposium in Honor of ChunShan Song

E. B. Fox, X. Guo, M. J. Janik, C. Song, *Organizers*
U. T. Turaga, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 ENFL 41. Multi-component catalysis: Limitations and potential. **M.J. Janik**

1:30 ENFL 42. Unique enhanced catalytic performance of PtFe/zeolite. **M. Matsukata**, R. Ushiki, M. Sakai

1:55 ENFL 43. Preparation of high performance MTA catalyst through combining alkali treatment and dry gel conversion. **M. Liu**, T. Cui, J. Li, X. Guo, C. Song

2:20 ENFL 44. It is not the catalyst-- it is the reactor! **B.I. Morsi**

2:45 Intermission.

3:00 ENFL 45. Metal oxide redox phenomena in chemical looping reforming systems. **L. Fan**

3:25 ENFL 46. Advances in catalysts and sorbents in energy and environment: From science to applications. **M. Namazian**, K.W. Lux, T. Imam



TECHNICAL PROGRAM

3:50 ENFL 47. CO₂ conversion to hydrocarbons with MOF-derived materials as catalysts. **A. Chaffee**

4:15 ENFL 48. Emergent opportunities for professors of practice: Keys to managing a successful transition from industry to academia. **T.F. Degnan**

4:40 Concluding Remarks.

Section B

Orange County Convention Center
West Hall B4 - Theater 13

Innovative Chemistry & Materials for Electrochemical Energy Storage

Li-Ion & Na-Ion

Cosponsored by CATL, INOR and PMSE
B. Gallant, W. Luo, Y. Mo, H. Sun, *Organizers*
D. Siegel, G. Yu, *Presiding*

1:00 Introductory Remarks.

1:05 ENFL 49. Fluorinated electrolytes for Li-ion batteries. **C. Wang**

1:35 ENFL 50. New cathode and anode materials for Na-ion batteries. **Y. Hu**

2:05 ENFL 51. Self-compensated reversible capacity in MnO-embedded carbon nanosheets for Li-ion battery anode with long cycle life. **y. xiao**

2:25 ENFL 52. Characterization of lithiation/delithiation of thick sintered lithium-ion battery electrodes using neutron imaging. **Z. Nie**, P. McCormack, H.Z. Bilheux, J. Bilheux, J.P. Robinson, **G. Koenig**

2:45 Intermission.

3:05 ENFL 53. Enabling the high capacity of lithium-rich anti-fluorite lithium-iron oxide by simultaneous anionic and cationic redox. **J. Lu**

3:35 ENFL 54. *In situ* characterization of the effect of stress on the Li diffusivity in Ge electrode. **S. Nadimpalli**

4:05 ENFL 55. Electrochemical performances and lithium intercalation mechanisms in bornite Cu₅FeS₄. **C. Mir**, D. Giaume, M. Chakir, P. Barboux

Section C

Orange County Convention Center
West Hall B4 - Theater 14

Carbon Dioxide Conversion & Utilization



TECHNICAL PROGRAM

CO₂ Conversion to Carbonates

Cosponsored by CATL, COMP and GEOC

Y. H. Hu, H. Lin, R. Motkuri, *Organizers*

S. Kawi, *Organizer, Presiding*

M. Aresta, C. J. Mota, *Presiding*

1:00 Introductory Remarks.

1:05 ENFL 56. Direct carboxylation of C5 acid to C6 diacids with inorganic carbonates: is CO₂ necessary? **M. Aresta**, A. Dibenedetto, F. Nocito

1:30 ENFL 57. Ceria-catalyzed CO₂ reaction with alcohols and amines into carbonates, ureas, and carbamates in the presence and absence of 2-cyanopyridine. **K. Tomishige**, M. Tamura, Y. Nakagawa

1:55 ENFL 58. Carboxylation of terminal alkynes with CO₂ over Ag loaded ZIF-8. **N. Sun**, J. Shi, L. Zhang, Q. Shen, Q. Gao, W. Wei

2:15 ENFL 59. Carbon dioxide as a building block for synthesis of cyclic carbamates. T. Niemi, I. Fernández, J. Mannisto, **T. Repo**

2:35 ENFL 60. Highly efficient, catalytic, cyclic carbonate formation by pyridyl salicylimines. **C.T. Yavuz**, S. Subramanian, J. Byun, D. Kim

2:55 Intermission.

3:05 ENFL 61. Synthesis of dimethyl carbonate over CeO₂ doped with Cu as catalysts and methyl trichloroacetate as dehydrating agent. **C.J. Mota**, A. Marciniak, L. Appel, O. Alves

3:30 ENFL 62. Integrated CO₂ capture, conversion, and storage to produce calcium and magnesium carbonates via amine looping strategies. **G. Gadikota**, **M. Liu**

3:50 ENFL 63. Direct synthesis of polycarbonate from CO₂ and α,ω -diols by a combination catalyst of CeO₂ and nitriles. **M. Tamura**, Y. Nakagawa, K. Tomishige

4:10 ENFL 64. Combining carbon mineralization with microalgae culture for biofuel production. **Z. Ye**, J. Abraham, C. Christodoulatos, V. Prigiobbe

Section D

Orange County Convention Center
West Hall B4 - Theater 15

Applied Electrocatalysis for Renewable Energy & Synthesis

Hydrogen Evolution Reaction

Y. Sun, H. Wang, *Organizers*

Y. Yang, *Organizer, Presiding*



TECHNICAL PROGRAM

1:00 Introductory Remarks.

1:05 ENFL 65. Two-dimensional transition metal carbides (MXenes) as electrocatalysts for hydrogen evolution reaction. X. Xiao, H. Wang, B. Anasori, L. Johnson, A. Vojvodic, **Y. Gogotsi**

1:45 ENFL 66. New insights regarding composition and practical limitations of Ni–Mo nanopowder hydrogen evolving electrocatalysts. **J.R. McKone**, R.B. Patil

2:15 ENFL 67. Vertically aligned metallic MoS₂ on plasma-treated mass transfer channels for hydrogen evolution reaction. **H. Zhu**

2:45 ENFL 68. Hydrogen evolution reaction catalyzed by atomically dispersed transition metals in carbon matrices. Y. Peng, B. Lu, **S. Chen**

3:15 Intermission.

3:20 ENFL 69. Designing efficient earth-abundant electrocatalysts for the conversion of energy and chemicals. **S. Jin**

4:00 ENFL 70. Bioinspired coordination complexes and polymers for energy applications. **S.C. Marinescu**

4:30 ENFL 71. Self-adjustable valence states of iron in pyramid-like Ni₃S₂ bifunctional electrocatalysts for highly enhanced electrochemical overall-water-splitting activity. **S. Sun**

Section E

Orange County Convention Center
West Hall B4 - Theater 16

Bioenergy & Bioproducts

Cosponsored by CELL

J. Fu, A. B. Padmaperuma, J. Shao, *Organizers*
W. Li, S. Turn, *Organizers, Presiding*

1:00 Introductory Remarks.

1:05 ENFL 72. Scale-up of a mechanocatalytic cellulose to sugar-conversion technology for cellulosic ethanol and bioproducts. **P.J. Cohen**, N. Corra

1:35 ENFL 73. Carbonyl alkylation of furan compounds to produce long-chain hydrocarbons from low molecular weight biomass oxygenates. **F.A. Agblevor**, H. Jahromi

2:05 ENFL 74. High temperature lubricants from novel hydroxylated fatty acid esters. **R.E. Minto**, X. Li, A. Teitgen, A. Shirani, T. Romsdahl, J. Ling, L. Busta, R.E. Cahoon, W. Zhang, Z. Li, K. Chapman, D. Berman, C. Zhang, E. Cahoon

2:25 ENFL 75. One-pot transformation of lignocellulosic biomass into crude bio-oil with metal chloride catalyst via hydrothermal and supercritical ethanol processing. **N. Hao**, A. Ragauskas, K. Alper, S. Karagoz, K. Tekin

2:45 ENFL 76. Biogas production using soluble biodegradable organic carbon in wastewater concentrated by adsorption. **S. Yoon**, W. Lee, Y. Choi



TECHNICAL PROGRAM

3:05 Intermission.

3:20 ENFL 77. Mechanism of scrap tire char induced cracking/deoxygenation in the catalytic pyrolysis of eucalyptus. **Q. Zhou**, A. Zarei, A.D. Girolamo, Y. Yan, L. Zhang

3:40 ENFL 78. Emission of inorganic PM from the combustion of the TOP pellets. **W. Cheng**, Y. Zhu, W. Yang, J. Fan, H. Liu, J. Shao, H. Yang, H. Chen

4:00 ENFL 79. Enhancement of algal biofeedstocks in a mixotrophic batch culture supplemented with exogenous glycerol. **A.L. Smythers**, E. Higginbotham, A.T. Holland, A. Stephenson, D. Kolling

4:20 ENFL 80. Extractive distillation approach for separation phenolic compounds from phenol oil fraction in medium-low temperature coal tar. **Y. Huang**, W. Wang, J. Kang, Q. Yi, W. Li, J. Feng

Section F

Orange County Convention Center
West Hall B4 - Theater 17

Simulations of Materials & Processes for Energy Applications

Y. Liu, D. Lu, B. Wood, H. Zhuang, *Organizers*
Y. Ping, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 ENFL 81. First-principles theory for understanding excitons in stacked organic assemblies. **S. Sharifzadeh**

1:35 ENFL 82. Plasmonic properties of transition metal nitrides. **A. Habib**, F. Florio, R. Sundararaman

2:05 ENFL 83. Plasmon-enhanced photocatalysis. **P.J. Nordlander**

2:35 ENFL 84. Time-domain modeling of excited state dynamics in halide perovskites. **O.V. Prezhdo**

3:05 Intermission.

3:20 ENFL 85. Cation alloying boosts structural stability and delocalizes polaron in hybrid lead-halide perovskites. **L. Zhou**, A. Neukirch, J. Even, C. Katan, S. Tretiak

3:50 ENFL 86. Discovery of new halide double perovskite photovoltaic materials using machine learning and electronic structure theory. **C. Musgrave**, C. Bartel, C. Sutton, B.R. Goldsmith, A. Holder

4:20 ENFL 87. *Ab initio* charge carrier dynamics and its application to materials for energy. **M. Bernardi**

Section G

Orange County Convention Center
West Hall B4 - Theater 18



TECHNICAL PROGRAM

Materials & Processes for Solar Energy

Y. H. Hu, Y. LIN, M. Long, *Organizers*
R. T. Koodali, W. Wei, *Organizers, Presiding*

1:00 Introductory Remarks.

1:05 ENFL 88. Designs of novel processes and advanced materials for solar energy conversions. **Y.H. Hu**

1:45 ENFL 89. Tailoring porphyrins for highly efficient (>9%) organic solar cells. v. cuesta, M. Vartanian, P. de la Cruz, G.D. Sharma, **F. Langa**

2:05 ENFL 90. Next-generation solar cells studied with GISANS. **P. Mueller-Buschbaum**

2:25 ENFL 91. Optoelectronics, charge carrier dynamics, and photoelectrochemistry of metal halide photoelectrodes. G.F. Samu, A. Balog, **C. Janaky**

2:45 Intermission.

3:00 ENFL 92. Pb-less perovskite solar cells. **M. Wang**, X. Gong, X. Shai

3:30 ENFL 93. Toward over 25% efficient 4-terminal perovskite/cigs thin-film tandem solar cells using mixed-dimensional wide-bandgap perovskite. **D. kim**, C. Muzzillo, J. Tong, A. Palmstrom, B. Larson, S. Harvey, J. Whitaker, F. Zhang, H. Lu, M. van Hest, J. Berry, L. Mansfield, Y. Yan, K. Zhu

3:50 ENFL 94. Chlorine atoms induced molecular interlocked network for non-fullerene solar cells. **F. He**

4:10 ENFL 95. P3HT-based high-efficiency solar cell using azadipyromethene-based Zn(II) complexes as electron acceptor. **C. Wang**, M. Zhao, G. Sauve

4:30 Concluding Remarks.

Section H

Orange County Convention Center
West Hall B4 - Theater 19

Sustainable Energy Conversion via Innovative Electrocatalysis & Photocatalysis

Electrocatalytic CO₂ Reduction

Y. Shao, G. Wu, *Organizers*
Y. Cheng, F. Jiao, *Organizers, Presiding*

1:00 Introductory Remarks.

1:05 ENFL 96. Designing flow cells for scalable CO₂ utilization. **C.P. Berlinguette**



TECHNICAL PROGRAM

1:35 ENFL 97. Electrification of the petrochemical industry through cost-effective electrochemical pathways. Z. Liu, J. Kaczur, H. Yang, S.D. Sajjad, L. Zhu, J.P. Sculley, Z.R. Ni, **R. Masel**

2:05 ENFL 98. PEM CO₂ electrolysis for fuels. **S. Ma**, E. Cave, N. Flanders, K. Kuhl

2:35 ENFL 99. Advanced Cu nanostructures for the electrochemical reduction of CO₂. D. Raciti, Y. Wang, **C. Wang**

3:05 Intermission.

3:10 ENFL 100. Electrochemical conversion of CO₂ using tandem strategy. **Q. Lu**

3:40 ENFL 101. Large-scale and highly-selective CO₂ electrocatalytic reduction on nickel single atom catalyst. **H. Wang**

4:10 ENFL 102. Electrocatalytic reduction of carbon dioxide over nanostructured catalyst. **G. Wang**, D. Gao, C. Yan, X. Bao

Symposium in Honor of Chuck Peden's Research Career: Catalysis for Energy & the Environment

Sponsored by CATL, Cosponsored by ENFL, ENVR, I&EC and PHYS

Data Science for Catalysis Research

Sponsored by CATL, Cosponsored by CINF, COMP and ENFL

Elucidation of Mechanisms & Kinetics on Surfaces

Reductions & Hydrogenations

Sponsored by CATL, Cosponsored by ENFL, ENVR, INOR and PHYS

Computational Electrocatalysis

Sponsored by CATL, Cosponsored by COMP and ENFL

MONDAY MORNING

Section A

Orange County Convention Center
West Hall B4 - Theater 12



TECHNICAL PROGRAM

George A. Olah Award in Hydrocarbon or Petroleum Chemistry: Symposium in Honor of ChunShan Song

X. Guo, M. J. Janik, C. Song, U. T. Turaga, *Organizers*
E. B. Fox, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 ENFL 103. Innovation in the new energy order. **U.T. Turaga**

8:30 ENFL 104. Intensifying natural gas utilization. **G. Vesper**

8:55 ENFL 105. Recent progress on fundamental studies of MTO reaction. **Z. Liu**

9:20 ENFL 106. Natural gas processing: Understanding of purification over the surface of oxide adsorbent. **S. Watanabe**

9:45 Intermission.

10:00 ENFL 107. Methane combustion over Pd/CeO₂ catalysts: Mechanistic distinctions between supported single atoms and nanoparticles. **R.M. Rioux**, M.J. Janik, L. Wang, S. Deo

10:25 ENFL 108. Methane conversion and utilization via catalysis. J. Zhang, G. Zeng, X. Li, **Y. Sun**

10:50 ENFL 109. Nano-structured Cu-based catalysts for efficient conversion of syngas to oxygenated compounds. **X. Ma**, Y. Wang, Y. Zhao

11:15 ENFL 110. Development of new syngas conversion routes beyond Fischer-Tropsch synthesis. **Y. Wang**

11:40 Concluding Remarks.

Section B

Orange County Convention Center
West Hall B4 - Theater 13

Innovative Chemistry & Materials for Electrochemical Energy Storage

Solid & Polymer Electrolytes

Cosponsored by CATL, INOR and PMSE
B. Gallant, W. Luo, Y. Mo, H. Sun, *Organizers*
H. Chen, K. Fu, *Presiding*

8:00 Introductory Remarks.

8:05 ENFL 111. High-energy density solid-state rechargeable battery based on Li/I₂. **E.S. Takeuchi**, A.C. Marschilok, K.J. Takeuchi

8:30 ENFL 112. Superior materials and *in situ* curing technologies for solid-state Li metal batteries. **Y. Guo**



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

8:55 ENFL 113. Design, synthesis, and characterization of oxides and sulfides solid state ionic conductors for all-solid-state Li-ion batteries. Z. Liu, S. Xiong, X. He, Y. Mo, **H. Chen**

9:20 ENFL 114. Lithium-graphite paste: An interface compatible anode for solid-state batteries. **J. Duan**, W. Wu, W. Luo

9:35 ENFL 115. Cooperative ion migration in Li-ion conducting glasses. **D. Siegel**, J. Smith

10:00 Intermission.

10:20 ENFL 116. Design and manufacturing of flexible, ion-conducting composite electrolytes for solid-state batteries. **K. Fu**

10:45 ENFL 117. Halide doping effect on lithium argyrodites from liquid-base synthesis. **H. Wang**, D. Ziolkowska, W. Arnold, T. Druffel, M. Sunkara

11:10 ENFL 118. Designing solid electrolytes for lithium-ion batteries: Experimental and computational studies. **F. Ramezanipour**, S. Fanah, M. Yu, A. Huq

11:25 ENFL 119. Dendrite-free Li metal deposition in ambient temperature solid-state lithium sulfur batteries with polymer-in-salt polysiloxane based electrolyte. **L. Chen, L. Fan**

11:40 ENFL 120. Novel mesoscale electrode structures for energy storage: Impact on functional electrochemistry. **A.C. Marschilok**, K.J. Takeuchi, E.S. Takeuchi

Section C

Orange County Convention Center
West Hall B4 - Theater 14

Carbon Dioxide Conversion & Utilization

CO₂ Capture & Separation

Cosponsored by CATL, COMP and GEOC
Y. H. Hu, S. Kawi, H. Lin, *Organizers*
R. Motkuri, *Organizer, Presiding*
S. Raveendran, H. Zhou, *Presiding*

8:00 Introductory Remarks.

8:05 ENFL 121. MOF-catalyzed CO₂ conversion: From structure to catalytic performance. **H. Zhou**, P. Zhang

8:30 ENFL 122. Carbon capture and recycling using inorganic phosphates. **B. Otoo**, M. Perez-Remirez

8:50 ENFL 123. CO₂ capture performance of Cu based metal-organic frameworks incorporated with amino acid functionalized layered materials. **Y. Zhao**

9:10 ENFL 124. CO₂ capture from flue gas over amine-functionalized activated semi-coke. **J. Jing**, X. Zhang, J. Feng, W. Li



TECHNICAL PROGRAM

9:30 ENFL 125. Understanding enhanced gas recovery from CO₂ competitive sorption in shale nanopores by molecular density functional theory. **J. Liu**, W.G. Chapman

9:50 Intermission.

10:05 ENFL 126. Metal-organic frameworks for volatile radionuclide separation. **P.K. Thallapally**, M. Sinnwell, R. Motkuri, D. Banerjee

10:30 ENFL 127. Dual functional catalytic materials for integrated CO₂ capture and conversion. **H. Sun**, B. Shen, J. Huang, C. Wu

10:50 ENFL 128. Metal-organic frameworks as a new platform for CO₂ chemical transformations. **S. Ma**

11:10 ENFL 129. Computational design of sorbents for effective capture of CO₂ through fine-tuning of molecular interactions. **S. Yarasi**, A. Parameswari, G. Sastry

Section D

Orange County Convention Center
West Hall B4 - Theater 15

Applied Electrocatalysis for Renewable Energy & Synthesis

Oxygen Evolution Reaction

H. Wang, Y. Yang, *Organizers*
Y. Sun, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 ENFL 130. Maximizing efficiencies of photocatalytic water splitting by engineering interfaces in multi-component photocatalysts. **S. Linic**

8:40 ENFL 131. Oxygen electrocatalysis on transition metal spinel oxides. **Z.J. Xu**, C. Wei

9:10 ENFL 132. Insights into the catalytically active phase of NiCoO_xH_y electrocatalysts by following the structural evolution during the oxygen evolution reaction (OER). **B.E. Koel**

9:40 ENFL 133. Understanding doping effects of iron group metals on morphology, composition, and electrocatalytic oxygen evolution activity of copper oxide nanoarray film. **Y. Yang**

10:05 Intermission.

10:10 ENFL 134. High-performance, transition-metal phosphide alloy catalyst for oxygen-evolution reaction. **Y. Zhu**

10:35 ENFL 135. Epitaxial design of functional oxides for electrocatalysis. **Y. Du**



TECHNICAL PROGRAM

11:00 ENFL 136. Role of proton transfer and transport coupled to electron transfer in mesoporous oxygen evolution electrocatalytic oxides. **C. Cyrille**

11:35 ENFL 137. Atomic-level insight into super-efficient electrocatalytic oxygen evolution on iron and vanadium co-doped nickel (oxy)hydroxide. **J. Jiang, M. Wang**

Section E

Orange County Convention Center
West Hall B4 - Theater 16

Bioenergy & Bioproducts

Bioenergy

Cosponsored by CELL
J. Fu, W. Li, S. Turn, *Organizers*
A. B. Padmaperuma, J. Shao, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 ENFL 138. Ultrafast synthesis of biodiesel fuel from waste cooking oil using nano-reactors. **N.N. Shaw**

8:35 ENFL 139. Chemical looping based biomass thermal catalytic conversion with Fe-Ca oxygen carrier for syngas production. **X. Zhang**, L. Chen, L. Sun, H. Chen, S. Yang, B. Zhao, M. Li, Y. Zhou, H. Si, X. Yi

9:05 ENFL 140. Comparison of biochar production from corn stover and cattle manure via hydrothermal carbonization and pyrolysis carbonization. **Z. Liu**, Z. Liu, Y. Zhang

9:25 ENFL 141. Catalytic oxidative lignin depolymerization by peracetic acid: Insights into reaction mechanisms. **R. Ma**, M.V. Olarte, X. Zhang

9:45 ENFL 142. *In situ* catalytic co-gasification of biomass and coal: Influence of catalysts on the gasification reactivity. **J. Hu**, H. Yang, J. Fan, **J. Shao**, **X. Wang**, H. Chen

10:05 Intermission.

10:20 ENFL 143. Importance of extraction solvents for assessing production of biocrude oil and energy efficiency of hydrothermal liquefaction. **J. Watson**, J. Lu, R. de Souza, B. Si, Y. Zhang, Z. Liu

10:40 ENFL 144. Catalytic conversion of sorbitol to C5/C6 alkanes over vanadium-modified Ir/SO₂ combined with HZSM-5 in a biphasic system. **L. Jin**, W. Li

11:00 ENFL 145. Hydrothermal catalytic conversion of biofeedstocks into high value special chemicals. **L. Kong**, G. Miao, Y. Sun

11:20 ENFL 146. Antimicrobial properties of depolymerized lignin compounds. **R. Kalinoski**, J. Shi

Section F



TECHNICAL PROGRAM

Orange County Convention Center
West Hall B4 - Theater 17

Simulations of Materials & Processes for Energy Applications

D. Lu, Y. Ping, B. Wood, H. Zhuang, *Organizers*
Y. Liu, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 ENFL 147. Discovery of new solar fuels photoanode materials with a combination of high-throughput theory and experiment. **J. Neaton**

8:35 ENFL 148. Simulation of technologically feasible potential for integrated photovoltaic and electrolyzer devices for solar hydrogen production. **I. Bayrak Pehlivan**, U. Malm, P. Neretnieks, L. Stolt, M. Edoff, T. Edvinsson

9:05 ENFL 149. Theory and modeling of correlated ionic and electronic motions in hybrid organic-inorganic perovskites. **A.M. Rappe**

9:35 Intermission.

9:50 ENFL 150. Simulation of energy conversion processes from first principles. **G.A. Galli**

10:20 ENFL 151. First-principles study of chemical doping in WSe₂. **D. Han**, W. Ming, H. Xu, S. Irle, S. Chen, M. Du

10:50 ENFL 152. Dimensionality dependence of radiative recombination in black phosphorus from first-principles. F. Wu, D. Rocca, **Y. Ping**

Section G

Orange County Convention Center
West Hall B4 - Theater 18

Materials & Processes for Solar Energy

Y. H. Hu, R. T. Koodali, Y. Lin, W. Wei, *Organizers*
M. Long, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 ENFL 153. Promoting charge carrier delocalization and conduction in perovskite quantum dots using conductive aromatic ligands. **J.Z. Zhang**

8:45 ENFL 154. Rational design and synthesis of TiO₂-based photocatalysts for H₂O₂ production. **M. Long**, L. Zheng, H. Su

9:15 ENFL 155. Atmospheric water harvesting using metal-organic frameworks powered by natural sunlight. **H. Kim**, S. Rao, E.A. Kapustin, S. Yang, L. Zhao, O.M. Yaghi, S. Lee, E. Wang



TECHNICAL PROGRAM

9:35 Intermission.

9:50 ENFL 156. Mixed cerium oxides as reactive materials for thermochemical water splitting. **H. Hagelin-Weaver**, S.J. Roberts

10:30 ENFL 157. Axially linked donor – aluminum(III) porphyrin – acceptor self-assembled triads as artificial photosynthetic reaction center models. **P. Poddutoori**

10:50 ENFL 158. Reduced graphene-oxide modified, sponge-compositing phase change materials for fast solar-thermal conversion and energy storage. **L. Liu**, Z. Liu, P. Hanyu, Q. Zhao, X. Ju, Y. Faraj, W. Wang, R. Xie, L. Chu

11:10 ENFL 159. High-performance TiO₂ nanostructured array photoanode for hydrogen production from water splitting. **X. Liu**, X. Cao, D. Zhang

11:30 Concluding Remarks.

Section H

Orange County Convention Center
West Hall B4 - Theater 19

Sustainable Energy Conversion via Innovative Electrocatalysis & Photocatalysis

Electrocatalytic & Photocatalytic CO₂ Reduction

Y. Shao, G. Wu, *Organizers*
Y. Cheng, F. Jiao, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 ENFL 160. Inorganic core-shell nanotube array for CO₂ photoreduction by H₂O. **H.M. Frei**

8:35 ENFL 161. Unveiling active sites of CO₂ reduction on nitrogen coordinated single atomic iron and cobalt catalysts. **Y. Li**, F. Pan, G. Wang, G. Wu

9:05 ENFL 162. Hierarchical zinc-oxide nanostructures for the photochemical reduction of bicarbonate to solar fuels. **H. Pan**, M. Heagy

9:30 ENFL 163. Identification of champion transition metals centers in metal and nitrogen-doped carbon catalysts for electrocatalytic reduction of carbon dioxide into fuels. **F. Pan**, Y. Li

9:55 Intermission.

10:00 ENFL 164. Controlling electrocatalytic performance of cobalt phthalocyanine for carbon dioxide reduction by modulating the catalyst's primary and outer coordination spheres. **C.C. McCrory**

10:30 ENFL 165. Influence of second coordination sphere functionality on electrocatalytic CO₂ reduction by Mn(α -diimine)(CO)₃⁻ catalysts. V. Blaszczak, M.E. McKinnon, D.C. Grills, M. Ertem, **J.J. Rochford**



TECHNICAL PROGRAM

11:00 ENFL 166. Improvement of Co porphyrin CO₂ electroreduction activity via its covalent immobilization on the surface of carbon cloth electrodes. **A. Marianov**, Y. Jiang

11:20 ENFL 167. Photocatalytic CO₂ reduction using hybrid nanoporous catalysts. **K. Kao**, A.R. Riscoe, A. Yang, W. Huang, A. Holm, C.W. Frank, M. Cargnello

11:40 ENFL 168. 2D ultrathin nanosheets for photocatalytic CO₂ reduction. B. Pan, Y. Wu, **C. Wang**

Section I

Orange County Convention Center
West Hall B4 - Theater 20

Celebrating 50 Years of ExxonMobil's Corporate Strategic Research Laboratories: A View Forward from a Retrospective

Cosponsored by CATL and I&EC⁺
C. W. Abney, *Organizer*
M. Afeworki, G. Cao, *Organizers, Presiding*

8:00 Introductory Remarks.

8:10 ENFL 169. Meeting the energy challenges: A 50-year journey for ExxonMobil corporate research. **M.G. Matturro**, M.C. Kerby

8:35 ENFL 170. Reflections on Mobil's Central Research Laboratory's culture and remarkable history of innovation. **T.F. Degnan**

9:00 ENFL 171. Tackling CO₂ issues by chemical conversion and by reducing CO₂ emission. **J.G. Chen**

9:25 ENFL 172. Mechanistic modeling of fast pyrolysis of biomass. X. Zhou, A. Yanez-McKay, L. Dellon, W. Li, R. Mabon, **L.J. Broadbelt**

9:50 Intermission.

10:20 ENFL 173. Clostridia in hot oil reservoirs of Texas. G. Christman, Z. Summers, **J. Biddle**

10:45 ENFL 174. Petroleomics: Dovetailing of academic and industrial research interests and objectives in ultrahigh-resolution mass spectral analysis of petroleum and its products. **A.G. Marshall**, M.L. Chacon, Y. Corilo, C.L. Hendrickson, A.M. McKenna, S.F. Niles, J.C. Putman, D.F. Smith, C.R. Weisbrod, R.P. Rodgers

11:10 ENFL 175. Studies to identify heteroatoms in aromatic molecules with non-contact atomic force microscopy. **Y. Zhang**, p. Zahl

11:35 Concluding Remarks.

Symposium in Honor of Chuck Peden's Research Career: Catalysis for Energy & the Environment



TECHNICAL PROGRAM

Sponsored by CATL, Cosponsored by ENFL, ENVR, I&EC and PHYS

Data Science for Catalysis Research

Sponsored by CATL, Cosponsored by CINP, COMP and ENFL

Frontiers in Catalysis for Energy & Sustainability

Sponsored by CATL, Cosponsored by ENFL⁺

Computational Electrocatalysis

Sponsored by CATL, Cosponsored by COMP and ENFL

Recent Advances in Plasma-Enhanced Catalysis

Sponsored by CATL, Cosponsored by ENFL, ENVR and PHYS

MONDAY AFTERNOON

Section A

Orange County Convention Center
West Hall B4 - Theater 12

George A. Olah Award in Hydrocarbon or Petroleum Chemistry: Symposium in Honor of ChunShan Song

E. B. Fox, X. Guo, C. Song, U. T. Turaga, *Organizers*
M. J. Janik, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 ENFL 176. Coal structural considerations in the production of highly naphthenic liquid fuels. **H.H. Schobert**

1:30 ENFL 177. Hydrocracking performance over nano-sized beta zeolite catalyst. **G. Wang**, J. Liu

1:55 ENFL 178. Software tools for molecular level kinetic modeling in thermochemical conversions. **M.T. Klein**

2:20 ENFL 179. Hydrodeoxygenation of phenols over Ni₃P-based catalysts. Z. Yu, **A. Wang**, Y. Wang, Z. Sun, Y. Liu



TECHNICAL PROGRAM

2:45 Intermission.

3:00 ENFL 180. Ethane activation using Mo-based sulfated zirconia catalysts. S. Kanitkar, A. Abedin, S. Bhattar, **J.J. Spivey**

3:25 ENFL 181. Adsorptive separation for ultra-deep desulfurization and ethane/ethylene separation in petrochemical industry. **J. Xiao**

3:50 ENFL 182. Computational study of hydrocarbons synthesis from CO₂ hydrogenation over Fe-based catalysts. **X. Nie**

4:15 ENFL 183. Catalytic hydrogenation of CO₂ to gasoline-range hydrocarbons over Na-Fe₃O₄/M-ZSM-5 catalysts. R. Yao, J. Wei, J. Sun, **Q. Ge**

4:40 Concluding Remarks.

Section B

Orange County Convention Center
West Hall B4 - Theater 13

Innovative Chemistry & Materials for Electrochemical Energy Storage

Supercapacitors

Cosponsored by CATL, INOR and PMSE
B. Gallant, Y. Mo, H. Sun, *Organizers*
W. Luo, *Organizer, Presiding*
Z. Zhou, *Presiding*

1:00 Introductory Remarks.

1:05 ENFL 184. Electrochemical energy storage mechanism of MXene pseudocapacitors. X. Wang, **Y. Gogotsi**

1:35 ENFL 185. Hierarchical porous carbon structures for supercapacitors. **Y. Li**

2:05 ENFL 186. Porous carbon fibers from block copolymers. **Z. Zhou**, T. Liu, A.U. Khan, G. Liu

2:25 ENFL 187. Flexible manganese (II,III) oxide nanowalls based electrodes for wearable supercapacitors. **J. Cherusseri**, K. Sambath Kumar, J. Thomas

2:45 ENFL 188. Mesoporous iron oxide pseudocapacitive electrodes with mutually high mass loadings and excellent rate capability. **T. Liu**, Y. Song, X. Liu, Y. Li

3:05 Intermission.

3:20 ENFL 189. Graphene quantum dots embedded V₂O₅ nanosheets as high-performance supercapacitor. **A.B. Ganganboina**, Y. Sheng-Mu, R. Doong

3:40 ENFL 190. Nature of carbon material determines the charge storage mechanism in 2H MoS₂. **B.A. Ali**, **N.K. Allam**



TECHNICAL PROGRAM

4:00 ENFL 191. 3D graphene frameworks for energy storage. **R. Kanungo**, J. Radich

4:20 ENFL 192. Defects-induced capacitance increase in supercapacitor via PEC process. **Y. Zhang**, L. Wang

4:40 ENFL 193. Pore engineering and heteroatom doping of carbon foams for ultrafast supercapacitors. **H. Peng**, Y. Li, Y. Zhang, P. Xiao

Section C

Orange County Convention Center
West Hall B4 - Theater 14

Carbon Dioxide Conversion & Utilization

CO₂ as an Oxidant

Cosponsored by CATL, COMP and GEOC
H. Lin, R. Motkuri, *Organizers*
Y. H. Hu, S. Kawi, *Organizers, Presiding*
J. J. Spivey, K. Tomishige, *Presiding*

1:00 Introductory Remarks.

1:05 ENFL 194. Study of dry reforming of methane over nickel-based pyrochlore catalysts. S. Bhattar, A. Krishnakumar, S. Kanitkar, A. Abedin, D. Haynes, D. Shekhawat, **J.J. Spivey**

1:30 ENFL 195. CO₂ steam bireforming of methane to syngas over Ni-supported on Sr-modified La₂O₃ and CeO₂ mixed-oxide catalysts. **L. Nakka**

1:50 ENFL 196. Highly active and stable Ni/SiO₂ catalyst for CO₂ reforming of methane prepared by modified impregnation method. **S. Das**, A. Jangam, S. Kawi

2:10 ENFL 197. High-temperature photothermal catalytic CO₂ reforming of methane on Pt/CeO₂-based catalysts using concentrated solar. **F. Pan**, X. Xiang, Y. Li

2:30 ENFL 198. Integrating methane dry reforming into calcium looping for the synergetic capture and conversion of carbon dioxide. **S. Tian**

2:50 Intermission.

3:05 ENFL 199. Effects of oxide supports on the dry reforming of ethane over Pt-Ni bimetallic catalysts. **Z. Xie**, J. Lee, J.G. Chen

3:25 ENFL 200. CO₂ methanation over Ni/Al@Al₂O₃ core-shell catalyst. T. Le, J. Kim, **E. Park**

3:45 ENFL 201. Enhanced performance and selectivity of CO₂ methanation over Ni-phyllsilicate-mesoporous SBA-15: Effect of preparation methods. **P. Hongmanorom**, S. Kawi

4:05 ENFL 202. New catalysts, adsorbents, and carriers for *in-situ* conversion of CO₂ to synthetic natural gas with dual function materials. **M.A. Arellano**, R.J. Farrauto



TECHNICAL PROGRAM

4:25 ENFL 203. Recycling mechanism of lattice oxygen over $\text{VO}_x/\text{CeO}_2(111)$ in the ethylbenzene oxidative dehydrogenation with CO_2 . **H. Fan**, W. Li, J. Feng, Q. Ge

Section D

Orange County Convention Center
West Hall B4 - Theater 15

Applied Electrocatalysis for Renewable Energy & Synthesis

CO₂ & N₂ Reduction

Y. Sun, Y. Yang, *Organizers*
H. Wang, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 ENFL 204. Mechanistic insights into selective CO_2 -to-fuels catalysis. A. Wuttig, M. Schreier, Y. Yoon, A. Hall, **Y. Surendranath**

1:40 ENFL 205. Catalytic plasticity of bismuth cathodes for conversion of CO_2 to fuels. **J. Rosenthal**

2:15 ENFL 206. Nano-sized manganese nitride in carbon matrix as electro-catalysis for CO_2 reduction. **Y. Hu**, J. Wang

2:35 ENFL 207. Structure sensitivity and structural dynamics of metal nanomaterials for CO_2 electrocatalysis. **Y. Li**, D. Kim, P. Yang

2:55 ENFL 208. Designing electroenzymatic interface for CO_2 reduction. **M. Yuan**, S. Sahin, R. Cai, S. Abdellaoui, D. Hickey, S.D. Minter, R. Milton

3:15 Intermission.

3:25 ENFL 209. Electrochemical synthesis of ammonia via nitrogen reduction using N_2 and H_2O under ambient conditions. **G. Wu**

4:00 ENFL 210. Nitrogenase bioelectrocatalysis: From electron-transfer mechanisms to energy applications. **R. Cai**, R. Milton, D. Hickey, S. Abdellaoui, S. Minter

4:20 ENFL 211. Investigating the generation of Ru(IV) imido from Ru(III) amine catalyst in homogeneous catalytic ammonia oxidation. **F. Habib-Zadeh**, A. Raithel, S.L. Miller, C.T. Dean, T. Hamann, M.R. Smith

4:40 ENFL 212. Electrochemical synthesis of ammonia on Fe/Fe oxide catalyst. **L. Hu**, X. Feng, W. Kaden, A. Khaniya

Section E

Orange County Convention Center
West Hall B4 - Theater 16



TECHNICAL PROGRAM

Bioenergy & Bioproducts

Green Chemistry

Cosponsored by CELL

W. Li, A. B. Padmaperuma, S. Turn, *Organizers*

J. Fu, J. Shao, *Organizers, Presiding*

1:00 Introductory Remarks.

1:05 ENFL 213. Fuel property first design of advantaged diesel blendstocks from biologically derived short chain carboxylic acids. N. Huq, X. Huo, J. Stunkel, G. Fioroni, P. St. John, S. Kim, R.L. McCormick, **D. Vardon**

1:35 ENFL 214. Flash points measurements and prediction of biofuels and biofuel blends with aromatic fluids. **J. Fu**, S. Turn

2:25 ENFL 215. Synergies in rate and extent of thermal decomposition of municipal solid waste by co-pyrolysis with microalgae. **A. Vuppaladiyam**, **M. Zhao**

2:45 ENFL 216. Isolation of endophytic fungus *Hypoxyton sp.* BS15 producing volatile organic compounds (VOCs) with fuel potential and epigenetically altering VOC production over time. **Y. Wang**, J. Harper

3:05 Intermission.

3:20 ENFL 217. Efficient aerobic oxidation of 5-hydroxymethylfurfural with α -MnO₂ catalyst. **L. Yu**, H. Chen, Y. Li

3:40 ENFL 218. Economic benefits of mixed biomass feedstocks for conventional and advanced biofuels production. **N.R. Baral**, M. Yang, C. Scown

4:00 ENFL 219. Exploring the hybrid conversion of lignin into biodiesel. **Z. Shang**, M.B. Foston

4:20 ENFL 220. Microalgal photolysis-mediated biohydrogen production in acetate-enriched wastewater. **J. Hwang**, K. Rodriguez, W. Lee

4:40 ENFL 221. Algal biofuel: Culture and optimization of *Scenedesmus obliquus* in untreated energetic-laden wastewater. **J. Abraham**, A. RoyChowdhury, T. Abimbola, Y. Lin, C. Christodoulatos, A. Lawal, P. Arrienti, B. Smolinsky, W. Braida

Section F

Orange County Convention Center
West Hall B4 - Theater 17

Simulations of Materials & Processes for Energy Applications

Y. Liu, D. Lu, Y. Ping, H. Zhuang, *Organizers*

B. Wood, *Organizer, Presiding*

1:00 Introductory Remarks.



TECHNICAL PROGRAM

1:05 ENFL 222. Two-dimensional materials design for photocatalytic water splitting from a theoretical perspective. **J. Yang**

1:35 ENFL 223. Impact of molecular structure on thermophysical properties of surrogate fuels: A molecular dynamics simulations study. **S. Maskey**, B.H. Morrow, P. Mikulski, D.J. Luning Prak, J.A. Harrison

2:05 ENFL 224. Novel 2D semiconductors: Effects of p-element chemistry and electrical polarization. **E. Kioupakis**

2:35 Intermission.

2:50 ENFL 225. Electrons in flat land: The electronic structure underlying electrochemistry of 2D materials. **Y. Liu**

3:20 ENFL 226. Hybrid method composed of cDFT and MD simulation for predicting electrokinetic energy conversion in slit nanochannels. **X. Hu**, Y. Nan, X. KONG, D. Lu, J. Wu

3:50 ENFL 227. High-throughput searches for novel two-dimensional materials and solid-state Li-ion conductors. **N. Marzari**

Section G

Orange County Convention Center
West Hall B4 - Theater 18

Materials & Processes for Solar Energy

Y. H. Hu, R. T. Koodali, M. Long, *Organizers*

Y. Lin, W. Wei, *Organizers, Presiding*

1:00 Introductory Remarks.

1:05 ENFL 228. Plasmonic metal-semiconductor heterojunctions for solar water splitting. **N. Wu**

1:35 ENFL 229. Morphological control of hydrogenated ZnO for enhanced photocatalytic activity of dye degradation under visible light. **Y. LIN**, H. Hu, Y.H. Hu

2:05 ENFL 230. Adsorption characteristics of small aromatic molecules on silica/Ru(0001). **M. Sajid**, W. Kaden, A. Kara

2:25 ENFL 231. Novel electrode materials for solar energy conversion devices. **W. Wei**, Y.H. Hu

2:45 ENFL 232. Surface passivation of lead halide perovskite quantum dots based on synergistic effect between phosphonic acid and (3-aminopropyl)triethoxysilane. **K. Xu**, J.Z. Zhang, X. Li

3:05 Intermission.

3:20 ENFL 233. Adsorption-determined hole transfer during photocatalytic oxidation. **C. Chen**

3:50 ENFL 234. Photocatalytic inactivating *E. coli* K-12 and degrading organic contaminants over AgBr-Ag-BiVO₄ under visible light. **S. Bao**, X. Gong, B. Tian



TECHNICAL PROGRAM

4:10 ENFL 235. Effects of dopants and pressure on the stability and optoelectronics of hybrid perovskite materials. **T. Xu**, J. Gong

4:30 ENFL 236. Photothermocatalytic degradation of typical VOCs over PtCu/CeO₂ ordered porous-catalysts under simulated solar irradiation. **J. Kong**, G. Li, **T. An**

4:50 Concluding Remarks.

Section H

Orange County Convention Center
West Hall B4 - Theater 19

Sustainable Energy Conversion via Innovative Electrocatalysis & Photocatalysis

Electrocatalysts for Chemical Conversion

Y. Cheng, F. Jiao, Y. Shao, G. Wu, *Organizers*
J. Holladay, L. C. Meyer, *Presiding*

1:00 Introductory Remarks.

1:05 ENFL 237. Exploring the effect of molecule functionality and metal on the electrocatalytic upgrading of biomass-derived oxygenated molecules. **J. Holladay**, J. Lopez-Ruiz, E. Andrews, S. Akhade, K. Koh, U. Sanyal, R. Rousseau, O.Y. Gutiérrez

1:30 ENFL 238. Building paths to fuels and chemicals: Mild aqueous electrocatalytic energy upgrading of lignin and related model compounds. **J.E. Jackson**, P. Hao, Y. Zhou, C.M. Saffron

1:55 ENFL 239. Exploring the design-space for economically-viable electrochemical carbon-dioxide processing. **F. Brushett**

2:20 ENFL 240. Furfural as a model reactant in the electrochemical conversion of biomass to fuels. **E.J. Biddinger**, S. Jung

2:45 Intermission.

2:55 ENFL 241. BCC-phased PdCu nanoparticles as a highly active electrocatalyst for hydrogen oxidation reaction in alkaline electrolytes. **W. Li**, Y. Qiu, L. Xin, Y. Li, I. McCrum, M. Janik

3:20 ENFL 242. Ion-free and organic-free synthesis of supported metal electrocatalysts. **T. Xu**

3:45 ENFL 243. Impact of surface modification of carbon, felt-supported Pd nanoparticles on electrochemical hydrogenation of oxygenates. **A.J. Karkamkar**

4:10 ENFL 244. Elucidating the reaction networks and mechanisms in electrocatalytic hydrogenation of carbonyl compounds. **L.C. Meyer**, U. Sanyal, K.A. Stoerzinger, O.Y. Gutiérrez, J.A. Lercher



TECHNICAL PROGRAM

4:35 ENFL 245. New discovery in energetics: Isothermal utilization of latent heat enthalpy by electrostatically localized protons at liquid-membrane interface. **J.W. Lee**

Section I

Orange County Convention Center
West Hall B4 - Theater 20

Celebrating 50 Years of ExxonMobil's Corporate Strategic Research Laboratories: A View Forward from a Retrospective

Cosponsored by CATL and I&EC
M. Afeworki, *Organizer*
C. W. Abney, G. Cao, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 ENFL 246. Direct methane conversion to ethylene and ethane by oxidative coupling in membrane/catalysts reacting systems. **S. Linic**, V. Igenegbai

2:00 ENFL 247. Tailoring the electronic structures of metal–organic frameworks for electrocatalysis. **S. Yuan**, Y. Shao-Horn

2:25 ENFL 248. Understanding and controlling active sites and their environments for catalysis in the liquid phase. **M. Neurock**

2:50 ENFL 249. Production of alcohols by biomass depolymerization and hydrodeoxygenation in supercritical methanol over a CuMgAl oxide catalyst. **G.W. Huber**, P. Galebach, D.J. McClelland, A.M. Wittrig, M.P. Lanci

3:15 Intermission.

3:30 ENFL 250. Quantitatively predicting the rates and products of reacting mixtures. **W.H. Green**

3:55 ENFL 251. Enabling widespread use of microporous membrane materials for challenging organic solvent separations. **R.P. Lively**

4:20 ENFL 252. Carbon dioxide capture in diamine-appended metal-organic frameworks. R. Siegelman, P.J. Milner, J. Martell, E. Kim, A. Forse, J. Lee, T. McDonald, J. Mason, J. Oktawiec, M. Gonzalez, T. Runcevski, D. Gygi, B. Dinakar, L. Porter-Zasada, S. Weston, J. Neaton, J.A. Reimer, **J.R. Long**

4:45 ENFL 253. Multi-level life cycle analysis tool for sustainable energy systems modeling. **E. Gencer**, **S. Torkamani**, F. O'Sullivan

5:10 Concluding Remarks.

Symposium in Honor of Chuck Peden's Research Career: Catalysis for Energy & the Environment

Sponsored by CATL, Cosponsored by ENFL, ENVR, I&EC and PHYS



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

Elucidation of Mechanisms & Kinetics on Surfaces

Experimental Surface Science

Sponsored by CATL, Cosponsored by ENFL, ENVR, INOR and PHYS

Frontiers in Catalysis for Energy & Sustainability

Sponsored by CATL, Cosponsored by ENFL[‡]

Computational Electrocatalysis

Sponsored by CATL, Cosponsored by COMP and ENFL

Recent Advances in Plasma-Enhanced Catalysis

Sponsored by CATL, Cosponsored by ENFL, ENVR and PHYS

MONDAY EVENING

Section A

Orange County Convention Center
West Hall C

Sci-Mix

H. Lin, *Organizer*

8:00 - 10:00

17-18, 35, 44, 52, 55-56, 58, 75, 123, 142, 160-161, 163, 167, 187, 189, 191, 193, 195-197, 201, 207-208, 236, 241, 245.
See previous listings.

259, 285, 292, 294, 324, 362, 385, 426, 466, 483, 485-486, 488, 492, 507, 514, 527, 530, 553, 579, 582, 588, 591, 602, 610, 619, 624, 644, 649, 657. See subsequent listings.

TUESDAY MORNING



TECHNICAL PROGRAM

Section A

Orange County Convention Center
West Hall B4 - Theater 12

George A. Olah Award in Hydrocarbon or Petroleum Chemistry: Symposium in Honor of ChunShan Song

E. B. Fox, M. J. Janik, C. Song, U. T. Turaga, *Organizers*
X. Guo, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 ENFL 254. CO₂ capture over molecular basket sorbents: Why fumed silica is better? **X. Wang**, C. Song

8:30 ENFL 255. Bimetallic Pd-Cu catalysts for CO₂ hydrogenation to methanol: Synergetic effect and alloy composition. **X. Jiang**, X. Nie, X. Guo, K.S. Walton, C. Song

8:55 ENFL 256. Novel hybrid CO₂ capture sorbents based on metal-organic frameworks. **A.A. Park**, G. Rim, T. Feric, B. Smit, K. Stylianou, B. Valizadeh

9:20 ENFL 257. Process considerations in using MOFs for large-scale CO₂ capture from flue gas and air. **D. Sholl**, R.P. Lively, K.S. Walton, C.W. Jones, M.J. Realff

9:45 Intermission.

10:00 ENFL 258. Heterogeneous single-atom catalysts for efficient CO₂ conversion. Y. Huang, X. Yang, B. Liu, **T. Zhang**

10:25 ENFL 259. Towards an economy based on carbon recycling: Innovative catalysts for the conversion of biomass and CO₂ as a renewable carbon source. **A. Dibenedetto**

10:50 ENFL 260. Cu₂O-based electrodes for photocatalytic CO₂ reduction in aqueous solutions. **J. Gong**

11:15 ENFL 261. Important role of carbon dioxide extraction from ambient air in climate stabilization. **C.W. Jones**

11:40 Concluding Remarks.

Section B

Orange County Convention Center
West Hall B4 - Theater 13

Innovative Chemistry & Materials for Electrochemical Energy Storage

Flow Batteries

Cosponsored by CATL, INOR and PMSE
B. Gallant, W. Luo, Y. Mo, H. Sun, *Organizers*
B. Helms, B. Li, *Presiding*



TECHNICAL PROGRAM

8:00 Introductory Remarks.

8:05 ENFL 262. Macromolecular design of porous polymer membranes for crossover-free aqueous alkaline energy storage devices. **B. Helms**, M. Baran, M. Braten, S. Sahu, M. Carrington

8:35 ENFL 263. Decay characterization of redox-flow battery materials utilizing a microelectrode. **F. Brushett**

9:05 ENFL 264. Low-cost and high-energy density aqueous flow batteries based on highly soluble organic/inorganic materials. **B. Li**

9:35 ENFL 265. Quinone redox flow battery with record stability at near-neutral pH. **Y. Ji**, M. Goulet, D.A. Pollack, D.G. Kwabi, S. Jin, D. De Porcellinis, E.F. Kerr, R.G. Gordon, M.J. Aziz

9:55 Intermission.

10:15 ENFL 266. Transition metal complexes supported by bridged bis-picolinamide ligands for use in non-aqueous redox flow batteries. **G. Andrade**, T. Chu, B.L. Davis

10:35 ENFL 267. High-performance quinone dimer for aqueous organic redox flow batteries. **L. Tong**, E.F. Kerr, M. Goulet, D. De Porcellinis, M.J. Aziz, R.G. Gordon

10:55 ENFL 268. Electrochemical properties of all-organic non-aqueous redox flow battery with highly soluble active materials. **J. Yuan**, Y. Li

11:15 ENFL 269. All-iron non-aqueous redox flow battery with a high performance and stability. **Y. Zhen**, Y. Li

Section C

Orange County Convention Center
West Hall B4 - Theater 14

Carbon Dioxide Conversion & Utilization

Electrocatalysis

Cosponsored by CATL, COMP and GEOC
S. Kawi, H. Lin, R. Motkuri, *Organizers*
Y. H. Hu, *Organizer, Presiding*
X. Guo, F. Jiao, *Presiding*

8:00 Introductory Remarks.

8:05 ENFL 270. Carbon utilization using electrochemical approaches. **F. Jiao**

8:30 ENFL 271. Selective CO₂ reduction at thiol-capped Au/Cu nanocatalysts. **D. Kauffman**, D.R. Alfonso

8:50 ENFL 272. Engineering SnO₂ electrocatalysts for expedited CO₂ activation and reduction. **C. Hu, L. Zhang, L. Li, J. Gong**



TECHNICAL PROGRAM

9:10 ENFL 273. Electrochemical conversion of CO₂ to formic acid under reduced CO₂ concentration. **H. Yang**, J. Kaczur, R. Masel

9:30 ENFL 274. Effect of CO₂ concentration on the electrolytic conversion of CO₂ to CO. **Z. Liu**, H. Yang, S.D. Sajjad, J. Kaczur, R. Masel

9:50 Intermission.

10:05 ENFL 275. Scalable electro-reduction of CO₂ to CO with a single atom nickel doped porous carbon electrocatalyst. **H. Jeong**, U. Sim, K. Nam

10:25 ENFL 276. Effects of electrolyte environment on carbon-dioxide reduction. **F.R. Lucci**, S. Baker

10:45 ENFL 277. Tetramethylimidazolium-functionalized alkaline anion exchange membranes for carbon dioxide electrolysis. **M.J. Pellerite**, M. Kaplun, J.C. Thomas, C. Hartmann-Thompson, T. Gregar, S.D. Sajjad, R. Masel

11:05 ENFL 278. Tuning the metal surface electronic state for effective CO₂ reduction. **Z. Wang**

11:25 ENFL 279. Chemical versatility of [FeFe]-hydrogenase models: Distinctive activity of [μ -C₆H₄-1,2-(κ^2 -S)₂][Fe₂(CO)₆] for electrocatalytic CO₂ reduction. **M. Cheng**

Section D

Orange County Convention Center
West Hall B4 - Theater 15

Applied Electrocatalysis for Renewable Energy & Synthesis

New Electrode Materials: Synthesis & Characterization

Y. Sun, Y. Yang, *Organizers*
H. Wang, *Organizer, Presiding*

8:00 Introductory Remarks.

8:45 ENFL 280. Pathway towards formation of colloidal semiconductor quantum dots. **K. Yu**

9:15 ENFL 281. MOF-derived, active materials for energy conversion and storage: Now and next. **J. Wang**

9:45 Intermission.

9:50 ENFL 282. New chemistry for development of novel electrode catalysts. **Y.H. Hu**

10:30 ENFL 283. Probing interfaces in heterogeneous catalysts at atomic scale: Current and emerging STEM techniques. **M. Chi**

11:00 ENFL 284. Understanding the electronic structure for electrocatalysis of 2D materials. **Y. Liu**



TECHNICAL PROGRAM

11:30 ENFL 285. Understanding triple-phase electrochemical reactions: *In-situ* visualization and ultralow catalyst loading. **F. Zhang**

Section E

Orange County Convention Center
West Hall B4 - Theater 16

Bioenergy & Bioproducts

Biofuel & Bioenergy

Cosponsored by CELL
W. Li, J. Shao, S. Turn, *Organizers*
J. Fu, A. B. Padmaperuma, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 ENFL 286. Food-energy-water nexus: Opportunities for advancement on nature-based solutions. **A. Waheed**, U. Siddique

8:35 ENFL 287. Analysis of measures to solve high sulfur petroleum coke. **J. Liu**

9:05 ENFL 288. Effect of ultrasonic pretreatment on microwave heating performance of zeolite-based catalysts mixed with SiC absorbers used in biomass pyrolysis/upgrading processes. **D. Boldor**, C. Marculescu, R. State, M. Patrascu

9:25 ENFL 289. Production of phenols from Kraft lignin over a tungsten phosphide catalyst. **Y. Sang**, Y. Li

9:45 ENFL 290. Elucidating neutral oil entrainment behavior during the dephenolization of coal-based liquid oil. **L. Yi**, J. Feng, W. Li

10:05 Intermission.

10:20 ENFL 291. Hydrogen sulfide removal from biogas on nitrogen-doped hierarchical carbons. **W. Quan**, X. Jiang, X. Wang, C. Song

10:40 ENFL 292. One-pot synthesis of high density and low freezing point jet-fuel-ranged blending from bio-derived phenols and cyclopentanol. **G. Nie**, X. Zhang, L. Pan, J. Zou

11:00 ENFL 293. Effect of support on nickel phosphide catalysts for the conversion of jatropha oil into hydrocarbons. **X. Du**, K. Zhou, D. Li, **C. Hu**

11:20 ENFL 294. Transformation of jatropha oil into high-quality bio-fuel over Ni-W bimetallic catalysts: Effect of alloy particle size. **R. Yang**, H. Xin, X. Du, K. Zhou, D. Li, **C. Hu**

11:40 ENFL 295. Valorization of humins for activated carbon production. **S. Kang**, Y. Xu, G. Zhang, H. Yin, X. Fu, Z. Peng

Section F



TECHNICAL PROGRAM

Orange County Convention Center
West Hall B4 - Theater 17

Simulations of Materials & Processes for Energy Applications

Y. Liu, D. Lu, Y. Ping, B. Wood, *Organizers*
H. Zhuang, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 ENFL 296. Stability of single-atom catalyst: Origin of sintering. **Y. Gao**

8:35 ENFL 297. Understanding lignin polymerization using kinetic Monte Carlo methods. **M. Orella**, T. Gani, M. Stone, E. Anderson, F. Brushett, Y. Roman-Leshkov

9:05 ENFL 298. Computational studies of CO₂ electrochemical reduction with metal electrodes. **S. Li**

9:35 Intermission.

9:50 ENFL 299. Computational investigation of electrochemistry on surfaces and interfacial structures. **P. Liao**

10:20 ENFL 300. Exploring free-energy surfaces of petroleum thermal cracking mechanisms. **F. Wang**, P. Tao

10:50 ENFL 301. Computational design of active and selective electrocatalysts for hydrogen peroxide and molecular hydrogen evolution. **J.R. Schmidt**

Section G

Orange County Convention Center
West Hall B4 - Theater 18

Emerging Materials for Renewable Energy

M. Hu, M. Lu, S. Nair, *Organizers*
Z. Li, D. Liu, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 ENFL 302. Influence of silanol densities on aldol condensation reactions in Ti-BEA. **D. Flaherty**, C. Berdugo Diaz, H. Zhang

8:40 ENFL 303. Understanding dehydration reaction and diffusion during biomass catalytic upgrading over ZSM-5 zeolite. L. Bu, K. Orton, K. Iisa, C. Mukarakate, **S. Kim**

9:10 ENFL 304. Atomistic modeling of vapor phase catalysis in H-ZSM5. **R. Surendran Assary**, L.A. Curtiss, M. Zhou



TECHNICAL PROGRAM

9:40 ENFL 305. Multifunctional zeolite catalyst for tandem ethanol conversion to C₃₊ olefins. J. Zhang, S. Adhikari, C. Yang, N. LiBretto, J.T. Miller, T. Krause, K.A. Unocic, **Z. Li**

10:10 Intermission.

10:25 ENFL 306. Coupling of methanol and carbon monoxide over H-ZSM-5 to form aromatics. Z. Chen, Y. Ni, W. Zhu, **Z. Liu**

11:00 ENFL 307. Acid catalyzed production of 1,3-butadiene from biomass derived tetrahydrofuran. **O. Abdelrahman**, P. Dauenhauer

11:30 ENFL 308. *Ab initio* molecular dynamics studies of the confinement effect of alcohols and water in in H-ZMS-5: Structure, spectroscopy, and adsorption free energy. M. Lee, s. yuk, V. Glezakou, **R. Rousseau**

Section H

Orange County Convention Center
West Hall B4 - Theater 19

Sustainable Energy Conversion via Innovative Electrocatalysis & Photocatalysis

Electrocatalysts for Chemical Conversion

Y. Cheng, F. Jiao, Y. Shao, G. Wu, *Organizers*
O. Y. Gutiérrez, A. J. Karkamkar, *Presiding*

8:00 Introductory Remarks.

8:05 ENFL 309. Metal-catalyzed hydrogenation of aromatic rings and carbonyl compounds in the presence of cathodic potential. U. Sanyal, L.C. Meyer, K.A. Stoerzinger, J. Holladay, J. Fulton, D.M. Camaioni, **O. Gutierrez-Tinoco**, J. Lercher

8:35 ENFL 310. Theoretical mechanistic studies of electrochemical hydrogenation of organic compounds. M. Lee, M. Nguyen, S. Akhade, D.C. Cantu, V. Glezakou, **R. Rousseau**

9:05 ENFL 311. Electrochemical processes intensification for the enhancement of carbon conversion. **L. Diaz Aldana**, T. Lister, N. Gao

9:35 ENFL 312. Anodic and cathodic restructuring of platinum electrocatalysts. **M. Koper**

10:05 Intermission.

10:10 ENFL 313. Pd-catalyzed electrohydrogenation of dinitrogen to ammonia. **X. Feng**

10:40 ENFL 314. Electrochemically forming and breaking the N-H bond in ammonia. **K. Manthiram**, N. Lazouski, Z. Schiffer

11:10 ENFL 315. Quantitative protocol for the electroreduction of N₂ to NH₃ under ambient conditions. **I. Stephens**, S.Z. Andersen, V. Colic, S. Yang, J. Schwalbe, A.C. Nielander, J.M. McEnaney, K. Enemark-Rasmussen, J. Baker, A. Singh,



TECHNICAL PROGRAM

B.A. Rohr, S. Blair, S. Mezzavilla, J. Kibsgaard, P. Vesborg, M. Cargnello, S. Bent, T.F. Jaramillo, J.K. Nørskov, I. Chorkendorff

11:40 ENFL 316. Proton control in electrochemical ammonia synthesis. **J. Schwalbe**, A. Singh, B. Rohr, M. Statt, A. Nielander, J.M. McEnaney, S.Z. Andersen, V. Colic, S. Yang, I. Chorkendorff, T.F. Jaramillo, J.K. Nørskov, M. Cargnello

Section I

Orange County Convention Center
Room W230D

ENFL Plenary: Chemistry for New Frontiers of Sustainable Energy & Fuels

L. Fan, J. W. Lee, *Organizers, Presiding*

9:00 Introductory Remarks.

9:05 ENFL 317. Catalysis for sustainable production of fuels and chemicals. **J.K. Nørskov**

10:05 Intermission.

10:15 ENFL 318. Using lessons from nature to achieve artificial photosynthesis. **M.R. Wasielewski**

Exploring the Frontiers of Chemistry through NASA Research

Getting There: Advanced Materials for Space Travel

Sponsored by COMSCI, Cosponsored by ANYL, BIOL, BIOT, CELL, COLL, ENFL, I&EC, INOR, NUCL, PHYS, PMSE and POLY

Elucidation of Mechanisms & Kinetics on Surfaces

Kinetic Modeling

Sponsored by CATL, Cosponsored by ENFL, ENVR, INOR and PHYS

Well-Defined Materials for Heterogeneous Catalysis: Synthesis, Characterization, & Performance Studies

Synthesis & Performance

Sponsored by CATL, Cosponsored by ENFL



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

Light-Driven Chemistry: Photoelectrochemistry & Photocatalysis

Sponsored by CATL, Cosponsored by COLL, ENFL, I&EC, INOR and PHYS

Frontiers in Catalysis for Energy & Sustainability

Sponsored by CATL, Cosponsored by ENFL[†]

Elucidating the Roles of Electric Fields in Catalysis

Sponsored by CATL, Cosponsored by ENFL and PHYS

TUESDAY AFTERNOON

Section A

Orange County Convention Center
West Hall B4 - Theater 12

George A. Olah Award in Hydrocarbon or Petroleum Chemistry: Symposium in Honor of ChunShan Song

E. B. Fox, X. Guo, M. J. Janik, C. Song, *Organizers*
U. T. Turaga, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 ENFL 319. Biomass valorization via catalysis in hot compressed water. **P.E. Savage**

1:30 ENFL 320. Oxidative cleavage of carbon-carbon bonds of lignin to aromatic chemicals. **F. Wang**

1:55 ENFL 321. Cross-surface migration of Ni and TiO₂-A induces formation of Ni/anatase TiO₂ catalyst for selective hydrodeoxygenation of guaiacol to phenolics. X. Zhang, P. Yan, B. Zhao, K. Liu, M. Kung, H. Kung, **Z. Zhang**

2:20 ENFL 322. Green synthesis of zeolites and zeolite-based green catalysis. **F. Xiao**

2:45 Intermission.

3:00 ENFL 323. Kinetic and spectroscopic studies of catalytic mechanisms: Hydrodeoxygenation of biomass feedstocks on transition metal phosphides. **S.T. Oyama**, G. Yun

3:25 ENFL 324. Biomass conversion in supercritical ethanol start from lignin. **Y. Li**, M. Chen



TECHNICAL PROGRAM

3:50 ENFL 325. Award Address (George A. Olah Award in Hydrocarbon or Petroleum Chemistry sponsored by the George A. Olah Award Endowment). Some new design approaches to adsorptive and catalytic processing for cleaner hydrocarbon fuels, CO₂ capture, and CO₂ conversion to chemicals and fuels. **C. Song**

4:50 Concluding Remarks.

Section B

Orange County Convention Center
West Hall B4 - Theater 13

Innovative Chemistry & Materials for Electrochemical Energy Storage

Beyond Li-Ion

Cosponsored by CATL, INOR and PMSE
W. Luo, Y. Mo, H. Sun, *Organizers*
B. Gallant, *Organizer, Presiding*
Y. Lu, *Presiding*

1:00 Introductory Remarks.

1:05 ENFL 326. Novel chemistry for automotive application: Lithium-selenium and selenium-sulfur couple. G. Xu, **K. Amine**

1:30 ENFL 327. Lithium-sulfur batteries: The next frontier in energy storage. **N. Koratkar**

1:55 ENFL 328. Suppressing dendritic lithium formation in lithium metal batteries. **B. Wei**

2:20 ENFL 329. Probing the intrinsic role of lithium fluoride in artificial solid electrolyte interphases. **B. Gallant**, M. He, R. Guo

2:45 ENFL 330. Dendrite suppression through charge and thermal management in lithium metal anode. D. Cao, A. Hafez, **H. Zhu**

3:10 Intermission.

3:25 ENFL 331. Stabilization of lithium electrodeposition via enhanced lithium ion transport properties at the electrode/electrolyte interface. **Y. Lu**

3:50 ENFL 332. Enabling ether-based electrolytes for high-voltage lithium-metal batteries. **W. Xu**, X. Ren, S. Jiao, J. Zhang

4:15 ENFL 333. Multi-shell metal-organic frameworks by fine-tuned hydrophilicity for O₂-battery. **W. Choi**, J. Kang

4:30 ENFL 334. Effects of polymer coatings on electrodeposited lithium metal. **J. Lopez**, A. Pei, Y. Cui, Z. Bao

4:45 ENFL 335. Effect of salt and co-solvents on electrolyte structure in Li-S batteries: A first-principles study. **B. Narayanan**, R.S. Assary, Q. Pang, A. Shyamsunder, M. Shin, T.S. Watkins, H. Wu, A.A. Gewirth, K.R. Zavadil, L. Nazar, L.A. Curtiss



TECHNICAL PROGRAM

Section C

Orange County Convention Center
West Hall B4 - Theater 14

Carbon Dioxide Conversion & Utilization

Photo, Electro & Plasma Catalysis

Cosponsored by CATL, COMP and GEOC
S. Kawi, H. Lin, R. Motkuri, *Organizers*
Y. H. Hu, *Organizer, Presiding*
F. Jiao, Y. Sun, *Presiding*

1:00 Introductory Remarks.

1:05 ENFL 336. Photocatalysis for reductive functionalization of CO₂. L. He, X. He, **K. Chen**

1:30 ENFL 337. New surface engineering strategy to promote photocatalytic CO₂ reduction by TiO₂ photocatalysts. X. Feng, F. Pan, **Y. Li**

1:50 ENFL 338. Dual photocatalytic roles of light: charge separation at the band gap and heat via localized surface plasmon resonance to photoconvert CO₂ into CO over silver-zirconium oxide. H. Zhang, T. Itoi, T. Konishi, **Y. Izumi**

2:10 ENFL 339. CO₂ photoreduction by artificial photosynthesis using hybrid multifunctional materials. **V.A. de la Peña O'Shea**, A. García Sanchez, L. Collado, P. Reñones, E. Alfonso-Gonzalez, M. Barawi, I. Villar, R. Pérez-Ruiz, F. Fresno, M. Liras

2:30 ENFL 340. Overview and outlook on CO₂ photothermal conversion by light alkanes. **X. Cao**, X. Liu, D. Zhang, T. Hanrath, D. Erickson

2:50 Intermission.

3:05 ENFL 341. Mechanochemical synthesis of all-Inorganic CsPbBr₃ nanorods and their use in selective photocatalytic hydrogenation of CO₂. **S. Kumar**, I. Poli, M. Isaacs, M. Regue, S. Eslava

3:25 ENFL 342. Electrochemical and photochemical reduction of CO₂ to CO: A cyanide-bridged di-manganese carbonyl complex. **H. Kuo**, T.S. Lee, S.E. Tignor, G.D. Scholes, A.B. Bocarsly

3:45 ENFL 343. CO₂ reduction by microwave plasma enabling efficient power-to-X conversion. **G. van Rooij**, D. van den Bekerom, A. van de Steeg, Q. Ong, T. Minea, R. Van de Sanden

4:05 ENFL 344. Tuning the chemistry in plasma-based CO₂ and CH₄ reforming processes using additives and scavengers. **R. Snoeckx**, M. Cha

4:25 ENFL 345. Plasma-driven hydrogenation of CO₂ to methanol at atmospheric pressure and room temperature. L. Wang, Y. Wang, **X. Tu**

Section D



TECHNICAL PROGRAM

Orange County Convention Center
West Hall B4 - Theater 15

Applied Electrocatalysis for Renewable Energy & Synthesis

Li-Ion Batteries & Fuel Cells

Y. Sun, H. Wang, *Organizers*
Y. Yang, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 ENFL 346. Li-oxygen battery: From open system to closed system. **J. Lu**

1:45 ENFL 347. Highly reduced aqueous polyoxometalate solutions for on-demand hydrogen generation and energy storage. **M. Symes**

2:15 ENFL 348. N_8^- polynitrogen stabilized on multi-wall carbon nanotubes for oxygen reduction reactions at ambient conditions. Z. Yao, Z. Iqbal, **X. Wang**

2:45 Intermission.

3:00 ENFL 349. Controlling catalytic reactions for production of hydrogen (HER), fuel cells (ORR), and carbon dioxide reduction (CO₂RR). **J.L. Mendoza-Cortes**

3:30 ENFL 350. Self-protection method to ultrasmall intermetallic PtM (M = Zn, Ga or Cu) nanocrystals as efficient electrocatalysts for oxygen reduction reaction. **J. Liang**, Q. Li

4:00 ENFL 351. Metallic, cotton, fiber-based biofuel cells. **C. Kwon**, Y. Ko, J. Choi, J. Cho

4:30 Concluding Remarks.

Section E

Orange County Convention Center
West Hall B4 - Theater 16

Energy Materials in Fuel Conversion & Utilization

L. Fan, L. Qin, *Organizers, Presiding*

1:00 Introductory Remarks.

1:05 ENFL 352. Multifunctional, Pr-doped ceria nanocrystal for advanced energy conversion technology. **Y. Liu**

1:30 ENFL 353. Mixed protonic-electronic membrane reactors: Converting hydrocarbon resources and CO₂ to fuels. **E.D. Wachsman**



TECHNICAL PROGRAM

2:10 ENFL 354. Perovskite-promoted mixed Co-Fe oxides for enhanced chemical looping air separation. **J. Dou**, E. Krzystowczyk, A. Mishra, X. Liu, F. Li

2:35 ENFL 355. Analysis and evaluation of torrefaction safety focusing on factors affecting self-heating phenomenon. **E. Arriola**, C. Wei-Hsin, M.G. de Luna

3:00 Intermission.

3:15 ENFL 356. Gas Conversion to clean liquid fuels and chemicals: Overview of recent advances and the challenges of catalytic Fischer-Tropsch multiphase reactors using sophisticated measurement and computing techniques. **M. Al-Dahhan**

4:20 ENFL 357. Reconstruction of Pt-Fe-Mn ternary alloys enclosed with high-index facets for enhanced electrocatalytic activity. **C. Qin**, A. Fan, X. Zhang

4:45 Concluding Remarks.

Section F

Orange County Convention Center
West Hall B4 - Theater 17

Simulations of Materials & Processes for Energy Applications

D. Lu, Y. Ping, B. Wood, H. Zhuang, *Organizers*
Y. Liu, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 ENFL 358. Low-temperature selective alkane activation on IrO₂(110) surfaces. **A.R. Asthagiri**, M. Kim, J.F. Weaver

1:35 ENFL 359. CH₄ dissociation and C-C coupling on metal-terminated carbide surfaces: A DFT study. **T. Zhang**, X. Yang, Q. Ge

2:05 ENFL 360. Density functional theory design and performance for molecular and materials problems, with example hydrogen storage applications. **M.P. Head-Gordon**

2:35 Intermission.

2:50 ENFL 361. When electrochemistry meets electrostatics: Implications and applications. **M. Coote**, B. Noble, C. Hammill, P. Norcott, S. Ciampi

3:20 ENFL 362. CO₂ hydrogenation over cubic and hexagonal In₂O₃ phases: Catalytic mechanism and structure-property-activity relationship. **S. Li**, B. Qin

3:50 ENFL 363. Toward a more accurate depiction of chemical-active site interactions using catalyst material parameters. X. Shen, Y. Pan, **Z. Peng**

Section G



TECHNICAL PROGRAM

Orange County Convention Center
West Hall B4 - Theater 18

Emerging Materials for Renewable Energy

Z. Li, D. Liu, *Organizers*
M. Hu, M. Lu, S. Nair, *Organizers, Presiding*

1:00 Introductory Remarks.

1:05 ENFL 364. Synthesizing hierarchical zeolites: A tale of two strategies. **K. Zhang**, S. Fernandez

1:35 ENFL 365. Elucidating the adsorption capacity of ETS-10 for rare earth element cations. **J. Thakkar**, B. Wissler, N. Dudenas, X. Zhang

2:05 ENFL 366. Zeolitic imidazolate framework membranes made by ligand-induced permselectivation for propylene/propane separation. **X. Ma**, P. Kumar, N. Mittal, A. Khlyustova, P. Daoutidis, A. Mkhoyan, M. Tsapatsis

2:35 ENFL 367. Recovery of xenon from air over ZIF-8 membranes. **T. Wu**, M.A. Carreon

3:00 ENFL 368. Emerging hybrid material membranes for biofuel processing and renewable energy applications. **M. Hu**, M. Lu

3:30 Intermission.

3:45 ENFL 369. Plasma-assisted formation of metallic nickel domains on nickel-iron-molybdenum oxyhydroxide for efficient, electrocatalytic oxygen-evolution reaction. **M. Byeongcheul**, J. Kang

4:10 ENFL 370. Hollow NiFeP@C derived from metal-organic framework for enhanced oxygen evolution reaction. **A. Fan**, C. Qin, X. Zhang

4:35 ENFL 371. Dual synergic effect in hybrid Co@Ni₁₂P₅/PPy for enhanced OER. **S. Ramani**, S. Cogal, J. Lowe, V. Bhethanabotla, J. Kuhn

Section H

Orange County Convention Center
West Hall B4 - Theater 19

Sustainable Energy Conversion via Innovative Electrocatalysis & Photocatalysis

Advanced Electrocatalyst for Fuel Cells

Y. Cheng, F. Jiao, *Organizers*
Y. Shao, G. Wu, *Organizers, Presiding*

1:00 Introductory Remarks.



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

1:05 ENFL 372. Non-precious metal electrocatalysts for clean energy applications. **P. Zelenay**

1:45 ENFL 373. Theoretical approaches for understanding the oxygen reduction reaction on PGM-free materials at the atomic scale. **E.F. Holby**, X. Yin, U. Martinez, H.T. Chung, S. Komini Babu, G. Purdy, P. Zelenay

2:15 ENFL 374. Carbon catalysis for high efficient making nanocarbon and aromatics. **F. Wei**

2:45 ENFL 375. Metal-organic framework-derived atomically dispersed metal site catalysts for oxygen reduction in acids. **G. Wu**

3:15 Intermission.

3:20 ENFL 376. *Ex-situ* and *operando* spectroscopic characterisation of inexpensive cathode catalysts for fuel cells. **F. Jaouen**

4:00 ENFL 377. Instability of Fe-N-C catalysts in acidic conditions. **C. Choi**

4:30 ENFL 378. Electrocatalyst stability and improvement for oxygen reduction reactions. X. Xie, V. Prabhakaran, J. Liu, C. Wang, **Y. Shao**

Section I

Orange County Convention Center
West Hall B4 - Theater 20

Energy Storage in Chemical Bonds: Advances in Chemistry & Materials for Hydrogen Storage

M. Jones, C. Yoon, *Organizers*
T. Autrey, *Organizer, Presiding*

1:00 Introductory Remarks.

1:10 ENFL 379. Liquid hydrogen carrier pathways for hydrogen supply and transmission. **D. Papadias**, J. Peng, R. Ahluwalia

1:30 ENFL 380. Highly efficient CO₂-formate based hydrogen storage system. **H. Lin**

1:50 ENFL 381. Understanding hydrogen release from formic acid and aqueous formate salt. **H. Jeong**, Y. Hwang, C. Yoon

2:10 Intermission.

2:20 ENFL 382. Characterising gas absorption by neutron scattering and dielectric resonance. **M. Jones**

2:40 ENFL 383. Violation of the Switendick criterion in metal hydrides evidenced by inelastic neutron scattering. **A. Ramirez-Cuesta**, A. Borgschulte, A. Pandey



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

3:00 ENFL 384. Observing hydrogen intercalation into palladium thin films using *in situ* grazing incidence x-ray diffraction and x-ray reflectivity. **A.T. Landers**, J.T. Feaster, K. Brown, J.C. Lin, M. Farmand, S. Fackler, Y. Nishimura, J. Beeman, M. Bajdich, D. Higgins, J. Yano, W. Drisdell, R. Davis, C. Hahn, A. Mehta, T.F. Jaramillo

3:20 ENFL 385. Highly monodisperse nano- and subnano-sized Ru particles on alkaline-exchanged zeolite Y for ammonia decomposition: Effect of surface acidity. J. Cha, Y. Jo, S. Nam, **H. Sohn**, C. Yoon

3:40 Intermission.

3:50 ENFL 386. Reversible hydrogen uptake/release over sodium phenoxide-cyclohexanolate pair. **T. He**, T. Autrey, P. Chen

4:10 ENFL 387. Thermodynamics and kinetics of formic acid as a H₂ carrier. **A.J. Karkamkar**

4:30 ENFL 388. Ammonia as an efficient CO_x-free hydrogen carrier: Fundamentals and applications. **Y. Jo**, J. Cha, C. Lee, H. Jeong, J. Han, S. Nam, C. Yoon

Elucidation of Mechanisms & Kinetics on Surfaces

Catalysis on Metal Interfaces with Metal Oxides

Sponsored by CATL, Cosponsored by ENFL, ENVR, INOR and PHYS

Exploring the Frontiers of Chemistry through NASA Research

Living There: Science for the Future of Manned Space Exploration

Sponsored by COMSCI, Cosponsored by ANYL, BIOL[‡], BIOT, CELL, COLL, ENFL[‡], I&EC[‡], INOR[‡], NUCL[‡], PHYS[‡], PMSE[‡] and POLY[‡]

Well-Defined Materials for Heterogeneous Catalysis: Synthesis, Characterization, & Performance Studies

Synthesis & Performance

Sponsored by CATL, Cosponsored by ENFL

Light-Driven Chemistry: Photoelectrochemistry & Photocatalysis

Sponsored by CATL, Cosponsored by COLL, ENFL, I&EC, INOR and PHYS



TECHNICAL PROGRAM

Frontiers in Catalysis for Energy & Sustainability

Sponsored by CATL, Cosponsored by ENFL[†]

Elucidating the Roles of Electric Fields in Catalysis

Sponsored by CATL, Cosponsored by ENFL and PHYS

TUESDAY EVENING

Section A

Orange County Convention Center
West Hall C

ENFL Poster Session

H. Lin, L. Yang, *Organizers*

6:00 - 8:00

ENFL 389. Novel, high-potential cathode materials for next-generation lithium-ion batteries. **Z. Alahmed**, H.A. Aly, A. Mussa, C. Arro, A. Aissaoui, J. abraham, S.Y. Al-Qaradawi, U. Nisar, A. Shakoor

ENFL 390. LiFePO₄/sulfur composite as a high-performance cathode material for hybrid lithium batteries. **L. Zhu**, X. Jiang, D. Jia, Y. Wu, W. Tang

ENFL 391. Designing stable SEI layers for long-lasting aqueous lithium-ion batteries. **C. Chua**, U. Subramanya, V. Leong, P. Singh, B. Yip, R. Robinson, A. Bokare, F. Erogbogbo, D. Oh

ENFL 392. Coalesced carbon onion anode: Towards high-rate anode materials for lithium-ion capacitor. **A. Aref Laleh**, R. Rajagopalan, C.A. Randall

ENFL 393. Conductive graphite incorporated carbon/silicon composites as negative electrode materials for lithium ion cells. C. Chou, J. Chen, C. Chang, **S. Yen**

ENFL 394. Synthesis of ceramic nanoparticles doped graphene as lithium-ion battery anode material. **Z. Zhang**, L. Ju, D. Fox, K. Liang, A.Z. Khater, L. Zhai

ENFL 395. Bifluoride ionic liquids with ultra-high electrochemical stability for metal-ion batteries. **T. Hmissa**, A. Mirjafari

ENFL 396. Zn-spinels as cathode materials for non-aqueous Zn-ion batteries. **C. Pan**, A.A. Gewirth, R.G. Nuzzo

ENFL 397. Alluaudite-based multicomponent cathode materials for Na-ion batteries. **A.A. Elwan**

ENFL 398. Layered electrode nanomaterials for sodium-ion batteries. **A.A. Mussa**, S.A. Qasim, M. Youssry



TECHNICAL PROGRAM

- ENFL 399.** *In-situ* reliability studies on vanadium flow batteries. **B. Li**
- ENFL 400.** Selection and optimization of stable heterocyclic aromatics for nonaqueous redox flow battery. **H. Yu, Y. Li**
- ENFL 401.** Toward performance enhancement in PffBT4T-2OD-based ternary polymer solar cells by optimizing morphology and efficient charge carrier transfer. **X. Zhang, J. Yu**
- ENFL 402.** Efficiency enhancement of Si-based solar cells with low-cost upgraded metallurgical-grade Si. **D. Lee**
- ENFL 403.** Optimize separation structure of donor-acceptor phase to adjust the fill factor in PBDB-T-based organic solar cells. **D. Zhang, J. Yu**
- ENFL 404.** Effect of ammonium salt on TiO₂ photoanode of dye-sensitized solar cells. **C. Su, P. Sireesha, S. Bai, W. Li**
- ENFL 405.** Boosting the efficiency of non-fullerene organic solar cell via isopropanol treatment. **T. Kong, J. Yu**
- ENFL 406.** New hybrid concept coupling photovoltaic and thermoelectric technologies for maximum solar energy exploitation. **M. Hajji**
- ENFL 407.** Characterizing screening methods for solar thermal fuel properties of norbornadiene. **K. Le, R. Szabo, T. Kowalczyk**
- ENFL 408.** Optimum process condition of zinc oxide layer in organic solar cell. **Y. Ma, D. Ko, S. Chu, G. Sim, J. Kim**
- ENFL 409.** All p-i-n hydrogenated amorphous silicon oxide thin film solar cells for semi-transparent solar cells. **J. Kwon, J. Yang, M. Shin**
- ENFL 410.** Rational design of the palladium nano-catalysts for selective CO₂ electrochemical reduction to formic acid and CO. **Z. Yin**
- ENFL 411.** Ligand-assisted formation of single-atom nickel sites over graphene sheets for selective electrochemical reduction of CO₂ to CO. **H. Jeong, M. Balamurugan, U. Sim, K. Nam**
- ENFL 412.** Pd@Cu as catalysts for CO₂ reduction reaction probing by *in-situ* XAS. **S. Chen**
- ENFL 413.** Decorated carbon nanotube/carbon nanosheet architecture enables improved CO₂ electroreduction. **F. Pan, Y. Li**
- ENFL 414.** CO₂ photoreduction by porous TiO₂ synergetically promoted by atomic layer deposited MgO and photodeposited Ag. **X. Feng, F. Pan, Y. Li**
- ENFL 415.** Photoelectrochemical strategy for discrimination of microbial pathogens using conjugated polymers. **Z. Xin, S. Wang**
- ENFL 416.** Photoelectrochemical properties and photocatalytic effect of doping nickel tungstate with group 11 elements. **A. Riley, S. Hosseini, M. Sutton, T.S. Zubkov, Z.J. Li**
- ENFL 417.** Constructing high-efficiency MoO₃-polyimide hybrid photocatalyst based on strong interfacial interaction. **C. Ma, H. Zhu, Y. Wang, Z. Zou**



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- ENFL 418.** Single-atoms as the active site with high selectivity for electrochemical application. **H. XU**, D. Liu, T. Xu
- ENFL 419.** Oxidation kinetics of electrospun compatibilized immiscible polymer blends. **S. Panangala**, C. Karunaweera, J.A. Garcia, J.P. Ferraris
- ENFL 420.** Biodiesel production by *Jatropha curcas*. **A.N. Gondal**
- ENFL 421.** Development of a novel spectro-electro-chemical technique for quantitative characterizations of major components of crude oil in Saudi Arabia. **A.N. Kawde**, M.A. Morsy, E. Al-Shafei
- ENFL 422.** Catalytic vs. non-catalytic synthesis of bio-oil via the conversion of biomass. **M. Perez**, **M. Pimentel**, W. Jang
- ENFL 423.** Thermal degradation of biofuels under simulated engine conditions. **A. Felix**, K.L. Chagoya, R.G. Blair
- ENFL 424.** Pd/C-CaO-catalyzed α -alkylation and hydrodeoxygenation of an ABE mixture for biogasoline synthesis. **H. Lee**
- ENFL 425.** Biodiesel. **T. Kupatadze**
- ENFL 426.** Biogas production from renewable resources through anaerobic digestion process: Experimental stage to the field. **O.O. Adetule**
- ENFL 427.** Depolymerization of alkali lignin in the presence of subcritical water and zeolite-supported catalysts. **B. Jadhav**, D.E. Raynie
- ENFL 428.** Effective and facile conversion of cellulose into platform chemicals over metal salts in sulfolane / water solvent. **K. Wang**, J. Jiang, J. Xu, J. Liu
- ENFL 429.** Enriched graphitic N in nitrogen-doped graphene as a superior metal-free electrocatalyst for oxygen reduction reaction. **P. Yang**, X. Lu, D. Wang, L. Ge, J. Zhang, M. An
- ENFL 430.** 3D, porous Fe-N-C catalyst based on oxide grapheme-phenolic resin for oxygen reduction reaction. C. Hou, **X. Zhang**, Y. Zhang, X. Liu
- ENFL 431.** Molybdenum carbide/reduced graphene oxide nanoribbon as an efficient hydrogen evolution reaction catalyst. **R. Wang**, S. Peng, X. Wang
- ENFL 432.** Hypersaline-oriented synthesis of 3D structure assembled from N/S-codoped hierarchically porous carbon nanosheets for supercapacitors. **D. Xue**, M. Liu, L. Gan
- ENFL 433.** Ni(OH)₂-MnO₂ nanosheets deposited on carbon nanotube networks for asymmetrical supercapacitors with high performance. **S. Peng**, R. Wang, X. Wang
- ENFL 434.** Reversibly deformable carbon-nanosheet based large-area electrochemical capacitors. **J. Lee**, J. Jun, I. Choi
- ENFL 435.** Metal-free porphyrins as water splitting catalysts. **Y. Ge**, Y. Wu, D. Villagran
- ENFL 436.** Electrodeposited non-noble metal phosphides: Active and stable catalysts for water splitting. **R. Wasalathanthri**, S.A. Jeffrey, N. Su, K. Sun, R. Awni, Y. Yan, D. Giolando



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- ENFL 437.** Synthesis of NiFe oxide-based metal-organic framework nanosheets on 3D reduced graphene oxide foams for water-splitting electrocatalysis. **C. Penthala**, D. Wang, A. Basurrah, D. Nde, W. Zhao
- ENFL 438.** Highly stable Ruddlesden-Popper/perovskite dual-phase membrane for O₂ permeation under pure CO₂ atmosphere. **N. Han**, X. Meng, Q. Wei, S. Zhang, B. Meng, S. Liu
- ENFL 439.** Nb and Ta co-doped cobalt-free perovskite cathode for intermediate-temperature solid oxide fuel cells. **J. Gan**, Z. Yicheng, Y. Li
- ENFL 440.** Hydrophilic hole transporting materials for inverted perovskite applications. **Y. Tingare**, C. Su, Y. Lin, W. Li
- ENFL 441.** Investigation of decomposition in lead halide perovskites via *in-situ* absorption spectroscopy and grazing incidence wide angle x-ray scattering. **S. Kundu**, T. Kelly
- ENFL 442.** Mapping spectroscopic signatures of Li_xV₂O₅ across lithiation-induced phase transformations. **H.L. Figueroa**, L.R. De Jesus, J.L. Andrews, S. Banerjee
- ENFL 443.** Toward Mg-doped tantalum oxynitrides for photocatalysis: Aerosol synthesis of oxide precursors with tunable dopant content. **D. Abeyasinghe**, Y. Losovyj, J.T. Gamler, S.E. Skrabalak
- ENFL 444.** Effects of promoters on SBA -15 supported iron catalysts for high temperature fischer tropesch synthesis. **S. Seby**, D. Weber, B. Joseph, J. Kuhn
- ENFL 445.** Hydrogen storage properties of pure, doped, and co-doped MgH₂ from first principle calculations and kinetic monte carlo simulation. **M. Lakhali**, M. Bhihi, M. Abdellaoui, M. El Khatabi, A. El Kenz, A. Benyoussef, M. Loulidi
- ENFL 446.** Porous liquid covalent organic frameworks. **R.E. Mow**, M.B. Martinez, T. Gennett, W.A. Braunecker
- ENFL 447.** Silver-palladium bimetallic nanoparticles on unsupported vulcan XC-72R as electrocatalysts toward oxygen reduction reaction in alkaline media. **M. Vega Cartagena**, C.R. Cabrera
- ENFL 448.** Molecular simulation of kerogen oil recovery using lean gas injection. **S. Baek**, I. Akkutlu
- ENFL 449.** Characterization and catalytic performance of high-active unsupported catalyst for diesel hydrofining. **J. Guo**, S. Ni, S. Chen
- ENFL 450.** Theoretical study on mechanism of hydrodeoxygenation of dibenzofuran catalyzed by supported transition metal catalysts. Z. Xie, **X. Wang**, W. Li
- ENFL 451.** Natural gas storage with hydrate technology at the ambient condition. **P. Rangsunvigit**
- ENFL 452.** Effects of Li₂TiO₃-coating on the structure and the electrochemical properties of LiNi_{0.5}Mn_{0.5}O₂ cathode materials at high voltages. **G. Jia**, S. Liu, M. Wang, Z. He
- ENFL 453.** Carbon dioxide removal from surrogate biogas using amine based silica sorbents. **U. Gopalakrishnan**, B. Joseph, J. Kuhn
- ENFL 454.** Developing effective catalysts: Sustainable fossil-free ammonia synthesis at atmospheric pressure. **N. Holliger**, P. Sharma, V. Chikan



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- ENFL 455.** Effect of methanol on stable methane hydrate decomposition. **X. Sun**, G. Zhou, G. Lu
- ENFL 456.** Paramagnetic fluorinated ionic liquids: Synthesis, characterization, and CO₂ adsorption. **J.E. Knoop**, J.R. Alston
- ENFL 457.** Fabrication and ionic transportation characterization of Biological ion channel array. **j. kim**, j. jung, i. kang, K. Choi
- ENFL 458.** Changing variables: Alternatives to an alternative and the self-assembly of better proton wire. **S. Pollozi**, H. Elshendidi, G. Reyes, G. Lopez, D.M. McGregor
- ENFL 459.** Asymmetric anodic aluminum oxide membrane with high ionic rectification and high currents. **K. Choi**, J. Jung, J. Kim, I. Kang
- ENFL 460.** Universal solvent viscosity reduction via hydrogen bonding disruptors. **X. Zhou**, H.B. Nulwala, H. Kim, S. Chen

WEDNESDAY MORNING

Section A

Orange County Convention Center
West Hall B4 - Theater 12

Lower Alkane Activation & Conversion

Y. Dai, H. Lin, *Organizers*
F. Huo, Y. Yang, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 ENFL 461. Alkane dehydrogenation on nanocarbon catalysts: From reaction mechanism to catalyst design. **W. Qi**, P. Yan, T. Cao

8:30 ENFL 462. Stable Co²⁺ sites incorporated in γ -Al₂O₃ sheet for catalytic propane dehydrogenation. **X. Gao**, Y. Dai, **Y. Yang**

8:55 ENFL 463. Role of oxygen carrier lanthanide oxides (La & Ce) doped Al₂O₃ supported chromium for propane dehydrogenation in the presence of CO₂ as a soft oxidant. **N. Dewangan**, M. Sethia, S. Das, A. Jangam, H. Kus, S. Kawi

9:20 ENFL 464. Study on a new Cr-K/zeolite- γ -Al₂O₃ microsphere catalyst and its propane dehydrogenation performance. **X. Wang**

9:45 Intermission.

10:00 ENFL 465. Iron-manganese oxide redox catalysts for chemical looping: Oxidative dehydrogenation of ethane. **S.M. Yusuf**, L.M. Neal, F. Li



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

10:25 ENFL 466. Highly selective conversion of methanol to propylene: Design of a MFI zeolite with selective-blockage of (010) surfaces. **D. Cai**, F. Wei

10:50 ENFL 467. Kinetic modeling of Na₂WO₄-promoted perovskite oxides for selective hydrogen combustion in the context of olefin production. **R. Dudek**, Y. Tian, G. Jin, F. Li

11:15 ENFL 468. Temperature hysteresis in dry reforming of methane on Ni/SBA-15 catalyst. **S. Wang**, Y. Wang, Q. Zhao, Y. Wang, **C. Hu**

Section B

Orange County Convention Center
West Hall B4 - Theater 13

Innovative Chemistry & Materials for Electrochemical Energy Storage

Beyond Li-Ion

Cosponsored by CATL, INOR and PMSE
B. Gallant, W. Luo, Y. Mo, H. Sun, *Organizers*
G. Cui, S. Guo, *Presiding*

8:00 Introductory Remarks.

8:05 ENFL 469. Developing calcium batteries: The good, the bad, and the ugly. **M. Palacin**

8:30 ENFL 470. Recent advances on advanced K-ion battery materials. **S. Guo**

8:55 ENFL 471. Architectural re-design of zinc anodes physically thwarts dendrite formation—with zinc batteries now rechargeable, what's next? **D.R. Rolison**, J. Parker, J.S. Ko, B.J. Hopkins, C.N. Chervin, J.W. Long

9:20 ENFL 472. Toward stable sodium metal anode in carbonate electrolyte: A compact, inorganic alloy interface. **X. Zheng**, W. Luo

9:35 ENFL 473. Relative solvating power as an indicator for the selection of electrolyte solvents in lithium-sulfur batteries. **C. Su**, M. He, R. Amine, Z. Chen, K. Amine

9:50 Intermission.

10:10 ENFL 474. Advanced rechargeable Zn and Mg batteries. **G. Cui**, J. Zhao, A. Du

10:35 ENFL 475. Effects of eutectic accelerators in sulfur cathodes for high-performance metal sulfur batteries. **J. Xie**

11:00 ENFL 476. Controlled titanium vacancies in titanium oxide for rechargeable magnesium batteries. **J. Ma**

11:25 ENFL 477. Rational design of layered, double hydroxide-based nanostructured host materials for advanced lithium-sulfur battery cathode. **J. Wang**, S. Chen, S. Deng



TECHNICAL PROGRAM

11:40 ENFL 478. Free-standing cathode from locked-in CNTs in as-spun mixed polymer fibers for Li-air batteries. **H. Kwon**, A. Lim, D. Lee, H. Lee, J. Seo, D. Im

Section C

Orange County Convention Center
West Hall B4 - Theater 14

Carbon Dioxide Conversion & Utilization

CO2 Capture & Conversion

Cosponsored by CATL, COMP and GEOC
H. Lin, *Organizer*
Y. H. Hu, S. Kawi, R. Motkuri, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 ENFL 479. Relationships between the charge-discharge methods and the gas adsorption performance of a supercapacitive swing adsorption module for CO₂ separation. **S. Zhu**, K. Ma, K. Landskron

8:25 ENFL 480. Efficiently screening surfactants at close to reservoir conditions via microfluidic chips for CO₂ foam applications. G. Jian, M.R. Kawelah, Z. Yousif, **A. Gizzatov**, A.I. Abdel-Fattah

8:45 ENFL 481. Synthesis and characterization of functional metal-organic framework materials. **O.K. Farha**

9:10 ENFL 482. Perovskite-oxide-based carbonate composite hollow fiber membrane for carbon dioxide separation. **S. Zhuang**, N. Han, F. Song, N. Yang, S. Liu

9:30 ENFL 483. High-performance catalytic perovskite SCFN hollow fiber membrane reactor for oxidative CO₂ reforming of methane. **Z. Wang**, Z. Li, N. Dewangan, Y. Cui, S. Das, S. Kawi

9:50 Intermission.

10:05 ENFL 484. Particle disintegration induced by formation of new interface over Ru/Al₂O₃. **Y. Yan**, A. Lapkin, Y. Yang, W. Liu

10:25 ENFL 485. Thermodynamics and kinetics control of photoelectrochemical CO₂ reduction reaction into liquid fuels. **Y. Kang**

10:45 ENFL 486. Beyond thermal equilibrium: A HI-Light reactor for reverse water-gas shift reaction. **X. Cao**, J. Akemi, Y. Kaminer, X. Liu, D. Zhang, T. Hanrath, D. Erickson

11:05 ENFL 487. Benzimidazoles as recyclable metal-free hydrides for CO₂ reduction to formate. **C. Lim**, J.T. Hynes, K. Glusac, C. Musgrave

11:25 ENFL 488. Bioelectrochemistry reduction of carbon dioxide by a molybdenum-containing formate dehydrogenase from *Cupriavidus necator*. **X. Yu**, D. Nicks, A.K. Mulchandani, R. Hille

Section D



TECHNICAL PROGRAM

Orange County Convention Center
West Hall B4 - Theater 15

New Frontiers in Petroleum Characterization, Transportation, Processing, Refining & Advanced Materials

Upstream Issues & Characterization

J. J. Adams, Y. Zhang, *Organizers*
C. F. Ovalles, P. Rahimi, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 ENFL 489. New green approach for extraction of diamondoids from petroleum source rock. **A. Akinlua**, M.A. Jochmann, T.S. Schmidt

8:30 ENFL 490. Controlling interfacial property through cost-efficient, CO₂-responsive assemblies for the enhancement of bitumen recovery. **Y. Lu**, Y. Zhu, D. Sun, Q. Liu, Z. Xu

8:55 ENFL 491. Dewatering process water-in-diluted bitumen emulsions using magnetically responsive Janus particles. **X. He**, C. Liang, Q. Liu, Z. Xu

9:20 ENFL 492. Fit-for-purpose counterion selection: Ammonium oxidation as a platform for on demand acid generation. **A. Cairns**, K. Hull, D. Schipper

9:45 Intermission.

10:00 ENFL 493. Towards a greener approach for microwave assisted acid digestion of refractory petroleum crude samples using a singler eaction chamber system followed by ICP techniques. F. Aguilar, J. Hernandez, L. Poirier, **F.A. Lopez-Linares**

10:25 ENFL 494. Simplification of heavy matrices by liquid-liquid extraction, the use of fractionation and GPC-ICP/MS. **C. Lienemann**, G. Gascon, J. Barbier, A. Socrates, B. Bouyssiere

10:50 ENFL 495. Accurate and sensitive method for the determination of inorganic chloride in petroleum hydrocarbons. **Z. Gajdosechova**, Z. Mester, E. Pagliano

11:15 Concluding Remarks.

Section E

Orange County Convention Center
West Hall B4 - Theater 16

Energy Materials in Fuel Conversion & Utilization

L. Fan, L. Qin, *Organizers, Presiding*

8:00 Introductory Remarks.



TECHNICAL PROGRAM

8:05 ENFL 496. Controllable synthesis of spherical Al-SBA-16 mesoporous materials with different crystal sizes and its high isomerization performance for hydrodesulfurization. **D. Hu**, A. Duan, C. Liu, Q. Meng

8:30 ENFL 497. Multiscale modeling of reactive interfaces for chemical storage of hydrogen fuel. **B. Wood**, T. Heo, S. Kang, K. Ray, L. Wan, A. Rowberg, A. Baker, J. Lee, J. White, F. El Gabaly, V. Stavila, L. Klebanoff

9:10 ENFL 498. Development and integration of new phase change materials for efficient energy storage in innovatively designed solar thermal water heating system. **j. prakash**, D. Roan, M. Ali, A.M. Kannan

9:35 ENFL 499. Novel epsilon-iron carbide Fischer-Tropsch catalysts with stable and low-CO₂ selectivity. **P. Wang**, Z. Guo, W. Chen, F. Chiang, A. Dugulan, Y. Song, R. Pestman, K. Zhang, J. Yao, B. Feng, P. Miao, W. Xu, Z. Men, E. Hensen

10:00 Intermission.

10:15 ENFL 500. Optimization of materials and processes for advanced energy systems. **D.C. Miller**

11:20 ENFL 501. Oxidation stability of unleaded alternative aviation gasolines. **C. Huang**

11:45 Concluding Remarks.

Section F

Orange County Convention Center
West Hall B4 - Theater 17

Simulations of Materials & Processes for Energy Applications

Y. Liu, D. Lu, B. Wood, H. Zhuang, *Organizers*
Y. Ping, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 ENFL 502. Simulation of the electrochemical reduction of CO₂. **A.T. Bell**

8:35 ENFL 503. Transition Metal (TM) promotion effects on the MoS₂ hydrodesulfurization nano-catalysts: First-principles studies. **P.H. Joo**, K. Yang

9:05 ENFL 504. Modeling out-of-equilibrium processes in energy materials. **M.K. Chan**

9:35 Intermission.

9:50 ENFL 505. Mesoscopic behavior of phase boundary migration in intercalation compounds for energy storage applications. K. Yang, L. Hong, Y. Zhang, **M. Tang**

10:20 ENFL 506. Effects of microstructure-sensitive gas diffusion on Cr poisoning in porous cathodes of solid oxide fuel cells. **W. Lyu**



TECHNICAL PROGRAM

10:50 ENFL 507. Origins and implications of interfacial capacitance enhancements in C₆₀-modified graphene supercapacitors. **T. Pham**, C. Zhan, M. Ceron, P. Campbell, V. Vedharathinam, M. Otani, D. Jiang, J. Biener, B. Wood, M. Biener

Section G

Orange County Convention Center
West Hall B4 - Theater 18

Emerging Materials for Renewable Energy

M. Hu, D. Liu, S. Nair, *Organizers*
Z. Li, M. Lu, *Organizers, Presiding*
Z. Zhou, *Presiding*

8:00 Introductory Remarks.

8:05 ENFL 508. Augmenting the photocurrent of CuWO₄ photoanodes by heat treatment in the nitrogen atmosphere. **A. Slabon**

8:30 ENFL 509. Visible-light-driven photocatalytic water splitting using CdS-TiO₂ coupled semiconductor dispersed on mesoporous SBA-15. **K. Thanabalasingam**, R.T. Koodali

8:55 ENFL 510. Correlating electron dynamics with photoelectrochemical efficiency in CuFeO₂ solar photocathodes. **E. Fugate**, S. Biswas, M. Clement, L. Baker

9:20 ENFL 511. Achieving the high phase purity in reduced-dimensional perovskite thin films by anti-solvent treatment. **C. Zhang**

9:45 Intermission.

10:00 ENFL 512. Frogspawn-coral-like hollow sodium sulfide nanostructured cathode for high-rate performance sodium-sulfur batteries. **C. Wang**, H. Wang, E. Matios, W. Li

10:25 ENFL 513. Atomically dispersed Mo-N/C as high performance sulfur host in Li-S battery. **f. ma**, Q. Li

10:50 ENFL 514. Controlled, temple-free fabrication of porous multilayered graphitic-like carbon nitride nanosheets doped with Pt and Cu for CO oxidation reaction under ambient conditions. K. Eid, M. H. Sliem, **A. Abdullah**

11:15 ENFL 515. Water-absorbable soft microcapsules-embedded heat transfer fluids for thermal energy storage and delivery. **T. Do**, U. Choi

Section H

Orange County Convention Center
West Hall B4 - Theater 19

Sustainable Energy Conversion via Innovative Electrocatalysis & Photocatalysis



TECHNICAL PROGRAM

Advanced Electrocatalyst for Fuel Cells

Y. Cheng, F. Jiao, *Organizers*
Y. Shao, G. Wu, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 ENFL 516. Gas-solid interactions by near-ambient pressure x-ray photoelectron spectroscopy: Challenges and approaches in characterization of complex electrocatalytic materials. **S. Pylypenko**

8:35 ENFL 517. Transmission electron microscopy investigation of structure-performance relation for electrocatalysis. **D. Su**

9:05 ENFL 518. Group IV metal oxynitride catalysts for polymer electrolyte fuel cells cathodes. **M. Chisaka**

9:35 ENFL 519. Ultrasmall structurally ordered PtM nanocrystals as efficient and robust oxygen reduction catalysts. **Q. Li, T. Wang, J. Liang**

10:05 Intermission.

10:10 ENFL 520. Nitrogen-doped graphene layers for electrochemical oxygen reduction reaction boosted by lattice strain. **Y. Song**

10:40 ENFL 521. Metal phthalocyanines to construct advanced single metal site electrocatalysts. **Y. Liang, Y. Wang**

11:10 ENFL 522. Molten salt mediated synthesis of highly active oxygen reduction electrocatalysts in acids. **K. Lu, Y. Cheng**

11:40 ENFL 523. Palladium-based antiperovskite as highly stable and efficient electrocatalysts for oxygen reduction in fuel cells. **S. Lee, I. Jang, P. Kim, S. Yoo**

Section I

Orange County Convention Center
West Hall B4 - Theater 20

Energy Storage in Chemical Bonds: Advances in Chemistry & Materials for Hydrogen Storage

T. Autrey, C. Yoon, *Organizers*
M. Jones, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 ENFL 524. Hydrogen production by formic acid dehydrogenation using iridium catalysts with pyridyl-pyrazole ligands. **Y. Himeda, N. Onishi, R. Kanega, E. Fujita**

8:25 ENFL 525. Modeling of thermodynamics and nucleation kinetics in the Mg-B-H system. **S. Kang, T. Heo, R. Shi, S. Bonev, T. Ogitsu, B. Wood**



TECHNICAL PROGRAM

8:45 ENFL 526. Role of additives on the H₂ storage properties of Mg(BH₄)₂. **N. Leick**, V. Stavila, K. Gross, M. Bowden, T. Gennett, S.T. Christensen

9:05 ENFL 527. Reversible hydrogen energy storage in Sc and Li decorated metal-BN-framework. **S. Kumar**, D. Thogluva Janardhanan

9:25 ENFL 528. Chemical approaches to fast, durable, high-capacity solid state hydrogen storage using organic/inorganic nanoscale interfaces. **J. Urban**

9:45 Intermission.

10:00 ENFL 529. Ionic liquid additives for lowering the melting point of magnesium borohydride. **R.T. Bell**, G. Russell-Parks, A. Huffer, S. Shulda, M.B. Martinez, P. Parilla, T. Gennett, B.G. Trewyn

10:20 ENFL 530. High-throughput study of metal dopants to improve the hydrogenation kinetics of MgB₂. H. Lefcochilos-Fogelquist, **L. Wan**, S. Kang, B. Wood

10:40 ENFL 531. Hydrogen chemi-sorption in condensed-phase frustrated Lewis acid-base pairs. **M. Bowden**, T. Autrey, M. Jones, B. Ginovska, T. Repo, A. Ramirez-Cuesta

11:00 ENFL 532. High-capacity organic hydrogen carriers based on biphenyl and diphenylmethane. **C. Yoon**, Y. Kim, Y. Jo, H. Jeong, H. Sohn, J. Han, S. Nam

11:20 ENFL 533. Electrolyte-assisted hydrogen storage reactions. J. Vajo, H. Tan, C. Ahn, D. Addison, S. Hwang, J. White, T. Wang, V. Stavila, **J.A. Graetz**

11:40 ENFL 534. Tracking the Mg(BH₄)₂/diglyme liquidus curve from room temperature to Mg(BH₄)₂-rich eutectic. **R.T. Bell**, G. Russell-Parks, A. Huffer, S. Shulda, M.B. Martinez, P. Parilla, B.G. Trewyn, T. Gennett

Elucidating the Roles of Electric Fields in Catalysis

Sponsored by CATL, Cosponsored by ENFL and PHYS

Activation of Light (C1-C4) Hydrocarbons: Theory & Experiments

Sponsored by CATL, Cosponsored by ENFL, ENVR, INOR and PHYS

Well-Defined Materials for Heterogeneous Catalysis: Synthesis, Characterization, & Performance Studies

Electrochemistry

Sponsored by CATL, Cosponsored by ENFL



TECHNICAL PROGRAM

Light-Driven Chemistry: Photoelectrochemistry & Photocatalysis

Sponsored by CATL, Cosponsored by COLL, ENFL, I&EC, INOR and PHYS

Chemical Catalysis for Bioenergy Consortium: Addressing Deactivation during Biomass Conversion

Sponsored by CATL, Cosponsored by ENFL, ENVR and INOR

WEDNESDAY AFTERNOON

Section A

Orange County Convention Center
West Hall B4 - Theater 12

Lower Alkane Activation & Conversion

H. Lin, Y. Yang, *Organizers*
Y. Dai, F. Huo, *Organizers, Presiding*

1:00 Introductory Remarks.

1:05 ENFL 535. Activity and selectivity of oxidative coupling of methane on doped La₂O₃ catalysts: A density functional theory study. Z. Wang, **X. Gong**

1:30 ENFL 536. Developing A₂B₂O₇ composite oxide catalysts for low temperature oxidative coupling of methane (OCM): on the relationship between the structure and reactivity. J. Xu, Y. Zhang, R. Xi, X. Xu, X. Fang, **X. Wang**

1:55 ENFL 537. Synthesis of ethanol from methane and water catalyzed by Ni-Cu/MoO₂. **Y. Wang**, Y. Wang, S. Wang, Q. Zhao, **C. Hu**

2:20 ENFL 538. High-temperature and pressure CH₄ partial oxidation catalysis over Ce- and Rh-promoted Ba_{0.75}NiAl₁₀O_{19-δ} catalysts: A structural and kinetic investigation. **T.H. Gardner**

2:45 Intermission.

3:00 ENFL 539. Designing a stable and efficient dual-functional catalyst for the sorption-enhanced steam reforming of glycerol. **Y. Hao**

3:25 ENFL 540. Simultaneous steam reforming of methane and CO water shift reaction on Ni/ZrO₂ catalyst. **Q. Zhao**, Y. Wang, S. Wang, G. Li, **C. Hu**

3:50 ENFL 541. Hydrogen production from the steam reforming of liquefied petroleum gas (LPG) over supported perovskites. **R. Pacheco Borges**, L. Gomes Moura, J.J. Spivey, F. Noronha, C. Hori



TECHNICAL PROGRAM

4:15 ENFL 542. Highly reactive Ni catalysts supported on Mg-Al oxides for efficient dry reforming of methane. **J. Huang**, Y. Yan, W. Liu, B. Liu

Section B

Orange County Convention Center
West Hall B4 - Theater 13

Innovative Chemistry & Materials for Electrochemical Energy Storage

Advanced Materials & Synthesis

Cosponsored by CATL, INOR and PMSE
B. Gallant, W. Luo, Y. Mo, H. Sun, *Organizers*
M. Doeff, Y. Li, L. Mai, *Presiding*

1:00 Introductory Remarks.

1:05 ENFL 543. Novel electrode structures made by freeze tapecasting. **M. Doeff**, E. Yi

1:30 ENFL 544. One-dimensional nanomaterials for emerging energy storage. **L. Mai**

1:55 ENFL 545. Controllable synthesis of multi-component metal oxide/graphene petal hybrid structure for energy storage system. **P. He**

2:10 ENFL 546. Layer-by-layer assembly of pillared MXene multilayers for high volumetric energy storage and beyond. **W. Tian**, A. VahidMohammadi, Z. Wang, L. Ouyang, M. Beidaghi, M. Hamed

2:25 ENFL 547. Blending ammonia in nitrogen: A facile synthesis strategy of nitrogen-doped carbon aerogels for electrochemical energy storage and catalysis. **T. Liu**, T. Kiu, J. Lu, G. Liu, Y. Li

2:40 ENFL 548. Facile preparation of hollow core-shell structure silicon/carbon anode by one-step magnesiothermic reduction. **J. Zhang**, Y. Chen, P. Yang, M. An, X. Chen

2:55 Intermission.

3:00 ENFL 549. Structural engineering of two-dimensional nanomaterials for electrochemical energy storage. **G. Yu**

3:25 ENFL 550. MOF-derived, nitrogen-doped ZnSe polyhedrons encapsulated by reduced graphene oxide as anode for lithium and sodium storage. X. Liu, **L. Fan**

3:50 ENFL 551. Promotion of co-production of ethylene and hydrogen by novel electrocatalysts via advanced electrochemical manufacturing processes at reduced temperatures. **D. Ding**, L. Wang, W. Wu

4:15 ENFL 552. Fluorescent thiazolothiazole viologen materials for energy storage: Photochemistry, electrochromism, and photoluminescence. A. Woodward, N. Sayresmith, J. Sailer, K. Sandor, **M.G. Walter**

4:30 ENFL 553. Real-time insight into the doping mechanism of redox-active organic radical polymers. **S. Wang**, F. Li, A. Easley, J.L. Lutkenhaus



TECHNICAL PROGRAM

4:45 ENFL 554. Poly(fluorene-*alt*-naphthalene diimide) energy storage electrodes. **K. Sarang**, A. Miranda, H. An, R. Verduzco, E. Oh, J.L. Lutkenhaus

Section C

Orange County Convention Center
West Hall B4 - Theater 14

Advanced Functional Materials in Harsh Conditions for Environmental & Energy Applications

S. Chang, S. Zhu, *Organizers*
H. Ow, W. Wang, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 ENFL 555. Nanoparticles under high pressure: Stability and formation of active nanostructures. **H. Fan**

2:05 ENFL 556. Evaluation of polymeric membranes for high pressure sour gas separations. **D.J. Harrigan**, B.J. Sundell, J. Yang, J.A. Lawrence, J. O'Brien, M.L. Ostraat

2:25 ENFL 557. Incorporating cathode materials into polymeric separator for lithium-ion batteries: Beyond additional capacity. **W. He**

2:45 ENFL 558. Fabrication of durable oxygen reduction electrodes with carbon nanotubes for proton exchange membrane fuel cell. **D. Lee**

3:05 Intermission.

3:20 ENFL 559. Core-shell structured TiO₂ as highly efficient photocatalyst for dye degradation under visible light. **Y. Lin**, H. Hu, Y.H. Hu

3:40 ENFL 560. Development of a dual, ionic, liquid-based electrolyte system for space exploration at extremely low temperatures. **Y. Xu**, W. Lin, M. Gliege, Z. Zhao, H. Yu, L. Dai

4:00 ENFL 561. Surface-Enhanced Raman Scattering (SERS) composite nanoparticles for dipicolinic acid detection. **S. Chang**, E. Shen, H. Ow, W. Wang

4:20 ENFL 562. Use of silanized fly ash as a low-cost coating agent to make water-wet surfaces highly hydrophobic. **J. Ok**, J. Jeong, D. Lee, C. Huh, H. Cho

4:40 ENFL 563. Controllable asymmetric functionalization of graphene oxide nanosheets in mass quantity. **W. Wang**, S. Chang

Section D

Orange County Convention Center
West Hall B4 - Theater 15

New Frontiers in Petroleum Characterization, Transportation, Processing, Refining & Advanced Materials



TECHNICAL PROGRAM

Characterization & Asphaltene Issues

C. F. Ovalles, P. Rahimi, *Organizers*
J. J. Adams, Y. Zhang, *Organizers, Presiding*

1:00 Introductory Remarks.

1:30 ENFL 564. Model compound study for the SAR-AD: Interpreting the SAR-AD fingerprint of different hydrocarbon liquids. **J.J. Adams**, J. Huo, J. Loveridge, N. Bolton

1:55 ENFL 565. Synchrotron X-ray Absorption Spectroscopy (XAS) characterisation of iron, vanadium, and nickel on FCC catalysts. Q. Zhou, B. Dai, Q. Liu, F. Ren, Y. Zhu, B. Etschmann, **L. Zhang**

2:20 ENFL 566. FT-ICR characterization of crude oil fractions obtained using n-pentane. **E. Rogel**, M. Witt

2:45 Intermission.

2:55 ENFL 567. Adsorption of long alkanes onto graphene, graphite, and asphaltenes. **E. Rogel**

3:20 ENFL 568. Advances in asphaltene petroleomics: Determining the role of heteroatoms in asphaltene chemistry. **M.L. Chacon**, D.F. Smith, J.C. Putman, A.M. McKenna, Y.E. Corilo, C.L. Hendrickson, A.G. Marshall, R.P. Rodgers

3:45 ENFL 569. Investigating the role of O-H functional groups in emulsion-stabilizing asphaltenes. **J.J. Adams**, S. Arulsamy, A. Sawaya, N. Bolton, J. Loveridge

4:10 ENFL 570. Mechanistic understanding of petroleum asphaltene conversion. **Y. Zhang**

4:35 ENFL 571. Evaluating the impact of process conditions on asphaltenes formation during visbreaking of vacuum residue deasphalted oil. **Y. Yan**, A. De Klerk, G.H. Prado

Section E

Orange County Convention Center
West Hall B4 - Theater 16

Energy Materials in Fuel Conversion & Utilization

L. Fan, L. Qin, *Organizers, Presiding*

1:00 Introductory Remarks.

1:05 ENFL 572. Framework for predicting ionic and electronic conductivity in disordered, mixed conducting perovskites. **E. Ertekin**

1:30 ENFL 573. Syngas production by CO₂ reforming of methane over iron-titanium composite oxygen carrier in a cyclic redox mode. **Z. Cheng**, D. Baser, L. Qin, S. Nadgouda, J. Fan, L. Fan



TECHNICAL PROGRAM

2:10 ENFL 574. Investigation on the electrical conductivity and microstructure of PLD-grown ScSZ/GDC bilayer electrolyte. **Y. Liu**, S. An, C. Cai, S. Li

2:35 ENFL 575. Cellulose nanocrystals as proton conductive filler and its composite membrane for DMFC. **S.S. Gaur**, P. Dhar, A. Kumar, **V. Katiyar**

3:00 Intermission.

3:15 ENFL 576. Redox oxygen transfer materials for carbon capture, hydrogen, and other interesting applications. **S. Scott**

3:55 ENFL 577. Defects engineering of 2D-TaS₂ and 2D-MoS₂: A route toward highly efficient CO hydrogenation and CO₂ reduction reactions. **M.M. Vaida**

4:20 ENFL 578. Nano-tailoring of infiltrated catalysts for high-temperature solid oxide regenerative fuel cells. **K. Yoon**

4:45 Concluding Remarks.

Section F

Orange County Convention Center
West Hall B4 - Theater 17

Simulations of Materials & Processes for Energy Applications

Y. Liu, D. Lu, Y. Ping, H. Zhuang, *Organizers*
B. Wood, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 ENFL 579. Statistical learning for small data materials challenges: Solid lithium-ion conductors for batteries. **E. Reed**

1:35 ENFL 580. High-throughput screening of Pb-free hybrid halide compounds for optoelectronic applications. **Y. Li**, K. Yang

2:05 ENFL 581. First-principles density functional theory modeling and machine learning approach for redox potential of carbon materials. **S. Jang**

2:35 Intermission.

2:50 ENFL 582. Oxygen off-stoichiometry and defect entropies in solar thermochemical water splitting materials. **C. Wolverton**

3:20 ENFL 583. Simple method to locate the optimal adsorption energy for the best catalyst directly. **J. Chen**, Y. Mao, H.F. Wang, P. Hu

3:50 ENFL 584. Properties of interfaces in all-solid-state rechargeable alkali-ion batteries. **S. Ong**



TECHNICAL PROGRAM

Section G

Orange County Convention Center
West Hall B4 - Theater 18

ENFL Distinguished Researcher Award: Symposium in Honor of Anne Gaffney

J. D. Allison, H. Lin, *Organizers*
M. M. Bhasin, F. Li, *Organizers, Presiding*

1:00 Introductory Remarks.

1:10 ENFL 585. Development and evaluation of supported Ir@Pt bimetallic catalysts for high temperature decomposition of SO₃ to SO₂ in the HyS process for thermochemical generation of H₂ and O₂ from H₂O. **J.R. Monnier**, W. Diao, J. Tengco, J.R. Regalbuto, D.M. Ginosar, B. Adhikari, C. Corgnale

1:35 ENFL 586. Probing the organization, transport, and adsorption behavior of confined light gases and heavy hydrocarbons for sustainable energy recovery. **G. Gadikota**, S. Mohammed, M. Liu

2:00 ENFL 587. Towards sustainable chemical manufacturing by creating synergy between CO₂ utilization and biorefinery. **H. Lin**

2:25 ENFL 588. From chemistry to interfaces and back. **A. Ulman**

2:50 Intermission.

3:10 ENFL 589. Pushing the limits of charge enhanced dry impregnation for supported metal catalyst preparation. S. Eskandari, L.T. De Castro, F. Rahman, J. Lipp, A. Dong, **J.R. Regalbuto**

3:35 ENFL 590. Use of zeta potential measurements in catalyst characterization. **S. Soled**, S. Miseo, W.A. Wachter

4:00 ENFL 591. Multiphase microreactors with in-situ spectroscopy as a gateway to process intensification in energy and fuels. **R.L. Hartman**

4:25 ENFL 592. Adsorbents for selectively removing H₂S from CO₂-containing gas streams. **X. Wang**, C. Song

Section H

Orange County Convention Center
West Hall B4 - Theater 19

Sustainable Energy Conversion via Innovative Electrocatalysis & Photocatalysis

Oxygen Reduction & Evolution Electrocatalysts

F. Jiao, G. Wu, *Organizers*
Y. Cheng, Y. Shao, *Organizers, Presiding*



TECHNICAL PROGRAM

1:00 Introductory Remarks.

1:05 ENFL 593. Well-defined surfaces show how Ti addition to IrO₂ and RuO₂ modifies oxygen electro-adsorption and oxygen evolution electrocatalysis. D. Kuo, H. Paik, J. Nelson, K. Shen, D. Schlom, **J. Suntivich**

1:35 ENFL 594. Interface engineering for efficient electrocatalysts. **G. Zou**

2:05 ENFL 595. Tungsten, cobalt, and iron ternary metal oxide as a carbon-free cathode catalyst for Li-O₂ batteries. **R. Yang**, X. Cao, Z. Sun, K. Zeng, X. Zheng

2:35 ENFL 596. Vertically aligned carbon nanofibers with reduced Pt loading as a highly active and methanol tolerant oxygen reduction electrocatalyst. **A. Elangovan**, J. Li

2:55 ENFL 597. Stable potential window of gamma-MnO₂ for water oxidation in acidic electrolyte for more than 6000 hours. **H. Han**

3:15 Intermission.

3:20 ENFL 598. Towards understanding the electrified RuO₂ water interface for the oxygen evolution reaction. **R.R. Rao**, Y. Shao-Horn

3:40 ENFL 599. Computational discovery of highly active and stable OER catalysts with unusual metal-ligand coordination. **M. Bajdich**

4:00 ENFL 600. Substitution strategy in designing spinel oxides for water oxidation. Y. Duan, S. Sun, Y. Sun, **Z.J. Xu**

4:20 ENFL 601. Direct observation of active catalyst redox states and the effect of dynamically increased crystallinity on efficient alkaline water splitting. **Z. Qiu**, T. Edvinsson

4:40 ENFL 602. Homogeneous cobalt and iron oxide hollow nanocages: Fe incorporation-dependent structural and electronic modulation for enhanced water oxidation. **X. Ren**, Q. Wang, X. Zhang

Section I

Orange County Convention Center
West Hall B4 - Theater 20

Energy Storage in Chemical Bonds: Advances in Chemistry & Materials for Hydrogen Storage

T. Autrey, M. Jones, *Organizers*
C. Yoon, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 ENFL 603. Transparent, mixed proton/electron conducting Nafion-PEDOT:PSS composite for tandem microwire array solar water splitting devices. **H.J. Fu**, S. Ardo, N.S. Lewis

1:25 ENFL 604. Synthesis of dendrimer-encapsulated nanoparticles via repetitively coupled chemical reduction and galvanic exchange for catalytic dehydrogenation of hydrogen storage compounds. **J. Kim**, T. Cho, C. Yoon



TECHNICAL PROGRAM

1:45 ENFL 605. Novel low temperature thermochemical heat storage system. **A. Dwivedi**, M.C. Rajagopal, S. Ganguly, B. Sharma, N. Rajagopalan, S. Sinha

2:05 ENFL 606. ‘On demand’ hydrogen release via an opto-thermal process. **E.A. Gaulding**, S.T. Christensen, N. Leick, J. Urban, T. Gennett

2:25 Intermission.

2:40 ENFL 607. Hydrogen sorption in fluorinated organic frameworks. **W.A. Braunecker**, M.B. Martinez, K.E. Hurst, S. Shulda, J.T. Koubek, A. Sellinger, T. Gennett, J.C. Johnson

3:00 ENFL 608. Assessment of the performance of density functionals for hydrogen storage in sorbents. **S. Veccham Krishna Prasad**, M.P. Head-Gordon

3:20 ENFL 609. Sustainable hydrogen storage in polyalcohols enabled by metal-organic framework catalysts. **V. Stavila**, L. Klebanoff, J. Su, G.A. Somorjai, D. Prendergast, T. Autrey, M. Allendorf

3:40 Intermission.

3:55 ENFL 610. First-principles study of hydrogen storage in Li- and Ca-decorated MOF designed with graphyne linker. S. Kumar, **D. Thogluva Janardhanan**

4:15 ENFL 611. Edge-functionalized graphene nanoribbon encapsulation to enhance stability and control kinetics of hydrogen storage materials. L. Wan, E. Cho, T. Marangoni, P. Shea, S. Kang, C. Rogers, E.W. Zaia, R. Cloke, B. Wood, F.R. Fischer, J. Urban, **D. Prendergast**

4:35 ENFL 612. Sustainable approach towards the fabrication of tunable graphene nanoscrolls and its application for energy storage. **P. Dhar**, **S.S. Gaur**, A. Kumar, **V. Katiyar**

Activation of Light (C1-C4) Hydrocarbons: Theory & Experiments

Sponsored by CATL, Cosponsored by ENFL, ENVR, INOR and PHYS

Light-Driven Chemistry: Photoelectrochemistry & Photocatalysis

Sponsored by CATL, Cosponsored by COLL, ENFL, I&EC, INOR and PHYS

Well-Defined Materials for Heterogeneous Catalysis: Synthesis, Characterization, & Performance Studies

Electrochemistry

Sponsored by CATL, Cosponsored by ENFL



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

Chemical Catalysis for Bioenergy Consortium: Addressing Deactivation during Biomass Conversion

Sponsored by CATL, Cosponsored by ENFL, ENVR and INOR

THURSDAY MORNING

Section A

Orange County Convention Center
West Hall B4 - Theater 12

Lower Alkane Activation & Conversion

F. Huo, H. Lin, *Organizers*
Y. Dai, Y. Yang, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 ENFL 613. Recent progress on anode materials for non-hydrogen solid oxide fuel cells. **Y. Li**

8:30 ENFL 614. Ordered mesoporous carbon confined gold nanocatalyst. X. Mu, **Y. Wan**

8:55 ENFL 615. Functional metal-organic frameworks for selective catalysis. **W. Zhang**, F. Huo

9:20 ENFL 616. Metal-organic framework nanocomposite materials. **F. Huo**

9:45 Intermission.

10:00 ENFL 617. Effect of competitive adsorption between methane and CO₂ on the activity of low temperature dry reforming of methane over Ni/ZrO₂ catalyst. **Y. Wang**, S. Wang, Q. Zhao, Y. Wang, C. Cui, **C. Hu**

10:25 ENFL 618. Preparation of highly efficient nanocatalysts and catalytic systems. **C. Cao**, W. Song

10:50 ENFL 619. Improved visible-light activities of rutile nanorod by co-modifying highly-dispersed SPR Au nanoparticles and HF groups for aerobic selective alcohol oxidation. **B. LINLU**

11:15 ENFL 620. Reaction pathways and mechanisms of nitrogen during the process of microalgae hydrothermal liquefaction. Y. Shao, **T. Bao**

11:40 Concluding Remarks.

Section B

Orange County Convention Center
West Hall B4 - Theater 13



TECHNICAL PROGRAM

Innovative Chemistry & Materials for Electrochemical Energy Storage

General

Cosponsored by CATL, INOR and PMSE
B. Gallant, Y. Mo, H. Sun, *Organizers*
W. Luo, *Organizer, Presiding*
L. Fan, *Presiding*

8:00 Introductory Remarks.

8:05 ENFL 621. Multi-walled carbon nanotubes as conductive additive in $\text{Li}_4\text{Ti}_5\text{O}_{12}$ micro/nanofibers by coaxial electrospinning as potential anodes in Li Ion batteries. **S. Montoya Bedoya, L. Sabogal Moncada, D. Echeverri Tamayo, N. Castaño Villa, E. García Tamayo, H. Martínez Tejada**

8:25 ENFL 622. Studies on ionic conductivity, structural and thermal behaviour of PVdF-HFP based ionic liquid gel polymer electrolyte. **M.Z. Dzulkpli, J. Karim, M. Suait, S. Mohd Noor, A. Ahmad, N. Hassan**

8:45 ENFL 623. Advanced electrolyte materials for high voltage lithium batteries. **G. Cui**

9:05 ENFL 624. Integration of lithium-rich, anti-perovskite electrolyte with cathode material. **J. Swanson, M. Dondelinger, G. Nasymov, C. Jahnke, A. Lannerd, A. Smirnova**

9:25 ENFL 625. Fundamentals of lithium and carbon substrates. **W. Luo**

9:45 Intermission.

10:00 ENFL 626. *In-situ* x-ray absorption spectroscopic investigation of the capacity degradation mechanism in Mg/S batteries. **Y. Xu**

10:20 ENFL 627. Dendrite-free Na metal plating/stripping onto 3D porous Cu hosts. **T. Wang, L. Fan**

10:40 ENFL 628. Achieving high-loading Si anode via employing triblock copolymer elastomer binder, metal nanowires, and a laminated conductive structure. **D. Wei, J. Mao**

11:00 ENFL 629. Surface-modified SiNPs applied as anode materials in lithium-ion battery. **S. Jiang**

Section C

Orange County Convention Center
West Hall B4 - Theater 14

Advanced Functional Materials in Harsh Conditions for Environmental & Energy Applications

H. Ow, W. Wang, *Organizers*
S. Chang, S. Zhu, *Organizers, Presiding*

8:00 Introductory Remarks.



TECHNICAL PROGRAM

8:05 ENFL 630. Flexible C-C bonded network polymers for high-density methane storage. **C.T. Yavuz**, V. Rozyyev, D. Thirion

8:55 ENFL 631. Stability of fluorescent carbon nanoparticles: Effect of solvent, temperature, and salinity. **A. Jalilov**

9:15 ENFL 632. Aramid nanofiber separators for energy storage application. **A. Patel**, K. Wilcox, I. George, R. Juneja, J.L. Lutkenhaus

9:35 Intermission.

9:50 ENFL 633. Bromate oxidation of ammonium salts under harsh reservoir temperatures for strategic acid placement. **K.L. Hull**, A.J. Cairns, M. Haq

10:10 ENFL 634. Fly ash nanoparticle-stabilized dry foams as fracturing fluids. **J. Jeong**, H. Cho, C. Huh, J. Ok

10:30 ENFL 635. Synthesis and evaluation of dipicolinic acid (DPA)-based interwell tracers for reservoir surveillance. **R. Shi**, G. Thomas, S. Chang, H. Ow

10:50 ENFL 636. Novel NiP-TiNi nanocomposite coatings for harsh oil and gas environments made by the electroless technology. **M.K. Hassan**, E.M. Fayyad, A.M. Abdullah, A. Mohamed, G. Jarjoura, Z. Farhat

11:10 Concluding Remarks.

Section D

Orange County Convention Center
West Hall B4 - Theater 15

New Frontiers in Petroleum Characterization, Transportation, Processing, Refining & Advanced Materials

Upgrading & Conversion

J. J. Adams, C. F. Ovalles, *Organizers*
P. Rahimi, Y. Zhang, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 ENFL 637. Partial upgrading: A closer reality for Canadian heavy oil producers. **P. Rahimi**

8:30 ENFL 638. Predicting coke morphology in delayed coking from feed characteristics. **C.F. Ovalles**, E. Rogel, M. Moir, P. Hajdu, T. Rea, K. Chaudhuri, K. Hench, D. Fuller

8:55 ENFL 639. Effect of chemical composition of coal tar pitches on mesophase formation and structure. **J.J. Adams**, K. Baig, S. Bassham, J. Loveridge

9:20 ENFL 640. Alternative technologies for olefin treatment in thermally cracked naphtha: Use of phosphoric acid. **S. Fong**, N. Montoya Sánchez, A. De Klerk



TECHNICAL PROGRAM

9:45 Intermission.

10:00 ENFL 641. Diesel engine combustion of military jet fuel: Fuel characterization and military fuel standards. **D.J. Luning Prak**, R. Gober, J. Fries, J. Cowart, P.C. Trulove

10:25 ENFL 642. Calorimetric adsorption study of light hydrocarbons on functionalized UiO-66 MOF. **T. Barrett**, M.D. Gross

10:50 ENFL 643. *N*-dodecane hydroisomerization over hierarchical ZSM-22 prepared by a dual-protected alkali treatment. **W. Xiangyu**, Q. Wang, X. Zhang, L. Wang

11:15 Concluding Remarks.

Section E

Orange County Convention Center
West Hall B4 - Theater 16

Energy Materials in Fuel Conversion & Utilization

L. Fan, L. Qin, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 ENFL 644. Enhancing the performance of partial oxidation of gasoline over Ni catalysts with Mo addition for SOFCs application: An experimental and DFT study. **Q. Bkour**, F. Che, J. McEwen, M. Norton, S. Ha

8:30 ENFL 645. Perovskite oxides for redox oxidative cracking of *n*-hexane. **F. Li**

9:10 ENFL 646. Biosilica from cultured diatom and its composite with Iron oxide for supercapacitors electrodes. **E. Karaman**, S. Mitra, Z. Wang

9:35 ENFL 647. Octane-on-demand: Onboard separation of oxygenates from gasoline. **J. Bays**, K. Grubel, W. Chouyyok, D.J. Heldebrant, J.C. Linehan

10:00 Intermission.

10:15 ENFL 648. CO₂ capture and conversion: Materials, activity, and stability. **C. Muller**, P. Abdala Macarena, A. Fedorov

10:55 ENFL 649. Investigation of the effect of surface and bulk properties of alkali salt@perovskite core-shell redox catalysts for CL-ODH of ethane. **Y. Gao**, F. Li

11:20 ENFL 650. Thermochemical gasification of biomass using chemical looping. **D. Xu**, Y. Zhang, T. Hsieh, M. Guo, C. Wang, E. Falascino, A. Tong, L. Fan

11:45 Concluding Remarks.



TECHNICAL PROGRAM

Section F

Orange County Convention Center
West Hall B4 - Theater 17

Simulations of Materials & Processes for Energy Applications

Y. Liu, D. Lu, Y. Ping, B. Wood, *Organizers*
H. Zhuang, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 ENFL 651. Understanding pseudocapacitive energy storage. **D. Jiang**

8:35 ENFL 652. Machine learning-assisted coarse-grained molecular dynamics for designing highly conductive polymer electrolytes. **Y. Wang**, T. Xie, A. France-Lanord, A. Berkley, J.A. Johnson, Y. Shao-Horn, J.C. Grossman

9:05 ENFL 653. Exploring electrochemical reaction dynamics of Li⁺-solvation structures with large-scale quantum mechanical simulations. **B.M. Wong**, J. Guo, C. Fu, L. Xu, F.W. Aquino

9:35 Intermission.

9:50 ENFL 654. High-throughput computational design of lead-free organic-inorganic halide compounds for optoelectronics. **K. Yang**, Y. Li

10:20 ENFL 655. Metal closo-borates as solid-state electrolytes. **Z. Lodziana**, R. Moury, H. Hagemann, A. Remhof, R. Cerny

10:50 ENFL 656. Fundamental studies of the bulk, surface, and tritium diffusivity properties in defective γ -LiAlO₂ pellets used in TPBAR. H.P. Paudel, Y. Lee, T. Jia, **Y. Duan**

Section G

Orange County Convention Center
West Hall B4 - Theater 18

ENFL Distinguished Researcher Award: Symposium in Honor of Anne Gaffney

M. M. Bhasin, F. Li, *Organizers*
J. D. Allison, H. Lin, *Organizers, Presiding*

8:00 Introductory Remarks.

8:10 ENFL 657. Innovation in mature technology spaces. **C.L. Tway**

8:35 ENFL 658. Robust supported metal catalysts for hydrocarbon conversions. **Y. Wang**



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

9:00 ENFL 659. Advances in hydrogen addition and carbon rejection routes to upgrading heavy, polyaromatic oil fractions. **M.P. Kaminsky**, O.S. Ali, S.C. Hayden, K.M. Shaik, L. Ding, E. Al-Sayed, W. Xu, S. Shaikh

9:25 ENFL 660. Mixed-metal oxide catalyst development for selective oxidation and ammoxidation of light hydrocarbons. **D.J. Buttrey**

9:50 Intermission.

10:05 ENFL 661. Catalytic ethane dehydroaromatization under microwave irradiation. **J. Hu**

10:30 ENFL 662. Ethane Oxydehydrogenation (EODH): Status and challenges. **M.M. Bhasin**

10:55 ENFL 663. Chemical looping oxidative dehydrogenation: Redox catalyst design, mechanism, and process evaluations. **F. Li**

11:20 ENFL 664. Selective catalytic routes for light hydrocarbon upgrading. **A.M. Gaffney**

Section H

Orange County Convention Center
West Hall B4 - Theater 19

Sustainable Energy Conversion via Innovative Electrocatalysis & Photocatalysis

Water Splitting & Photocatalysis

F. Jiao, G. Wu, *Organizers*
Y. Cheng, Y. Shao, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 ENFL 665. Atomically dispersed hybrid sites for photoelectrocatalysis. **C. Cui**

8:35 ENFL 666. Design and synthesis of novel perylenemonoimide dyes for solar energy conversion devices. **A. Curtze**, Y. Wu

9:00 ENFL 667. Understanding photoelectrocatalysis on epitaxial oxide surfaces. **K.A. Stoerzinger**, L. Wang, Y. Ye, M. Bowden, E.J. Crumlin, Y. Du, S. Chambers

9:20 ENFL 668. Transition-metal phosphides as efficient electrocatalysts for water electrolysis. **S. Chen**

9:40 ENFL 669. Unifying the HER/HOR kinetics in base by identifying the catalytic roles of hydroxyl-water-cation adducts. **Q. Jia**, E. Liu, J. Li, J. Li, S. Mukerjee, Y. Huang

10:00 Intermission.

10:05 ENFL 670. Two-dimensional metal carbide (MXene) electrocatalysts with active basal planes for hydrogen evolution. **Z. Seh**



TECHNICAL PROGRAM

10:25 ENFL 671. Localized surface plasmons and hot carriers in aluminium nanoclusters. **A. Goebel**, J. Lischner, A. Rubio

10:45 ENFL 672. Bioinspired approaches for solar light-driven water splitting. **S. Luber**, M. Schilling

11:05 ENFL 673. Coupling surface science, electrochemistry, and computation to quantify electrocatalytic structure-property relationships. **D. Kauffman**, X. Deng, D. Sorescu

11:25 ENFL 674. Hydrogen production from sugar beet wastewater in the presence of perovskite type catalysts by photocatalysis. **A. Yuksel Ozsen**, C. Orak

11:45 ENFL 675. Improved photo-electrochemical properties of strained SnO₂. **Z. Kerrami**

Well-Defined Materials for Heterogeneous Catalysis: Synthesis, Characterization, & Performance Studies

Selectivity

Sponsored by CATL, Cosponsored by ENFL

Chemical Catalysis for Bioenergy Consortium: Addressing Deactivation during Biomass Conversion

Sponsored by CATL, Cosponsored by ENFL, ENVR and INOR

Elucidation of Mechanisms & Kinetics on Surfaces

Sponsored by CATL, Cosponsored by ENFL, ENVR, INOR and PHYS

THURSDAY AFTERNOON

Well-Defined Materials for Heterogeneous Catalysis: Synthesis, Characterization, & Performance Studies

Characterization

Sponsored by CATL, Cosponsored by ENFL

Activation of Light (C1-C4) Hydrocarbons: Theory & Experiments

Sponsored by CATL, Cosponsored by ENFL, ENVR, INOR and PHYS



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

Elucidation of Mechanisms & Kinetics on Surfaces

Sponsored by CATL, Cosponsored by ENFL, ENVR, INOR and PHYS

ENVR

Division of Environmental Chemistry

S. Obare, *Program Chair*

SUNDAY MORNING

Section A

Orange County Convention Center
Valencia Ballroom B-D - Theater 9

Abiotic & Biotic Pollutant Transformation in Soils

G. Chen, H. Cheng *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 ENVR 1. Back conversion from product to parent: Methyl triclosan to triclosan in soil, earthworms, and plants. X. Du, Q. Fu, J. Gan

8:35 ENVR 2. Reduction of nitro explosives RDX and NTO by iron-bearing minerals: A study on the kinetics and using compound specific isotope analysis to assess mechanisms. Y. Tong, J.H. Strehlau, B. Ulrich, J. Bolotin, T.B. Hofstetter, W. Arnold

8:55 ENVR 3. Compound specific isotope analysis of nitroaromatic compounds during reaction with Fe-bearing minerals. M.J. Berens, B. Ulrich, J.H. Strehlau, T.B. Hofstetter, W. Arnold

9:15 ENVR 4. Determine mechanistic causes for antagonism in PAH mixture degradation in mycobacterium species. X. Liu

9:35 ENVR 5. Destruction and transformation of pyrene by mineral surfaces during thermal desorption. C. Oden, C.J. Werth, L.E. Katz

9:55 Intermission.



TECHNICAL PROGRAM

10:10 ENVR 6. Effects of compositions and chemical structures of sedimentary organic matter on mineralization efficiency of benzo(a)pyrene by hydrogen peroxide. **Y. Ran**, C. Zhuo, D. Zhang, Y. Yang

10:30 ENVR 7. Preferential molecular fractionation of dissolved organic matter by iron minerals with different oxidation states. **K. Sun**, Z. Zhang, L. Han, Y. Wang

10:50 ENVR 8. Abiotic dechlorination of chlorinated solvents by iron(II) in fractured rocks. **A. Haluska**, P. Grathwohl

11:10 ENVR 9. Simulation of intermediate accumulation during trichloroethene dechlorination in a H₂-based biofilm. **B. Wang**, R. Krajmalnik-Brown, C. Zhou, Y. Luo, B.E. Rittmann, Y. Tang

11:30 ENVR 10. Pentachlorophenol removal pathways in thermal conduction heating-soil vapor extraction (TCH-SVE). **J. Davis**, H. Liljestrand, L.E. Katz

Section B

Orange County Convention Center
Valencia Ballroom B-D - Theater 10

Polymer Degradation Processes in Environmental Systems

K. P. McNeill, M. Sander, *Organizers, Presiding*

8:15 Introductory Remarks.

8:20 ENVR 11. Degradation of polymeric organics in domestic wastewater using iron-activated persulfate. **H. Vu**, C.J. Miller, D. Waite

8:40 ENVR 12. Polyacrylamide degradation by mesophilic anaerobic digestion. **M. Akbar**, H. Wang, M. Khan

9:00 ENVR 13. What happens to microplastics when they enter the sea: A two week characterization study. **E. McGivney**, L. Cedarholm, M. Ogonowski, A. Barth, M. Hakkarainen, E. Hamacher-Barth, A. Motiei, E. Gorokhova

9:20 ENVR 14. Evaluation of biodegradability and biodegradation control by reductive stimuli of polyesters. **Y. Tachibana**, T. Baba, S. Suda, K. Kageyama, K. Kasuya

9:40 ENVR 15. Hydrolysis by extracellular enzymes and its importance for the biodegradation of polyesters in the environment. **M.T. Zumstein**, H. Kohler, K.P. McNeill, M. Sander

10:00 Intermission.

10:15 ENVR 16. Evaluating polymer photodegradation processes in environmental systems. **R.G. Zepp**, B. Acrey, D.C. Bouchard, A. Andrady, A. Commodore, O. Okungbowa, M. Davis

10:35 ENVR 17. Using stable carbon isotope labeling to study the biodegradation of synthetic polymers in agricultural soils. **T. Nelson**, R. Baumgartner, H. Kohler, K.P. McNeill, M. Sander

10:55 ENVR 18. Photochemical reactivity of dissolved organic matter in the St. Louis River and implications for contaminant fate. **S.M. Berg**, J.A. Herrli, Q.T. Whiting, R. Winkels, K.H. Wammer, C.K. Remucal



TECHNICAL PROGRAM

11:15 ENVR 19. Nano-FTIR spectroscopy: Nanoscale resolved infrared spectroscopy of self-assembled monolayers. **T. Gokus**, S. Mastel, A. Huber

11:35 ENVR 20. Effect of environmental factors such as pH on the hydrolytic degradation of aliphatic polyesters. R. Vaid, M.W. King, **M.A. Pasquinelli**

11:55 Closing Remarks.

Section C

Orange County Convention Center
Valencia Ballroom B-D - Theater 8

Contributions of a Simple Chemist: How Professor Ronald Atlee Hites Changed Environmental Chemistry

Cosponsored by PROF†
E. T. Furlong, S. T. Glassmeyer, S. L. Simonich, *Organizers*
E. M. Ulrich, M. Venier, *Organizers, Presiding*
A. Salamova, *Presiding*

8:30 Introductory Remarks.

8:35 ENVR 21. Pedagogic Legacy of Professor Ronald A. Hites. **S.T. Glassmeyer**, E.T. Furlong, E.M. Ulrich

8:55 ENVR 22. Portable chromatography for environmental analysis. **M.L. Lee**, X. Xie, L. Patil, A. Ghosh, L. Tolley, D. Tolley

9:15 ENVR 23. My amazing learning experience as a Ph.D. student in Professor Hites' Lab at MIT in the mid 70's. **V. Lopez-Avila**

9:35 ENVR 24. Dissolved organic matter characterization along a river continuum: Composition control based on ecological concepts vs. watershed land use. **R. Jaffe**

9:55 Intermission.

10:30 ENVR 25. I'm just a simple chemist: The environmental mass spectrometry contributions of Professor Ronald Atlee Hites. **E.T. Furlong**, R. Jaffe, D. Swackhamer

11:00 ENVR 26. Simple chemistry: Tracking honey bee pesticide exposure at ornamental nurseries. **B.D. Eitzer**, R. Cowles, K. Stoner, A. Nurse

11:20 ENVR 27. Everything I ever needed to know about PAHs I learned from Ron Hites. **S. Simonich**

11:40 ENVR 28. Dissolved organic matter alterations by permanganate during drinking water treatment. **J.R. Laszakovits**, A.A. MacKay

Section D

Orange County Convention Center
Valencia Ballroom B-D - Theater 12



TECHNICAL PROGRAM

Nanotechnology at the Water-Agriculture-Energy Nexus

A. A. Keller, G. Lowry, C. Sabilov, J. C. White, Y. Yang, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 ENVR 29. Cu-based nanoparticles for sustainable agriculture: toward a molecular-level understanding of how CuO and Cu₃(PO₄)₂ nanoparticles influence plant growth and susceptibility to disease.. **R.J. Hamers**, J.C. White, C.L. Haynes, W. Elmer, J. Borgatta, C. Ma

8:25 ENVR 30. Improving plant stress tolerance and resource use through chloroplast nanobiotechnology. H. Wu, P. Hu, I. Santana, J. An, G.M. Newkirk, **J. Giraldo**

8:45 ENVR 31. Effects of polymeric nanoparticles on plant health. **C.E. Astete**, S.M. Navarro, H. Waldvogel, S. Sondh, J.A. Davis, C. Sabilov

9:05 ENVR 32. Advanced environmentally-friendly crop protection chemicals for agricultural sustainability. M. Young, A. Ozcan, P. Rajasekaran, A. Strayer-Scherer, Y. Liao, M. Myers, E. Johnson, J. Graham, J. Jones, M. Paret, **S. Santra**

9:25 ENVR 33. Engineered nanomaterials for the suppression of fungal and viral crop disease. **J.C. White**, C. Ma, R.J. Hamers

9:45 ENVR 34. Carbon Nanoparticles Reduce Nitrate Leaching Through Soil and Improve Yield of Lettuce (*Lactuca sativa*). **P.K. Westerhoff**, M. Pandorf

10:05 Intermission.

10:20 ENVR 35. Nano-polymer-urea composite for improved fertilizer applications: study of their effect on soil enzymatic activities and microflora dynamics in N-cycle of potato (*Solanum tuberosum* L.). K. Rohini, A. Kalia, S. Sharma, Y. Vikal, K. Luthra, G. Dheri, **C.L. Gomes**

10:40 ENVR 36. Combining molecular recognition and nanotechnology: Towards smart fertilizers. **M.C. Derosa**, C. Monreal

11:00 ENVR 37. CuO NPs improve plant health in high pH (calcareous) soils by affecting microbiome structure, network, and nitrogen-related functions. **X. Gao**, X. Guan, A. Avellan, E. Spielman-Sun, E. Casman, G. Lowry

11:20 ENVR 38. Development and application of analysis method for carbon nanotubes in plant tissues. K.K. Das, V. Nava, C. Chang, J. Chan, B. Xing, **Y. Yang**

11:40 ENVR 39. Toxicity of graphene materials to freshwater algae as affected by environmental factors. **J. Zhao**, B. Xing

Section E

Orange County Convention Center
Valencia Ballroom B-D - Theater 13

Aquatic Photochemistry



TECHNICAL PROGRAM

Photoproducts & Reactive Intermediates

W. Arnold, K. P. McNeill, *Organizers*
S. G. Pati, *Organizer, Presiding*

9:00 Introductory Remarks.

9:05 ENVR 40. Photochemical production of sulfate and methanesulfonic acid from dissolved organic sulfur. **R. Ossola**, J. Tolu, B. Clerc, P.R. Erickson, L. Winkel, K.P. McNeill

9:25 ENVR 41. Dissolved organic matter mediated indirect photochemical formation of COS and CS₂ in natural waters: kinetics and reaction mechanisms. **M. Modiri Gharehveran**, A. Shah

9:45 ENVR 42. Understanding sulfate production from photosensitized cysteine degradation. **R. Ossola**, B. Clerc, K.P. McNeill

10:05 ENVR 43. Atmospheric aquatic organic chemistry. **A. Carlton**, K. Fahey

10:25 ENVR 44. Direct pH measurement with SERS in the micro aquatic system - aerosol droplets. **Q. Huang**, L.C. Marr, P.J. Vikesland

10:45 Intermission.

11:00 ENVR 45. Effects of ozone on the dissolved organic matter and insights on the photophysics that govern to the formation of reactive intermediates photoproduction. **F. Leresche**, T. Kurtz, J.A. Torres-Ruiz, G. McKay, S. Canonica, U. von Gunten, F.L. Rosario

11:20 ENVR 46. Prediction of photochemically produced reactive intermediates in surface waters via satellite remote sensing. **Y. Chen**, R.M. Hozalski, L. Olmanson, C. Griffin, P. Brezonik, J. Finlay, W. Arnold

11:40 ENVR 47. Phototransformation and flocculation of dissolved organic matter to new organic compounds: the biogeochemical implications. **H. Chen**, P.G. Hatcher

Section F

Orange County Convention Center
Valencia Ballroom B-D - Theater 14

Emerging Issues on & Horizon Technologies for Water Disinfection

X. Xie, *Organizer*
N. B. Saleh, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 ENVR 48. Emerging DBPs: State of the Science and New Impacts. **S.D. Richardson**



TECHNICAL PROGRAM

8:45 ENVR 49. Rejection of Disinfection Byproducts by Commercial Forward Osmosis Membranes for Wastewater Recycling. **J. Xu**, T.N. Tran, H. Lin, N. Dai

9:10 ENVR 50. Mitigating NDMA formation during disinfection with oxidants: Two precursor case studies. **E. Marti**, C. Glover, E. Dickenson

9:35 ENVR 51. Drinking water chlorination and chloramination in water distribution system: Release of lead, formation of disinfection byproducts (DBPs) and toxicity of tap water. **J. Liu**, W. Li, Y. Li, X. Zhang, H. Lujan, C.M. Sayes, V.K. Sharma

10:00 Intermission.

10:15 ENVR 52. Chlorination of phenols revisited: Formation of electrophilic dicarbonyl ring cleavage products. **C. Prasse**, U. von Gunten, D.L. Sedlak

10:40 ENVR 53. General acid catalysis of bromide oxidation by free chlorine. **S. Brodfuehrer**, D. Wahman, L.E. Katz, G. Speitel

11:05 ENVR 54. Formation of total and specific nitrosamines from amine containing micropollutants in wastewater. **C. Pu**, T. Zeng

11:30 ENVR 55. Linking disinfectant residuals, metagenomics, and water quality during the recovery of two Texas drinking water systems following Hurricane Harvey. **M.R. Landsman**, L. Rowles, S. Brodfuehrer, J. Maestre, K. Kinney, M. Kirisits, L.E. Katz, D. Lawler

11:55 Concluding Remarks.

Symposium in Honor of Chuck Peden's Research Career: Catalysis for Energy & the Environment

Sponsored by CATL, Cosponsored by ENFL, ENVR, I&EC and PHYS

Elucidation of Mechanisms & Kinetics on Surfaces

Mechanisms on Surfaces: C-C Coupling, C-H & C-O Bond Manipulations

Sponsored by CATL, Cosponsored by ENFL, ENVR, INOR and PHYS

SUNDAY AFTERNOON

Section A

Orange County Convention Center
Valencia Ballroom B-D - Theater 9

Abiotic & Biotic Pollutant Transformation in Soils



TECHNICAL PROGRAM

H. Cheng, *Organizer*
G. Chen, *Organizer, Presiding*
H. Cheng, *Presiding*

1:30 ENVR 56. Colloid-mediated transport of antibiotics through chemically heterogeneous porous media. **J. Zhuang**, X. Chen

2:00 ENVR 57. Trends of uranium (IV) adsorption onto clay minerals. **A. Satpathy**, D. Giammar

2:20 ENVR 58. Uranium-bacteria complexation and bacteria-facilitated uranium transport in the presence of phytate at Savannah River site. **R. Li**

2:40 ENVR 59. Extent and rates of chromium (VI) leaching from weathered chromium ore processing residue (COPR)-impacted soils. **M. Bhattacharya**, A. Singh

3:00 ENVR 60. Source apportionment of heavy metals in surface soils based on their chemical speciation and stochastic modeling. **Y. Hu**

3:20 Intermission.

3:35 ENVR 61. Impact of aging on sulfidated nanoscale zerovalent iron. **D. O'Carroll**, A. Nunez Garcia, D. Appleton, K. Chen, M. Lee

3:55 ENVR 62. Abiotic processes controlling the fate of phenylarsenic compounds in soil and aquatic environment. **H. Cheng**, X. Xie, W. Zhao

4:15 ENVR 63. Kinetics, mechanisms, and pathways of oxidative degradation of phenylarsonic compounds by birnessite (δ -MnO₂). **W. Zhao**, H. Cheng

4:35 ENVR 64. Quantitative analysis of dsRNA biopesticides for the ecological risk assessment of RNAi agricultural biotechnology. K. Zhang, K.K. Das, M. Sander, **K.M. Parker**

4:55 ENVR 65. Rapid kinetics and modeling of two-stage Fenton and solar-Fenton process. **Y. Li**, H. Cheng

5:15 Concluding Remarks.

Section B

Orange County Convention Center
Valencia Ballroom B-D - Theater 10

Science & the Perception of Climate Change

S. O. Obare, *Organizer*
E. Schoffers, *Organizer, Presiding*

1:30 Introductory Remarks.



TECHNICAL PROGRAM

1:35 ENVR 66. The Fourth National Climate Assessment: Highlighting impacts, risks, and responses across sectors of the United States. **C.W. Avery**

2:05 ENVR 67. Climate Justice and Voices of the Disenfranchised. **K.E. Peterman**

2:30 ENVR 68. The Power of Innovation and Implementation in Climate Science Literacy. **G.P. Foy**, R. Foy

2:55 ENVR 69. Climate Disruption: Change, the “New Normal”. **J.A. Bell**

3:20 Intermission.

3:30 ENVR 70. Chemists need science communication to do their job and to help save the climate. **E. Schoffers**

3:55 ENVR 71. Climate Change – A “Third Rail” of American Politics? **D. Kriner**, J. Goldfarb

4:20 ENVR 72. Science and society: Opportunities and challenges. **B.Z. Shakhshiri**

4:45 Discussion.

5:10 Closing remarks.

Section C

Orange County Convention Center
Valencia Ballroom B-D - Theater 8

Contributions of a Simple Chemist: How Professor Ronald Atlee Hites Changed Environmental Chemistry

E. M. Ulrich, M. Venier, *Organizers*

E. T. Furlong, S. T. Glassmeyer, S. L. Simonich, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 ENVR 73. Heroic history of Hitesisms. **M.F. Simcik**

1:55 ENVR 74. Environmental signals of the anthropocene: POPs in sediments and Ron Hites as a first ‘anthropocener’. **S.J. Eisenreich**

2:15 ENVR 75. Coupling of atmosphere-land-ocean fluxes and concentrations of persistent organic pollutants at coastal Antarctica. **J. Dachs**, P. Casal, G. Casas, A. Cabrerizo, M. Vila-Costa, M. Pizarro, B. Jiménez

2:35 ENVR 76. Identifying unknowns and why a thoughtful, expert mass spectral interpretation is still needed: Lessons learned from Ron Hites. **S.D. Richardson**

2:55 Intermission.

3:15 ENVR 77. Ron Hites: The scientist as editor. **D.L. Sedlak**



TECHNICAL PROGRAM

3:35 ENVR 78. Don't call it a spec(k). **E.M. Ulrich**

3:55 ENVR 79. Biotransformation and bioconcentration of polyfluoroalkyl phosphate diesters in common carp (*Cyprinus carpio*). **L. Zhu**

4:15 ENVR 80. In gratitude to my students, colleagues, and family. **R.A. Hites**

4:45 Concluding Remarks.

Section D

Orange County Convention Center
Valencia Ballroom B-D - Theater 12

Nanotechnology at the Water-Agriculture-Energy Nexus

A. A. Keller, G. Lowry, C. Sabilov, J. C. White, Y. Yang, *Organizers, Presiding*

1:30 ENVR 81. Nanomaterial-Driven Electrochemistry as a Water Treatment and Sensing Tool. **D. Jassby**, A.K. Mulchandani

1:50 ENVR 82. Nanoscale structures for enabling and enhancing membrane processes at the water-energy nexus. **S. Lin**

2:10 ENVR 83. Investigating the Food Safety Implications of Two Broadly Applied Nano-agricultural chemicals. **X. Ma**

2:30 ENVR 84. Coating chemical identity and size of gold nanoparticles affect pathways of foliar uptake, translocation and leaf-to-rhizosphere transport in wheat plants. **A. Avellan**, J. Yun, E. Spielman-Sun, Y. Zhang, G. Lowry

2:50 ENVR 85. Potential application of few layered black phosphorus in water treatment. **Q. Zhao**, S. Zhang, X. Zhang, B. Xing

3:10 ENVR 86. Withdrawn

3:30 Intermission.

3:50 ENVR 87. Study of the transport mechanism in a freestanding graphene oxide forward osmosis membrane. **S. Liu**, **X. Tong**, **J.C. Crittenden**, **Y. Chen**

4:10 ENVR 88. Taking a systems approach to nano-enabled agrochemical design to advance sustainability at the water-agriculture-energy nexus. **L.M. Gilbertson**, J. Urso, A. Smith, G. Lowry, L. Pourzahedi

4:30 ENVR 89. Electrochemical CO conversion to valuable chemicals. **F. Jiao**

4:50 ENVR 90. High-performance nanomaterials for the recovery of nitrogen and phosphorus nutrients. M. Manto, **C. Wang**

5:10 ENVR 91. Impact of CuO Nanomaterials on Bacterial Co-Cultures. **N.V. Hudson-Smith**, S. Mitchell, J. Borgatta, R.J. Hamers, E.E. Carlson, C.L. Haynes



TECHNICAL PROGRAM

Section E

Orange County Convention Center
Valencia Ballroom B-D - Theater 13

Aquatic Photochemistry

Photochemically Produced Reactive Intermediates

W. Arnold, S. G. Pati, *Organizers*
K. P. McNeill, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 **ENVR 92.** Photochemical formation methylhydroperoxide (MHP) in natural water under solar irradiation. J. Sun, **W. Song**

1:55 **ENVR 93.** Production of hydroxylating species from DOM model sensitizers. **K.D. Couch**, G. McKay, F.L. Rosario

2:15 **ENVR 94.** Singlet oxygen quantum yields of dissolved organic matter by time-resolved singlet oxygen phosphorescence. **K. Moor**, P.R. Erickson, D.E. Latch, K.P. McNeill

2:35 **ENVR 95.** Exploring the role of photoexcited triplet states in the formation of halide radicals: implications for advanced oxidation processes. **S. Snow**, M. Kamat, K. Moor, K.P. McNeill

2:55 **ENVR 96.** Single-electron oxidation of *N*-cyclopropylanilines by triplet-state dissolved organic matter. **N.C. Pflug**, M. Schmitt, K.P. McNeill

3:15 Intermission.

3:30 **ENVR 97.** Impact of pH and wavelength on the production of reactive oxidants during chlorine photolysis. **D. Bulman**, C.K. Remucal

3:50 **ENVR 98.** Nitrate removal via formate radical-induced photochemical process. **H. Liu**

4:10 **ENVR 99.** Stable oxygen isotopes as a novel, sensitive tracer of hydrocarbon oxidation on the sunlit sea surface. **C.P. Ward**, K. Sutherland, S. Wankel, C. Reddy

4:30 **ENVR 100.** Impact of pH on iron redox transformations under dark and light conditions in simulated freshwaters containing natural organic matter. S. Garg, C. Jiang, **T. Waite**

Section F

Orange County Convention Center
Valencia Ballroom B-D - Theater 14

Emerging Issues on & Horizon Technologies for Water Disinfection



TECHNICAL PROGRAM

N. B. Saleh, *Organizer*
X. Xie, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 **ENVR 101.** Comparing the quality of water produced by O3/BAC vs. MF/RO for potable reuse of municipal wastewater. **W. Mitch**, Y. Chuang

2:15 **ENVR 102.** Polyamide Membrane Monomer Degradation Kinetics and Mechanisms during Chlorination of Halide-impacted Waters. **K. Huang**, K. Reber, M. Toomey, J.A. Howarter, A. Shah

2:40 **ENVR 103.** Mechanisms of single and triple layered RNA virus inactivation by UV irradiation. **T.H. Nguyen**, E. Araud

3:05 **ENVR 104.** Investigation of bacteria sensitivity to pulsed electric field electroporation using a lab-on-a-chip platform. **T. Wang**

3:30 Intermission.

3:45 **ENVR 105.** Controlling the ionic release and surface passivation of silver nanoparticles with a natural polymer: Integrating ancient Navajo techniques into ceramic water filters. L. Rowles, D. Lawler, **N.B. Saleh**

4:10 **ENVR 106.** Silver nanowire-modified filter with controllable silver ion release for pathogen inactivation in water. **W. Chen**

4:35 **ENVR 107.** Biological mechanisms behind disinfection and the development of bacterial resistance to disinfectants: Comparisons between hypochlorite and ferrate. **K. Ikuma**, S. Daer

5:00 **ENVR 108.** Mechanistic Investigation of Bromamines Decomposition in the Presence of Cu(II). **W. Hu**, S. Allard, J. Croué

5:25 Concluding Remarks.

Symposium in Honor of Chuck Peden's Research Career: Catalysis for Energy & the Environment

Sponsored by CATL, Cosponsored by ENFL, ENVR, I&EC and PHYS

Elucidation of Mechanisms & Kinetics on Surfaces

Reductions & Hydrogenations

Sponsored by CATL, Cosponsored by ENFL, ENVR, INOR and PHYS

MONDAY MORNING



TECHNICAL PROGRAM

Section A

Orange County Convention Center
Valencia Ballroom B-D - Theater 9

Environmental Chemistry Undergraduate Education in the Classroom, Laboratory, and Beyond

M. A. Benvenuto, M. Berger, E. Roberts-Kirchhoff, L. A. Welch, *Organizers, Presiding*

8:45 Introductory Remarks.

8:55 ENVR 109. Integrated teaching strategies for improved student learning in environmental chemistry curriculum. **M. Li**

9:15 ENVR 110. Design and development of a student-centered environmental competition focusing on water desalination and purification. **A. Mlynarski, J.J. Keleher**

9:35 ENVR 111. Innovative approaches for implementing environmental chemistry in an ACS local chapter. **F. Ocasio Idorwatt, G. Hernandez**, L.I. Santiago

9:55 ENVR 112. Extracurricular undergraduate research and education in environmental chemistry and sustainability through EPA P3 projects. **W. Lee**, J. Hwang, K. Rodriguez

10:15 Intermission.

10:30 ENVR 113. Preparing for water-related graduate school in the United States: Online mentorship in water education for students from underserved communities. **S. Kum**, L. Rowles III, R. Alcalde, F. Diaz, A. Mikelonis, D. Lawler

10:50 ENVR 114. Taking the “mud” out of the muddy river: Engaging students in chemical analysis. **M. Berger**

11:10 ENVR 115. Design Considerations When Developing an Undergraduate Research Project that Measures Heavy Metals in the Environment and Beyond. **J. Duggan**

11:30 ENVR 116. Connecting environmental engineering to introductory chemistry in the freshmen year. **L.E. Katz**, S. Brodfuehrer, J. Davis, J. Grundy, M.R. Landsman

11:50 Concluding Remarks.

Section B

Orange County Convention Center
Valencia Ballroom B-D - Theater 10

Per- & Polyfluoroalkyl Substances in the Environment: From Legacy To Emerging Contaminants

C. I. Olivares, *Organizer*
K. A. Barzen-Hanson, A. Robel, *Organizers, Presiding*
C. Olivares, *Presiding*



TECHNICAL PROGRAM

8:45 Introductory Remarks.

8:50 ENVR 117. Reference Materials for the Quality Assurance and Quality Control of the Measurements of Per- and Polyfluoroalkyl Substances. **B.J. Place**, J.L. Reiner

9:10 ENVR 118. Retention of per- and polyfluoroalkyl substances during filtration: Implications for proper sample pretreatment. **K. He**, A. Feerick, H. Jin, L.M. Blaney

9:30 ENVR 119. Identification of per- and polyfluoroalkyl substances (PFAS) from samples near US industrial manufacturing and use facilities. **M. Strynar**, J. McCord, A. Lindstrom, J. Washington, J. Offenberg, J. Ryan, R. Theran, D.G. Tabor, I. George, T. Buckley, M. Medina-Vera, A. Gillespie, E. Bergman, S. Goodrow, E. Peduto, B. Kernen, C. Beahm

9:50 ENVR 120. Identification of novel chlorinated and hydrogenated polyfluoroalkyl ether sulfonates in sewage sludge by high-resolution mass spectrometry. Y. Lin, **T. Ruan**, G. Jiang

10:10 Intermission.

10:25 ENVR 121. Perfluoroalkyl substances in landfill leachates produced from different waste types. **H. Solo-Gabriele**, A. Jones, H. Zhang, J. Lang

10:45 ENVR 122. Per- and polyfluoroalkyl substances in source and treated drinking waters of the United states. **S.T. Glassmeyer**, J. Boone, E.T. Furlong, D.W. Kolpin, R. Benson, J. Donohue, J. Simmons

11:05 ENVR 123. Per- and poly-fluoroalkyl substances (PFASs) in drinking water and human blood from a Colorado community impacted by aqueous film-forming foam (AFFF) contamination: The PFAS-AWARE Study. **C.A. McDonough**, K. Barton, A. Starling, J.L. Adgate, C.P. Higgins

11:25 ENVR 124. Impacts of tetrafluoro-2-(Heptafluoropropoxy)-propanoate (GenX) on growth, reproduction, and neurological behaviors in *Caenorhabditis elegans*. **X. Pan**, T. Thornburg, D. Collier

11:45 Closing Remarks.

Section C

Orange County Convention Center
Valencia Ballroom B-D - Theater 8

Accurate Mass/High Resolution Mass Spectrometry for Environmental Monitoring & Remediation

T. Anumol, R. Marfil-Vega, T. M. Young, C. Zwiener, *Organizers, Presiding*

9:00 Introductory Remarks.

9:05 ENVR 125. Unknown identification of transformation products and disinfection by-products in wastewater impacted drinking water. **D. Westerman**, H.K. Liberatore, K. Cochran, C. Montagner, D.D. Dionysiou, L. Cizmas, S.D. Richardson

9:25 ENVR 126. Application of non-target high resolution mass spectrometry for quantitative source apportionment. **K.T. Peter**, Z. Tian, C. Wu, E.P. Kolodziej



TECHNICAL PROGRAM

9:45 ENVR 127. Quantification and suspect-screening of a broad range of quaternary ammonium compounds in wastewater effluents and sediment cores from across Minnesota. **S.G. Pati**, W. Arnold

10:05 ENVR 128. LC-HRMS screening of poly- and perfluorinated alkyl substances (PFAS) and their transformation products in contaminated soil. B. Bugsel, S. Tisler, **C. Zwiener**

10:25 Intermission.

10:40 ENVR 129. 8 Years after the *Deepwater Horizon* spill: The evolution of oil transformation compounds in Louisiana Salt Marsh Sediments revealed by FT-ICR mass spectrometry. **H. Chen**, A.M. McKenna, C. Davis, R.P. Rodgers, A. Hou

11:00 ENVR 130. Improving non-target identification of organic contaminants by probabilistic ranking of putative structure assignments by HR/AM MS(MS) and computational mass spectrometry. **G.J. Getzinger**, L. Ferguson

11:20 ENVR 131. Metabolomics for environmental monitoring: Developing tools for monitoring the remediation activity of microbial consortia, SDC-9. **S.R. Campagna**, A. May, Y. Xie, F. Loeffler, M. Michaelsen

11:40 Discussion.

Section D

Orange County Convention Center
Valencia Ballroom B-D - Theater 12

Micro- & Nano-Plastics in the Environment: Detection, Characterization, Fate & Impact

S. R. Al-Abed, M. J. Gallagher, P. Potter, *Organizers, Presiding*

8:00 Introductory Remarks.

8:10 ENVR 132. Plastics increasing chemical contamination in ocean and coast. H. Kimukai, H. Sato, **K. Koizumi**, K. Takatama, S. Chung, M. Nishimura, Y. Kodera, **K. Saïdo**

8:30 ENVR 133. Chemical Mechanisms and Toxicological Effects of Microplastics in the Aqueous Environment. **C. Sayes**

8:50 ENVR 134. Preliminary assessment of FTIR and IRMS for characterization of microplastics. **Q.T. Birch**, S.R. Al-Abed, P. Pinto, P. Potter, D.D. Dionysiou

9:10 ENVR 135. Rapid, automated analysis of microplastics using laser direct infrared imaging and spectroscopy. D. Mainali, M.R. Kole, **A. Ghetler**, M. Rault, **C.R. Moon**

9:30 ENVR 136. Identification of microplastics via FTIR micro-spectroscopy for potential source tracking in freshwater. **G.A. Arbuckle-Keil**, K. Sipps, K. Parker, N. Fahrenfeld

9:50 Intermission.

10:05 ENVR 137. Reliably quantifying microplastics within a wastewater matrix. **T.R. Mayo**, **B. Sturm**, E.F. Peltier



TECHNICAL PROGRAM

10:25 ENVR 138. Textile micro fibers released to the environment during home laundering: Aerobic biodegradation in aquatic environments. M. Zambrano, **R.A. Venditti**, J. Pawlak, J.J. Cheng, C. Goller, J. Daystar, M. Ankeny

10:45 ENVR 139. Transfer of additives from ingested plastics to seabirds and their accumulation in the tissue. **H. Takada**, K. Tanaka, R. Yamashita, Y. Watanuki

11:05 ENVR 140. Studies of Persistent Organic Pollutants in Some Selected Locations in Jos North Metropolis, Jos, Plateau State, Nigeria. **E.G. Ibrahim**

11:25 Panel Discussion.

Section E

Orange County Convention Center
Valencia Ballroom B-D - Theater 13

Aquatic Photochemistry

Photolysis of Pesticides & Personal Care Products

W. Arnold, K. P. McNeill, *Organizers*
S. G. Pati, *Organizer, Presiding*

9:00 Introductory Remarks.

9:05 ENVR 141. Photolysis of neonicotinoid insecticides on model and real leaf surfaces. **Y. Chen**, S. Todey, A. Itkin, W. Arnold

9:25 ENVR 142. Safener benoxacor induces herbicide metolachlor photolysis on simulated soil surface. **L. Su**, J.D. Sivey, N. Dai, L. Caywood

9:45 ENVR 143. Degradation of strobil fungicides in aquatic and soil environments. **M. O'Connor**, W. Arnold

10:05 ENVR 144. Investigating the indirect photolysis of commonly used pesticides. **J. Apell**, N.C. Pflug, K.P. McNeill

10:25 Intermission.

10:40 ENVR 145. Photolysis of select QACs in sunlit surface water. **P.I. Hora**, W. Arnold

11:00 ENVR 146. Direct and indirect phototransformation of triclosan in wetland water. **K. Lam**, S. Nelieu, P. Benoit, E. Passeport

11:20 ENVR 147. Degradation of 4-methylbenzylidene camphor by sunlight photolysis in the presence of free chlorine. **W. Lai**, K. Chen, A.Y. Lin

11:40 ENVR 148. Aquatic Photochemistry of a Fragrance Ingredient and its Use in Environmental Persistence Assessment. **J. Lin**, V. Hewins, M. Emberger, S. Gimeno



TECHNICAL PROGRAM

Section F

Orange County Convention Center
Valencia Ballroom B-D - Theater 14

Emerging Issues on & Horizon Technologies for Water Disinfection

N. B. Saleh, X. Xie, *Organizers*

8:00 Introductory Remarks.

8:05 ENVR 149. Edible dye-enhanced solar disinfection with safety indication. **J. Kim**, E. Ryberg, C. Chu

8:45 ENVR 150. Nanowire-assisted coaxial-electrode electroporation disinfection cell enabling low-voltage water disinfection in pipelines. **J. Zhou**

9:10 ENVR 151. Pilot Testing of Peracetic Acid – Ultraviolet Disinfection and Advanced Oxidation for Wastewater Treatment. **N. Dai**, A. Hassaballah, K. Naas, L. Sassoubre

9:35 ENVR 152. Structural equation modeling to identify social drivers for water use in low-income communities in Southern Texas. **L. Rowles**, D. Lawler, **N.B. Saleh**

10:00 Intermission.

10:15 ENVR 153. Electrode development for electroporation disinfection cells. **X. Xie**, C. Yu

10:40 ENVR 154. Visible-light-responsive photocatalyst of graphitic carbon nitride for biofilm control. **H. Shen**, D. Shuai

11:05 ENVR 155. Disinfection of *Legionella pneumophila* within drinking water biofilms using various treatment technologies. **H. Buse**, B. Morris, I. Struewing, J. Szabo

11:30 ENVR 156. Withdrawn

11:55 Closing Remarks.

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Sponsored by PROF, Cosponsored by AGFD, ANYL, BIOL, BIOT, CARB, CELL, CHED, CMA, COLL, COMP, ENVR, GEOC, I&EC, MEDI, MPPG, NUCL, ORGN, PHYS, PMSE, POLY, PRES, WCC and YCC

Symposium in Honor of Chuck Peden's Research Career: Catalysis for Energy & the Environment

Sponsored by CATL, Cosponsored by ENFL, ENVR, I&EC and PHYS



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

Recent Advances in Plasma-Enhanced Catalysis

Sponsored by CATL, Cosponsored by ENFL, ENVR and PHYS

MONDAY AFTERNOON

Section A

Orange County Convention Center
Valencia Ballroom B-D - Theater 9

Research Experiences in Environmental Chemistry Projects for Undergraduate & Graduate Students

M. A. Benvenuto, M. Berger, E. Roberts-Kirchhoff, L. A. Welch, *Organizers, Presiding*

1:00 Introductory Remarks.

1:10 ENVR 157. Quantification of heterocyclic aromatic amines in particulate matter by high performance liquid chromatography-tandem mass spectrometry. **A.N. Fagundes**, O.K. Pham, A.N. Whitmore, M.R. Olson, J.J. Schauer, H.T. To, T. Norimichi, J. Miller-Schulze

1:30 ENVR 158. Undergraduate Research and CURE Development in MOF Materials for Water Remediation. **D. Kissel**

1:50 ENVR 159. Investigation of Oleaginous Yeast and *Azolla caroliniana* as viable biomass feedstocks for renewable energy. **L.A. Welch**, C.A. Coccie

2:10 ENVR 160. Reusable biodegradable solvents from biodiesel coproduct glycerol. L.S. Ott, **R.E. Bumbaugh**

2:30 Intermission.

2:45 ENVR 161. Antibiotic resistance induced by endocrine-disrupting chemicals. **D.E. Novoa**, S. Key, O. Conroy-Ben

3:05 ENVR 162. Development and implementation of a course-based undergraduate research experience in quantitative analysis laboratory. **K.R. Evans**, K.C. Lanigan, E. Roberts-Kirchhoff

3:25 ENVR 163. Development of methods for copper and atrazine removal from aqueous solutions using fruit peel waste. Z. Smith, K. Desai, T. Patel, N. DeOrnellas, A. Almouseli, A.M. Lopez, A. Chaney, E. Leever, I. Muqbil, K.E. Yacoo, K.R. Evans, **K.C. Lanigan**

3:45 Closing Remarks.

Section B

Orange County Convention Center
Valencia Ballroom B-D - Theater 10



Per- & Polyfluoroalkyl Substances in the Environment: From Legacy To Emerging Contaminants

C. I. Olivares, *Organizer*
K. A. Barzen-Hanson, A. Robel, *Organizers, Presiding*
C. Olivares, *Presiding*

1:00 Introductory Remarks.

1:05 **ENVR 164.** Interrelationships between PFAS and *in situ* microbial communities at an AFFF field site. **D. O'Carroll**, M. Lee, S. Le, A. Yeung, M. Manefield, K. Weber, S. Wallace, N. Battye, T. Jeffries

1:25 **ENVR 165.** Biotransformation of zwitterionic polyfluoroalkyl compounds in aerobic soils. M. Liu, G. Munoz, S. Vo Duy, S. Sauve, **J. Liu**

1:45 **ENVR 166.** Identification of Biotransformation Products of 6:2 Fluorotelomer Thioether Amido Sulfonate under Nitrate-Reducing Conditions Using Automated Mass Spectrometry Analysis. **S. Yi**, W. Zhuang, L. Alvarez-Cohen, K. Harding-Marjanovic¹, E. Houtz

2:05 **ENVR 167.** Drinking water quality and treatment challenges associated with per- and polyfluoroalkyl substances. **D. Knappe**, Z. Hopkins, J. McCord, M. Strynar, A. Lindstrom

2:25 Intermission.

2:40 **ENVR 168.** Removal of persistent polyfluoroalkyl pollutants from water using paramagnetic ionic liquids. **D. Bwambok**, M. Peralta, J. Woodtle

3:00 **ENVR 169.** Sorption of PFAS by Cationic Hydrophobic Polymers. **Y. Olshansky**, J.D. Chorover, L.M. Abrell, J. Field, A. Gomeniuc, J. Hatton, R. Sierra Alvarez

3:20 **ENVR 170.** Field demonstration design of heat-activated persulfate in situ chemical oxidation (ISCO) of PFASs in Jacksonville, FL. **E. Cook**, C. Olivares, D. Ocasio, R. Deeb, E. Hawley, B. Marvin, J. Kornuc, D.L. Sedlak, L. Alvarez-Cohen

3:40 **ENVR 171.** Bioelectrochemical oxidation of per- and polyfluoroalkyl substances and non-fluorinated co-contaminants in aqueous film forming foam. **J. Blotevogel**, N. Pica, R. Young, S.S. Kalra, Y. Miao, H. Chen, A.M. McKenna, T. Borch, S. Mahendra

4:00 Discussion.

4:30 Closing Remarks.

Section C

Orange County Convention Center
Valencia Ballroom B-D - Theater 8

Accurate Mass/High Resolution Mass Spectrometry for Environmental Monitoring & Remediation



TECHNICAL PROGRAM

T. Anumol, R. Marfil-Vega, T. M. Young, C. Zwiener, *Organizers, Presiding*

1:00 Introductory Remarks.

1:05 ENVR 172. Advancing throughput for comprehensive HRMS screening of drinking water: Combined approach of online SPE and direct injection. **L. Tölgyesi**, S. Lebertz, T. Anumol

1:25 ENVR 173. Cheminformatics approaches to support chemical identification delivered via the EPA CompTox Chemicals Dashboard. **A.J. Williams**, A. McEachran, C. Grulke, E.M. Ulrich, J. Sobus

1:45 ENVR 174. High-throughput identification and prioritization of ToxCast chemicals in airborne fine particulate matter. Y. Lin, **T. Ruan**, G. Jiang

2:05 ENVR 175. Profiling of environmental contaminants using GC/Q-TOF. **S. Nieto**, K. Chen, C. Milner, C. Alaimo, T. Young, **A. Andrianova**

2:25 Intermission.

2:40 ENVR 176. Identifying estrogenic compounds with High Resolution LC/MS effects-directed analysis in California sewage sludge. **G. Black**, T.M. Young

3:00 ENVR 177. Evaluating photolysis products of brominated estrogens with high resolution mass spectrometry. **C. Hutchinson**, K. Nance, R. Milstead, B. Dwyer, D.R. Griffith

3:20 ENVR 178. Quantitative and qualitative environmental water analysis using Orbitrap® technology. **R. Jack**

3:40 Discussion.

4:00 Concluding Remarks.

Section D

Orange County Convention Center
Valencia Ballroom B-D - Theater 12

Photocatalytic & Electrochemical Processes in Green Energy & Environmental Remediation: A Symposium in honor of Professor Krishnan Rajeshwar

D. D. Dionysiou, N. Wu, *Organizers*
C. Janaky, V. K. Sharma, *Organizers, Presiding*

1:00 Introductory Remarks.

1:05 ENVR 179. Photosensitization aspects of semiconductor quantum dots in photovoltaics. **P.V. Kamat**

1:35 ENVR 180. Size dependence of exciton dynamic in organo-metal halide perovskite nanocrystals. **J.Z. Zhang**



TECHNICAL PROGRAM

- 2:05 ENVR 181. Optoelectronic properties of semiconductor photoelectrodes. **Á. Balog**, G.F. Samu, C. Janaky
- 2:25 ENVR 182. Place in the sun for artificial photosynthesis. **L. Vayssieres**
- 2:55 Intermission.
- 3:10 ENVR 183. CO₂ conversion on N-doped carbon electrodes: Morphological and mechanistic insights. **D. Hursán**, A. Samu, K. Artyushkova, P.B. Atanassov, C. Janaky
- 3:30 ENVR 184. Photocatalytic reduction of gaseous carbon dioxide by cuprous oxide/graphitic carbon nitride composite photocatalyst. **P. Chang**, I. Tseng
- 3:50 ENVR 185. Electrodeposition of semiconductor/nanocarbon photoelectrodes. **E. Kecsenvity**, B. Endrodi, C. Janaky
- 4:10 ENVR 186. Development of platinum/graphene counter electrode based DSSCs. **Y. Zhang**
- 4:30 ENVR 187. Plasmon-enhanced photocatalysis for environment remediation and solar fuel generation. **N. Wu**

Section E

Orange County Convention Center
Valencia Ballroom B-D - Theater 13

Aquatic Photochemistry

Transformation Mechanisms of Contaminants During Photolysis

K. P. McNeill, S. G. Pati, *Organizers*
W. Arnold, *Organizer, Presiding*

1:00 Introductory Remarks.

- 1:05 ENVR 188. Substituent effect on the direct photodegradation of benzotrifluorides. **A. Manfrin**, G.J. Getzinger, A. Hänggli, K.P. McNeill
- 1:25 ENVR 189. Reaction mechanisms, efficiency, and optimization of reductive transformation of PFASs by hydrated electrons in contaminated groundwater. **G. McKay**, R. Tenorio, D.J. Van Hoomissen, J. Liu, C. Bellona, C.P. Higgins, S. Vyas, T.J. Strathmann
- 1:45 ENVR 190. Assessing the suitability of traditionally employed reactive species sensitizers and probes to study photochemical reaction kinetics of ebselen, an organoselenium compound. **M. Hopanna**, L.M. Blaney
- 2:05 ENVR 191. Phototransformation of halophenolic disinfection byproducts (DBPs) in receiving seawater: Kinetics, products, and toxicity. **J. Liu**, X. Zhang, Y. Li, W. Li, C. Hang, V.K. Sharma
- 2:25 ENVR 192. UV-initiated photooxidation process of disinfection byproducts: mechanism of the degradation of tribromoacetic acid by femtosecond transient absorption spectroscopy and density functional theory study. **Y. Chi Shun**, D. Phillips, S. Leu, H. Tse



TECHNICAL PROGRAM

2:45 Intermission.

3:00 **ENVR 193.** Photodegradation of trace organic contaminants by singlet oxygen: a kinetic/transport model. **I.I. Marquez**, H. Vo, T. Zhang, B. Barnett, A. Nienhauser, P. Yang, D. Quanrud, R. Arnold, A.E. Saez

3:20 **ENVR 194.** Reversible photo-nucleophilic addition for trienone steroids. **K.H. Wammer**, N.C. Pflug, A.K. Kral, J.E. OBrien, E.P. Kolodziej, J.B. Gloer, D.M. Cwiertny

3:40 **ENVR 195.** Unusual bioactive rearrangement products from aqueous photolysis of pharmaceutical steroids and their enrichment through diurnal light-dark cycling. **N.C. Pflug**, C. Knutson, D. Martinovic-Weigelt, K.C. Breuckman, E.E. Meyer, D. Swenson, K.H. Wammer, J.B. Gloer, D.M. Cwiertny

4:00 **ENVR 196.** Studies of the singlet oxygenation of Domoic acid: Mechanisms, kinetics and biological significance.. **M. Jaramillo**, K.E. O'Shea

4:20 Concluding Remarks.

Section F

Orange County Convention Center
Valencia Ballroom B-D - Theater 14

Transdisciplinary Approaches to Sustainable Solutions at the Food-Energy-Water Nexus

J. L. Goldfarb, D. Kriner, *Organizers, Presiding*

1:00 Introductory Remarks.

1:10 **ENVR 197.** Analyzing life expectancies in terms of sustainability criteria and impacts. **D.J. Nelson**

1:40 **ENVR 198.** Polymer-clay composites for sorptive removal of trace organic compounds and metals during urban stormwater treatment. **J. Ray**, I. Shabtai, M. Teixido, Y. Mishael, D.L. Sedlak

2:05 **ENVR 199.** Deeper understanding of co-digestion of domestic wastewater settled solids and food industry waste using molecular biological tools. **A.R. St. James**, R.E. Richardson, M. Rodriguez, J. Lin

2:30 Intermission.

2:45 **ENVR 200.** Bridging science and policy: Raising public support for renewable energy by increasing public understanding. **D. Kriner**, J.L. Goldfarb

3:15 **ENVR 201.** Thermochemical conversions of mixed waste streams to engineer sustainable biofuels and water treatment materials. L. Gao, **J. Goldfarb**

3:40 **ENVR 202.** Coupling hydrothermal liquefaction and membrane distillation to treat anaerobic digestate from food and dairy farm waste. **U. Rao**, R. Posmanik, L.E. Hatch, J. Tester, S.L. Walker, K. Barsanti, D. Jassby

4:05 **ENVR 203.** Optimization of an automated, pilot-scale reactor for struvite recovery from poultry litter. **C.R. Portner**, M.A. Fleming, U. Shashvatt, S. Musa, L.M. Blaney



TECHNICAL PROGRAM

4:30 Panel Discussion.

4:50 Closing Remarks.

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Sponsored by PROF, Cosponsored by AGFD, ANYL, BIOL, BIOT, CARB, CELL, CHED, CMA, COLL, COMP, ENVR, GEOC, I&EC, MEDI, MPPG, NUCL, ORGN, PHYS, PMSE, POLY, PRES, WCC and YCC

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Symposium in Honor of Chuck Peden's Research Career: Catalysis for Energy & the Environment

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Elucidation of Mechanisms & Kinetics on Surfaces

Experimental Surface Science

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Recent Advances in Plasma-Enhanced Catalysis

Sponsored by CATL, Cosponsored by ENFL, ENVR and PHYS

Undergraduate Research Posters

Environmental Chemistry

Sponsored by CHED, Cosponsored by ENVR and SOCED

MONDAY EVENING



TECHNICAL PROGRAM

Section A

Orange County Convention Center
West Hall C

Sci-Mix

S. O. Obare, *Organizer*

8:00 - 10:00

275, 277, 278, 281, 282, 285, 287, 290, 291, 292, 293, 294, 295, 296, 297, 299, 300, 301, 304, 314, 315, 324, 325, 330, 331, 332, 334, 338, 340, 344, 354, 358, 361, 367, 372, 375, 379, 382, 388, 404, 405, 406, 407, 408, 418, 422, 425, 426, 432, 434, 435, 437, 442, 448, 451, 455, 463, 465, 469, 470, 471, 472, 473, 476, 480, 481, 483, 488, 489, 492, 494. See subsequent listings.

TUESDAY MORNING

Section A

Orange County Convention Center
Valencia Ballroom B-D - Theater 9

Current Status of Environmental Research on Water Contaminants

S. Ahuja, B. G. Loganathan, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 ENVR 204. Contaminants of emerging concern in Chesapeake Bay rivers fed by urban and agricultural areas. **E.R. Hain**, K. He, J.A. Andrade, A. Feerick, A.L. Timm, M. Tarnowski, L.M. Blaney

8:55 ENVR 205. Legacy pesticides in riverine marsh sediment cores from the tidal freshwater, oligohaline, and mesohaline zones of the Potomac River. **E. Lang**, R. McBride, T.B. Huff, D. Velinsky, G.D. Foster

9:15 ENVR 206. Degradation of naled in natural waters collected from areas impacted by aerial spray activities. A. Jones, D. Cohen, F. Alberdi, A. Sanabria, N. Clausell, M. Roca, **H. Solo-Gabriele**, E.M. Zahran

9:35 ENVR 207. Levels, tissue distribution and health risk assessment of organochlorine pesticides associated with *Pomadasy Commersonii* and *Mugil Cephalus* from selected estuaries in Eastern Cape Province, South Africa. **C. Olisah**, O.O. Okoh, A. Okoh

9:55 Intermission.

10:10 ENVR 208. Monitoring hydraulic fracturing indicator chemicals in produced water. **A. Hill**, J. Lee, R.M. Tinnacher, W.T. Stringfellow



TECHNICAL PROGRAM

10:30 ENVR 209. Treatment of bromide-containing brines with ammonium persulfate produces bromate. **R.E. Bishop**

10:50 ENVR 210. Sorption of ciprofloxacin to perfluorinated compounds determined through fluorescence quenching. **C. Ajjan, G.D. Foster**

11:10 ENVR 211. Kinetics and application of artificial neural network in the modeling and optimization of cartap removal by Fenton oxidation in a fluidized-bed reactor. **A. Rabongue, M.G. de Luna**

11:30 ENVR 212. Identification of disinfection byproducts and its precursors in River Yamuna in India: First case study of the situation. **S. Tak, B. Vellanki**

11:50 Concluding Remarks.

Section B

Orange County Convention Center
Valencia Ballroom B-D - Theater 10

Per- & Polyfluoroalkyl Substances in the Environment: From Legacy To Emerging Contaminants

C. I. Olivares, *Organizer*
K. A. Barzen-Hanson, A. Robel, *Organizers, Presiding*
C. Olivares, *Presiding*

8:30 Introductory Remarks.

8:35 ENVR 213. Enhancing the total oxidizable precursor assay for environmental samples containing per- and polyfluoroalkyl ether acids. **C. Zhang, Z. Hopkins, J. McCord, M. Strynar, A. Lindstrom, D. Knappe**

8:55 ENVR 214. Degradation of perfluorooctanoic acid by sulfate radical produced from thermally activated persulfate: Novel insights into mechanistic pathways from DFT and experimental investigations. **Y. Zhang, A.H. Moores, J. Liu, S. Ghoshal**

9:15 ENVR 215. Beyond legacy PFAS: Models to inform assessment across structural classes and species. **W. Cheng, M. Khazaee, C. Ng**

9:35 ENVR 216. Structure-based categorization of Per- & Polyfluoroalkyl substances in the DSSTox database and EPA's ToxCast inventory using Markush representations. **C. Grulke, G. Patlewicz, B. Meyer, A.J. Williams, A. Richard**

9:55 Intermission.

10:10 ENVR 217. US-EPA comptox chemicals dashboard: an information hub for over five thousand per- & polyfluoroalkyl chemical substances. **A.J. Williams, C. Grulke, G. Patlewicz, A. Richard**

10:30 ENVR 218. Towards the Virtual Bioprofiling of PFAS Derivatives. **D. Fourches**

10:50 ENVR 219. Protein pairing and lipid linking: Mechanistic studies reveal the effects of environmental conditions and PFAS mixtures. **J. Orr, M. Fedorenko, G.D. Bothun**



TECHNICAL PROGRAM

11:10 ENVR 220. Monitoring PFAS in the environment: From regulatory to emerging methods. **T. Anumol**, J. Pyke, R. Rhindle, T. Coggan, B. Clarke

11:30 Discussion.

11:55 Concluding Remarks.

Section C

Orange County Convention Center
Valencia Ballroom B-D - Theater 8

Applications & Implications of Nanomaterials & Their Toxic Effects

S. Hussain, N. Mallikarjuna, B. A. Manning, *Organizers*
S. R. Kanel, R. O'Hara, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 ENVR 221. Silver nanoparticle stability and oxidative dissolution by metal oxide soil minerals. B.A. Manning, **S.R. Kanel**, E. Guzman, S.W. Brittle

8:45 ENVR 222. Nanoscience in cosmetics. **H. Kumari**, X. Kang, M. Mirzamani, A. Dawn

9:05 ENVR 223. In vitro pulmonary toxicity of reduced graphene oxide-nano zero valent iron nanohybrids and comparison with parent nanomaterial attributes. **N. Aich**, A. Masud, Q. Wang, Y. Wu

9:45 ENVR 224. Toxicity evaluation of particles and additives used in the semiconducting industry. **E. Andreescu**, E. Dumitrescu, K. Wallace

10:05 Intermission.

10:20 ENVR 225. Impact of engineered nanoparticles on aquatic microbial communities. **Y. Liang**, N. Londono, A. Donovan, M. Geisler, H. Shi

11:00 ENVR 226. Qualitative and quantitative evaluation of nanomaterial release from multi-walled carbon nanotubes epoxy composite after weathering treatment. **Y. Zhao**, G. Ramakrishnan, D. Goodwin, L. Sung, E. Petersen, A. Orlov

11:20 ENVR 227. Determining what really counts: Modeling and measuring nanoparticle number concentrations. E. Petersen, **A. Montoro**, B. Toman, M. Johnson, M. Ellefson, G. Caceres, A. Neuer, Q. Chan, J. Kemling, B. Mader, K. Murphy, M. Roesslein

11:40 ENVR 228. Easily-recoverable, micron-sized TiO₂ hierarchical spheres decorated with cyclodextrin for enhanced photocatalytic degradation of organic micropollutants. **D. Zhang**, P.J. Alvarez

Section D

Orange County Convention Center
Valencia Ballroom B-D - Theater 12



TECHNICAL PROGRAM

Photocatalytic & Electrochemical Processes in Green Energy & Environmental Remediation: A Symposium in honor of Professor Krishnan Rajeshwar

D. D. Dionysiou, *Organizer*
C. Janaky, V. K. Sharma, N. Wu, *Organizers, Presiding*

8:15 Introductory Remarks.

8:20 ENVR 229. Combination of insulating boron nitride and inert Au substrate as an efficient electrocatalysts for oxygen reduction reaction and hydrogen evolution reaction. **K. Uosaki**, G. Elumalai, H. Noguchi

8:50 ENVR 230. Synthesis of a graphene-coated cathode for the electro-Fenton treatment of TMDD. Z. Wang, H. Olvera-Vargas, O. Garcia-Rodriguez, M. Surmani Martins, S. Garaj, **O. Lefebvre**

9:20 ENVR 231. FTO-TiO₂ photoelectrocatalytic degradation of triphenyltin chloride coupled to photoelectro-Fenton. **H. Olvera-Vargas**, X. Jianxiong, O. Lefebvre

9:40 ENVR 232. Capacitive performance of heteroatom-enriched activated carbon prepared from waste plastic bottles. **D. Shu**, H. Chen

10:00 Intermission.

10:15 ENVR 233. Enhanced oxidation of organic pollutants in water by activated ferrate(VI): Electron-transfer versus oxygen-atom transfer reductants. M. Feng, C. Jinadatha, T. McDonald, **V.K. Sharma**

10:45 ENVR 234. Efficient Photocatalytic Reduction of Environmental Pollutants in Water. **Q. Li**

11:15 ENVR 235. Boron, phosphorus co-doped one dimensional graphitic carbon nitride for photodegradation of diclofenac. **A.B. Ganganboina**, N. Luong, R. Doong

11:35 ENVR 236. Nanofabrication of N-doped graphene oxide with magnesium ferrite for effective Pb (II) and As (III) sequestration: A comparative study. **M. Kaur**, M. Kaur, D. Singh, A.C. Oliveira, V. Garg, V.K. Sharma

Section E

Orange County Convention Center
Valencia Ballroom B-D - Theater 13

Great Achievements in ES&T: James J. Morgan Environmental Science & Technology Early Career Award Symposium

W. Aumiller, D. L. Sedlak, *Organizers*
D. Sedlak, *Presiding*

9:00 Introductory Remarks.

9:05 ENVR 237. "Everything is everywhere": A network analysis of SVOCs indoors with implications for human exposure. **M.L. Diamond**, C. Yang, A. Anderson, S.A. Harris, L.M. Jantunen, L. Melymuk



TECHNICAL PROGRAM

9:30 ENVR 238. Toxicity of novel two-dimensional material. G. Qu, **G. Jiang**

9:55 Intermission.

10:10 ENVR 239. High-resolution air pollution mapping with Google Street View cars: Exploiting big data. **J. Apte**

10:35 ENVR 240. Discovery of neonicotinoid insecticides in finished drinking water and formation of novel products with altered pharmacophores during chlorination. **G.H. LeFevre**, D.M. Cwiertny, K.K. Wong, D. Webb, D.W. Kolpin, M.L. Hladik

11:00 ENVR 241. Technology horizon for photocatalytic water treatment: Sunrise or sunset? **J. Kim**, S. Loeb, P.J. Alvarez, J. Brame, E.L. Cates, W. Choi, J.C. Crittenden, D.D. Dionysiou, Q. Li, G. Li Puma, X. Quan, D.L. Sedlak, D. Waite, P.K. Westerhoff

11:25 ENVR 242. Understanding and mitigating the emerging microbial-associated threats in our treated wastewaters. D. Mantilla-Calderon, N. Ausburger, H. Cheng, N. Aljassim, **P. Hong**

11:55 Concluding Remarks.

Section F

Orange County Convention Center
Valencia Ballroom B-D - Theater 14

Photooxidation in Engineered and Natural Systems

G. Li Puma, K. E. O'Shea, W. Song, *Organizers*
D. D. Dionysiou, D. Minakata, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 ENVR 243. New insight into removal of trace organic contaminants in chloramine-impacted UV-H₂O₂ system for water reuse. **K. Mangalgi**, S.D. Patton, L. Wu, K.P. Ishida, H. Liu

9:00 ENVR 244. Ciprofloxacin (CIP) Degradation and CIP resistant *E. faecium* inactivation by UV-LED/Chlorine Process. **T. Kim**, K. Zoh, T. Kim

9:25 ENVR 245. Novel disinfection process by peracetic acid combined with UV irradiation (i.e. PAA-UV/PAA): Underlying photooxidation chemistry. **T. Zhang**, B. Mejia-Tickner, P. Sun, T. Wang, X. Xie, C. Huang

9:50 ENVR 246. Coupling Experimental and Theoretical Investigation of Fate of Photochemical Oxidation of Nitrosamine and Nitrogen-containing Species. **D. Minakata**, E. Coscarelli

10:15 Intermission.

10:30 ENVR 247. Degradation Kinetics and Cytotoxicity Analysis of Contaminants of Emerging Concern Treated by UV/H₂O₂ and UV/NO₃⁻. **D.D. Dionysiou**, Y. Huang, M. Kong, S. Coffin, D. Westerman, K. Cochran, E. Xu, D. Schlenk, S.D. Richardson



TECHNICAL PROGRAM

11:00 ENVR 248. Degradation of chloroform and chlorobenzene by pulsed streamer plasma: A comparative study. J. Jose, **L. Philip**

11:25 ENVR 249. Ultrasonic degradation of the flame retardant tris (2-chloroethyl) phosphate (TCEP) in aqueous solution: Kinetics and mechanistic investigation. **A. Abdullah**, K.E. O'Shea

11:50 Concluding Remarks.

Section G

Orange County Convention Center
Valencia Ballroom B-D - Theater 11

When Chemistry Meets Biology: Novel Solutions for Emerging Challenges in Pollutant Control, Remediation & Resource Recovery

C. M. Sales, W. Zhuang, *Organizers*
X. Mao, Y. Men, S. Yi, *Organizers, Presiding*
C. Sales, *Presiding*

8:30 Introductory Remarks.

8:35 ENVR 250. Withdrawn

8:55 ENVR 251. Synthesis of novel terpyridine functionalized superparamagnetic nanoparticles and its effectiveness for the removal of rhodamine B from wastewater. **M.O. Ojemaye**, O.O. Okoh, A. Okoh

9:15 ENVR 252. Development of a bioelectrochemical system for simultaneous energy and nutrient recovery from wastewater treatment. **C. Dykstra**

9:35 ENVR 253. Simultaneous chemical-free nitrogen and phosphorus recovery from municipal wastewater. **M.K. Perera**, J. Englehardt

9:55 ENVR 254. Microbial Electrochemical Nutrient Recovery from Wastewater. X. Chen, D. Hou, **Z.J. Ren**

10:25 Intermission.

10:40 ENVR 255. Biogeochemistry of depleted uranium in US army shooting site and potential remediation. **F.X. Han**, L. Chen, J. Li, Q. Zhang, Z. Arslan

11:00 ENVR 256. Engineering a light-responsive biofilm to mitigate membrane biofouling. M. Mukherjee, Y. Hu, **B. Cao**

11:20 ENVR 257. Environmental fate of carbon nanotubes: New insights into microbial activities. **Y. You**, K.K. Das, H. Guo, C. Chang, M. Navas-Moreno, J. Chan, P. Verburg, S. Poulson, X. Wang, B. Xing, Y. Yang

11:40 ENVR 258. Predation and parasitism induces community stability and performance within EBPR reactors. **J.R. Price**, Y. Nan, Y. Wang, M. Cheng, S. Keshani, S. Woloszynek, G. Rosen, L. Yuan, C.M. Sales



TECHNICAL PROGRAM

Elucidation of Mechanisms & Kinetics on Surfaces

Kinetic Modeling

Sponsored by CATL, Cosponsored by ENFL, ENVR, INOR and PHYS

TUESDAY AFTERNOON

Section A

Orange County Convention Center
Valencia Ballroom B-D - Theater 9

Current Status of Environmental Research on Water Contaminants

S. Ahuja, B. G. Loganathan, *Organizers, Presiding*

1:00 Introductory Remarks.

1:05 **ENVR 259.** Challenges with lead and copper sampling: Case study in Puerto Rico. **M.R. Warren**, F.L. Rosario, J.A. Korak

1:25 **ENVR 260.** Effectiveness of orthophosphate addition for controlling lead levels in water conveyed through lead service lines during a switch in disinfectant. **Y. Bae**, V. Liu, J.D. Pasteris, D. Giammar

1:45 **ENVR 261.** Effects of sodium silicate on surface chemistry of fresh copper-lead galvanic joints in a prepared chlorinated water. X. Ma, **M. Alam**, F. Ribeiro, V. Sidorkiewicz, D. Lytle, W. Lee

2:05 **ENVR 262.** Effects of sodium silicate corrosion inhibitors on lead release from pipe materials. **A. Mishra**, D. Giammar

2:25 Intermission.

2:40 **ENVR 263.** Lead-catalyzed redox-driven recrystallization of lead oxide. **W. Pan**, D. Giammar

3:00 **ENVR 264.** Removal of Arsenic from water using iron oxide precipitated Douglas fir biochar. **C. Navarathna**, A. Karunanayake, T. Mlsna

3:20 **ENVR 265.** Destruction of γ -hexachlorocyclohexane versus hexachlorobenzene in an acidified ethanol using ball-milled ZVMg. **A.M. Garbou**, J.A. Gomez, C. Yestrebky

3:40 **ENVR 266.** Biochar adsorbent with enhanced hydrophobicity for oil spill removal. C. Navarathna, N. Dewage, C. Keeton, J. Pennisson, **E. Henderson**, T. Mlsna

4:00 **ENVR 267.** Utilization of fly ash permeable reactive barrier to remove heavy metals from contaminated water. **H. Rostami**, **M. Bahadory**

4:20 Closing Remarks.



TECHNICAL PROGRAM

Section A

Orange County Convention Center
West Hall C

Abiotic & Biotic Pollutant Transformation in Soils

G. Chen, H. Cheng, *Organizers*

4:00 - 6:00

ENVR 268. Degradation of chlorantraniliprole in california rice field soils. **Z. Redman**, R.S. Tjeerdema

ENVR 269. Environmental fate and ecotoxicity of explosives in contaminated sites. **C.S. Chen**, C. Tien

ENVR 270. Computational approach for quantifying the interactions of mercury with low molecular weight organic compounds. **D. Devarajan**, P. Lian, S. Brooks, J. Parks, J. Smith

ENVR 271. Thallium bioaccessibility in 13 contaminated soils from China: Correlation to thallium relative bioavailability and thallium in different fractions. **H. Deng**, M. Luo, M. Liu, T. Xiao, Y. Chen, J. Luo

ENVR 272. Optimized combination of fillers in constructed wetlands. **Z. Duan**, S. Xie, N. Li

ENVR 273. Optimized combination of fillers in constructed wetlands for eutrophication control. **Z. Duan**, S. Xie, N. Li

ENVR 274. Effect of sludge fermentation broth as pH buffer solution on hydrogen production efficiency of MEC-AD coupling reaction system. **H. Bao**, X. ZHANG, H. Su, X. Zhang

Section A

Orange County Convention Center
West Hall C

Accurate Mass/High Resolution Mass Spectrometry for Environmental Monitoring & Remediation

T. Anumol, R. Marfil-Vega, T. M. Young, C. Zwiener, *Organizers*

4:00 - 6:00

ENVR 275. Diurnal variation of PM_{2.5}-bound polycyclic aromatic hydrocarbons in Ho Chi Minh City, Vietnam during 2013-2014 using TD-GC/MS. **O.K. Pham**, H.T. To, Y. Itano, D. Asakawa, N. Takenaka

ENVR 276. Identification of biotic and abiotic transformation products of the antidepressant fluoxetine by LC-HRMS. S. Tisler, F. Zindler, T. Braunbeck, **C. Zwiener**

ENVR 277. Determination of bromate in drinking water using ion chromatography-single quadrupole mass spectrometry. **J. Hu**, J. Rohrer



TECHNICAL PROGRAM

ENVR 278. Withdrawn

Section A

Orange County Convention Center
West Hall C

Applications & Implications of Nanomaterials & Their Toxic Effects

S. Hussain, S. R. Kanel, N. Mallikarjuna, B. A. Manning, R. O'Hara, *Organizers*

4:00 - 6:00

ENVR 279. Environmental exposures to titanium dioxide engineered. **M. Baalousha**

ENVR 280. Selective oxidation of hydroxymethylfurfural to furandicarboxylic acid using air and chitosan-derived porous nitrogen-enriched carbonaceous carbon nitride catalyst. **S. Verma**, R.S. Varma, M. Nadagouda

ENVR 281. C-H activation and oxidative cyanation of amines using protuberant lychee-like goethite. S. Verma, R.S. Varma, **M. Nadagouda**

ENVR 282. Quantification of TiO₂ engineered nanoparticles in natural soils. **J. Wang**, S. Mohanty, M. Baalousha

ENVR 283. Interaction of graphene oxide and reduced graphene oxide nanomaterials with model biological surfaces. **D.C. Bouchard**, X. Chang, M. Henderson, R.G. Zepp

ENVR 284. Enhanced immobilization of U(VI) using a new type of FeS-modified Fe⁰ core-shell particles. J. Duan, **D. Zhao**

ENVR 285. Water dispersible and magnetically recoverable carbon-coated iron carbide for organic and arsenic adsorption. **C. Powell**, S. Guo, K. Ventura, A.W. Lounsbury, R. Turley, J.L. Gardea-Torresdey, D. Villagran, J.B. Zimmerman, A. Atkinson, P.K. Westerhoff, M.S. Wong

ENVR 286. Cobalt oxyhydroxide: a novel and highly efficient peroxymonosulfate activator for degradation of 2,4-chlorophenol in water. **C. Lyu**, Y. Lyu, T. Xi, X. Li

ENVR 287. High fluorescence carbon dots from kappa-carrageenan for fluorescence imaging, chemical and metal ion sensor applications. **M. Sinoy**, M.G. de Luna, P. Paoprasert

ENVR 288. VOC emissions from carbon nanotube composites used in 3D printing. **P. Potter**, S.R. Al-Abed, D. Lay, S.M. Lomnicki

ENVR 289. Exposure of hepatocellular carcinoma (HEP-G2) to CdSTe quantum dots. **A. Ponton**, L. Alamo-Nole

ENVR 290. Comparative study of methods for the synthesis of silica nanoparticles from sugarcane waste ash. **S. Rovani**, D.A. Fungaro, F.B. Carvalho, J.J. Santos

ENVR 291. Development of a chemi-assay battery for nanoparticle biotransformation. **M. George**, C.M. Sayes



TECHNICAL PROGRAM

Section A

Orange County Convention Center
West Hall C

Aquatic Photochemistry

W. Arnold, K. P. McNeill, S. G. Pati, *Organizers*

4:00 - 6:00

ENVR 292. Photolysis of aqueous atmospheric aerosol mimics. **M.M. Galloway**, D. Grace, J.R. Sharp, R.E. Holappa, A.M. King

ENVR 293. Disinfection byproducts formation in UV/chlorine process for micro-polluted water treatment. **X. Zhang**

ENVR 294. Electroactive polymer nanocomposites for photocatalysis. **M. Ocampo**, **V.G. Marin-Ponce**, K.K. Burke, J.A. Irvin

ENVR 295. Estrogenic properties and removal of tetrabromobisphenol-a (TBBPA) by UV advanced oxidation. **B.A. Taylor**, P.A. Ruiz-Haas

ENVR 296. Study of the photolysis and cellular toxicity of the organic ultraviolet filter chemical 3-(4-methylbenzylidene) camphor and its photoproducts. **N. Derosier**, S.R. Kearing, L. MacManus-Spencer

ENVR 297. Investigation of the photolysis of the common UV filter chemical octyl dimethyl para-amino benzoic acid and its photoproducts. **S.R. Kearing**, N. Derosier, L. MacManus-Spencer

ENVR 298. Source and influence of hydroxyl radicals on the photoaging of particulate matter in the environment. **F. Leresche**, J. Salazar, D.J. Pfothenauer, M.P. Hannigan, B.J. Majestic, F.L. Rosario

ENVR 299. Phototransformation and residual antimicrobial activity of five macrolide antibiotics in UV-254 engineered systems. **T. Ibitoye**, M. Hopanna, B.M. Anger, E.R. Hain, K. He, L.M. Blaney

Section A

Orange County Convention Center
West Hall C

Aqueous Contaminant Separation, Resource Recovery & Clean Energy Generation by Electrochemical Processes

D. F. Call, O. Coronell, M. Hatzell, *Organizers*

4:00 - 6:00

ENVR 300. Simultaneous selenate removal, elemental selenium recovery and electricity generation by a biocathode microbial fuel cell. **Z. Zhang**, Y. Tang



TECHNICAL PROGRAM

- ENVR 301.** Surveying faradaic electrode materials for efficient electrochemical water desalination. **V. Pothanamkandathil**, C. Gorski
- ENVR 302.** Hydrogen production via proton exchange membrane water electrolyzer with non-noble cathode. **S. Ahn**, J. Kim, H. Kim, J. Kim
- ENVR 303.** Boron removal from water by electrocoagulation, and comparison with chemical coagulation. **M. Chen**, O. Dollar, S. Waseem, K. Shafer-Peltier, S. Randtke, E.F. Peltier
- ENVR 304.** Electrodialysis pretreatment to reduce fouling of nanofiltration membranes for treatment of produced water. **M.R. Landsman**, S. Kum, D. Lawler, L.E. Katz
- ENVR 305.** Novel anaerobic electrochemical membrane bioreactor with CNTs hollow fiber membrane cathode to mitigate membrane fouling and enhance energy recovery. **S. Qiao**, Y. Yang, X. Quan, J. Zhou
- ENVR 306.** Effect of electrode orientation on salt removal in flow-through capacitive deionization. **Y. Algurainy**, S. Zhu, D.F. Call
- ENVR 307.** Mass transport in ion exchange membrane: a percolation simulation study. **H. Gao**, B. Zhang, Y. Chen
- ENVR 308.** Water-Energy Nexus: Electrochemical Removal of Silica from Alternative Cooling Water Sources. **L. Valentino**, Y.J. Lin
- ENVR 309.** Withdrawn
- ENVR 310.** Electrochemical water desalination: Framework for selecting among manganese oxide electrode materials. **J. Fortunato**, C. Gorski
- ENVR 311.** Enhancing forward osmosis water recovery from landfill leachate by desalinating brine and recovering salts in a microbial desalination cell. **S. Iskander**, Z. He, J. Novak
- ENVR 312.** Redox-Active Metallopolymer Electrodes for Selective Heavy-Metal Oxyanion Capture and Remediation. **X. Su**, T. Hatton
- ENVR 313.** Low energy desalination using a novel capacitive deionization-electrodialysis process. **T. Chen**, C. Hou
- ENVR 314.** Characteristics of Natural Organic Matter Foulants on Nano-filtration Surfaces: The Effect of Electrodialysis Pretreatment. **S. Kum**, D. Lawler, L.E. Katz

Section A

Orange County Convention Center
West Hall C

Combined Biological-Chemical Reactions for Contaminant Transformation

J. Blotevogel, K. T. Finneran, S. Jin, *Organizers*

4:00 - 6:00



TECHNICAL PROGRAM

ENVR 315. Biologically mediated abiotic degradation of bisphenol A. **Y. Sun**, N. Shobnam, J. Im, G. Chen, Y. Yin, S. Campagna, F. Loeffler

ENVR 316. Biochar-mediated microbial dehalogenation. Y. Zhou, **Y. Yang**

ENVR 317. Quantifying biodegradation rates of 17 β -estradiol in sewage impacted rivers at environmentally relevant concentrations. **M. Carolan**, A. Romig, C. Hutchinson, D.R. Griffith

ENVR 318. Biodegradation of nonylphenol in waste activated sludge during anaerobic fermentation production and mechanisms. **X. Duan**, L. Feng, Q. Zhou, X. Wang, J. Xie, Y. Yan, F. Wang

ENVR 319. Characterization of nitrogen transformation in the nitrification layer of both lab-scale and pilot-scale Nitrogen Removing Biofilters (NRB). **Z. Maleki Shahraki**, X. Mao, S. Waugh, H. Walker, F. Russo, C. Gobler

ENVR 320. Transformation of neonicotinoid insecticides and their mammalian toxic metabolites by bio-augmented black carbon. **D. Webb**, G.H. LeFevre

ENVR 321. Engineering surface-display laccase biocatalyst for treating emerging organic contaminants: Kinetics and enzyme catalytic properties in acetaminophen degradation. **Y. Wu**, Y. Chen, N. Wei

ENVR 322. Novel enzymatic formate production from carbon monoxide using CO hydratase system. **H. Hwang**, J. Lee, Y. Kim

ENVR 323. Effect of dissolved oxygen for subsurface flow constructed wetlands for wastewater treatment. **Y. Gao**, J. Liu

Section A

Orange County Convention Center
West Hall C

Contributions of a Simple Chemist: How Professor Ronald Atlee Hites Changed Environmental Chemistry

E. T. Furlong, S. T. Glassmeyer, S. L. Simonich, E. M. Ulrich, M. Venier, *Organizers*

4:00 - 6:00

ENVR 324. Emissions and fate of organophosphorus flame retardants in the indoor environment using a natural environmental chamber model and the implications for human exposures. **Y. Ma**

ENVR 325. Isotope fingerprints as natural gas fugitive emission source constraints. **C.R. Nelson**

Section A

Orange County Convention Center
West Hall C

Current Status of Environmental Research on Water Contaminants



TECHNICAL PROGRAM

S. Ahuja, B. G. Loganathan, *Organizers*

4:00 - 6:00

ENVR 326. Occurrence and fate of Fluoroquinolone resistant bacteria in a sewage treatment plant in India. **J. Kurasam**, S. Sarkar, P. K. Mandal

ENVR 327. Withdrawn

ENVR 328. Determination of total Hg in ASGM Samples via ICP-OES in comparison to DMA-80 Analysis. **C.S. Seney**, A.M. Kiefer, S. Aljic

ENVR 329. Method development/determination of the disposition of Hg in tissues of rats exposed to Hg(CN)₂. **C.S. Seney**, A.M. Kiefer, C.C. Bridges, M.E. Moore, L. Joshee

ENVR 330. New antimicrobial approaches for the treatment of antibiotic-resistant bacteria in water. **S. Joo**, S. Baek

ENVR 331. Cytotoxic effects of urban watersheds on HT29 Cells. **D. Abdullah-Smoot**

ENVR 332. Evaluation of volatile organic compounds and polyaromatic hydrocarbons in Barker Reservoir in Houston, Texas after the 2017 Hurricane Harvey. **T. Phan**

ENVR 333. Evaluation of granular activated carbon performance to remove 1,4-dioxane degradation byproducts and residual H₂O₂ from UV/H₂O₂ treatment system. **Y. Tang**, C. Lee, A. Venkatesan, X. Mao, C. Gobler, H. Walker

ENVR 334. Biosorption of steroidal hormones onto sorbents prepared from *Chlorella vulgaris* biomass. **C. Engelhard**, A. Cadkova, T. Potocar, T. Branyik

ENVR 335. Lead levels in ocean water near Culebra Island in Puerto Rico are substantially above EPA permissible limits for coastal and estuarine water. **L. Vazquez-Szendrey**, P. Das, D. Giacherio, S. Zamule, A. Gimler, R. Pacella

ENVR 336. Withdrawn

ENVR 337. Using EEM-PARAFAC to probe membrane fouling potential of stabilized landfill leachate pretreated by various options. **J. Hur**, B. Aftab, J. Cho

ENVR 338. Assessing rural groundwater for atrazine contamination in central Pennsylvania. **F.M. Ferguson**, U.J. Williams, S.S. Yohn

ENVR 339. Light adsorption and fluorescence properties of fractionated natural organic matter upon loading with arsenic and selenium. **Z. Zhang**, **P. Pham**, D.D. Dionysiou, K.E. O'Shea

ENVR 340. Phosphate removal from waste water using novel renewable resource-based, cerium/manganese oxide-based nanocomposites. **A. Nakarmi**, S.E. Bourdo, T. Viswanathan

ENVR 341. Enhanced membrane distillation using nanomaterial based membranes for organic solvent separation from their aqueous mixtures. **O. Gupta**, S. Roy, S. Mitra

ENVR 342. Functionalized Carbon Nanotube Enhanced Membrane Distillation. **M.s. Humoud**, S. Mitra



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

ENVR 343. Graphene oxide immobilization on the permeate side of the PTFE membrane to enhance flux in membrane distillation. **W. Intrchom**, S. Mitra, S. Roy, M.s. Humoud

ENVR 344. Roteoneone attenuation in high latitude lakes and laboratory assessment of photolytic vs. microbial degradation. **J. Couture**, J. Bozzini, B. Briggs, R. Massengill, P.L. Tomco

ENVR 345. Produced water filtration using clay filters. **A. Johnson**, M. Montes

Section A

Orange County Convention Center
West Hall C

Electrochemical Water Treatment

J. Blotevogel, B. P. Chaplin, C. Schaefer, *Organizers*

4:00 - 6:00

ENVR 346. Use of electroflocculation in remediating industrial wastewaters in the Philippines. **E.E. Mojica**, L.S. Arcillas, C.C. Ramos, D.O. Alabat, V.P. Migo

ENVR 347. Flower-like MgAl layered double hydroxides grown on carbon paper as a free-standing electrode for efficient electrochemical sensing of nitrite. **X. Xiang**, F. Pan, Y. Li

ENVR 348. Electrocatalytic Oxidation Degradation of Ammonia Nitrogen Wastewater. **Z. Yang**, G. Yan, S. Guo

Section A

Orange County Convention Center
West Hall C

Emerging Issues on & Horizon Technologies for Water Disinfection

N. B. Saleh, X. Xie, *Organizers*

4:00 - 6:00

ENVR 349. Efficient reduction of bromate by iodide-assisted UV/sulfite process. X. Liu, **J. Wang**, D. Yan

ENVR 350. Comparing bromination and chlorination kinetics of the herbicide dimethenamid in natural and in synthetic waters. **M.H. Schammel**, T.L. Swanson, R.P. Dias, J.D. Sivey

ENVR 351. Formation of by-products during the chlorination disinfection on UV filter 2,4-dihydroxybenzophenone. **D. Wei**

ENVR 352. Protein phosphatase inhibition assays (PPIA) for the evaluation of microcystin oxidation products. **A. Herppich**, B. Spies, D. Szlag



TECHNICAL PROGRAM

Section A

Orange County Convention Center
West Hall C

General Posters

S. O. Obare, *Organizer*

4:00 - 6:00

ENVR 353. Three-dimensionally Ordered Macroporous $\text{La}_{1-x}\text{K}_x\text{MnO}_3$ Perovskite-type Metal Oxides Catalysts for the Simultaneous Removal of PM and NO_x from Diesel Engines. **R. Li, Z. Zhao**

ENVR 354. Flower-like bismuth metal-organic frameworks grown on carbon paper as a free-standing electrode for efficient electrochemical sensing of Cd^{2+} and Pb^{2+} in water. **X. Xiang, F. Pan, Y. Li**

ENVR 355. Combining nanoplastics characterization and metabolomic approach to assess polymers biodegradation. **B. Eyheraguibel, M. Lerembour, M. Brissy, B. Diem, M. Sancelme, A. Delort**

ENVR 356. Liquid crystal electrode assisted-hybrid bio-electrochemical reactor for enhanced biofilm attachment and sustainable wastewater treatment. **R. Srinivasan, I. Nambi, J. Senthilnathan**

ENVR 357. Withdrawn

ENVR 358. Tunable effect of dopants on the carbon support on the catalytic properties of a single gold atom catalyst in CO oxidation. **S. Ali**

ENVR 359. Gold recovery from electronic waste by nanoporous polymers. **C.T. Yavuz, Y. Hong, D. Thirion, S. Subramanian**

ENVR 360. Improving Mg/S battery performance by YCl_3 additive and magnesium polysulfide. **Y. Xu**

ENVR 361. Detection of nitro aromatics with MOF's. **J. Kaur**

ENVR 362. High efficiency water desalination via 2D MoS_2 layer membranes of near atomic thickness. **H. Li, Y. Jung**

ENVR 363. Withdrawn

ENVR 364. One-pot synthesis of hierarchical porous carbon from polyvinyl chloride for high performance supercapacitor: Nano-ZnO as an antichlor and activator. **Z. Xiaoli, H. Zhang, L. Shao, F. Lü, P. He**

ENVR 365. Investigation on the Catalytic Performance of $\text{La}_{0.9}\text{Ce}_{0.1}\text{Co}_{0.8}\text{Fe}_{0.2}/3\text{DOM Al}_2\text{O}_3/$ Honeycomb Ceramic Monolith Catalyst for Soot Combustion and Acid Modification. **K. Zhao, Z. Zhao**

ENVR 366. Preparation of aluminosilicate gel from coal fly ash for the removal of toxic metals from wastewater. **B. Wang, L. Li, H. Xu, Y. Wang**



TECHNICAL PROGRAM

- ENVR 367.** Water quality chemistry in the Great Lakes region: Crowd sourcing classroom data to bring researchers and classrooms together. **R. Adams**, D.J. Lecaptain, J.H. Tomasik
- ENVR 368.** Effect of cation doping on reversible CO₂ adsorption on promoted MgO-CaO solid solutions: A first-principles based study. **S. Kang**, J. Jang
- ENVR 369.** Development of bimetallic Pd-based catalyst supported on the hollow carbon spheres for selective nitrate and nitrite reduction. **K. Hong**, Y. Choi, J. Choe
- ENVR 370.** Effect of Low Molecular Weight Organic Acids on the Kinetics of Disjunctive Ligand Exchange: Lewis base identity and chelate ring size. **L. Briody-Pavlik**, **Z. Huang**, N.E. Boland
- ENVR 371.** High Pressure CO₂ Adsorption on Hierarchical Porous Carbon with N-Functional Group. **T. Chaisuwan**, N. Manmuanpom, S. Wongkasemjit
- ENVR 372.** Establishing Ecological Interrelationships Between Manufactures, Products and Consumers Using A Returnable or Take Back System. **T. Clardy**
- ENVR 373.** Investigating the utility of silicone bands as passive samplers to monitor the health of honey bee hives. **E. Bullock**, A. Schafsnitz, R. Broadrup, A. Macherone, C. Mayack, H.K. White
- ENVR 374.** Advanced oxidation processes used to disinfect wastewater: Role of electrode material. **M. Carlson**, N. Barashkov, L. Lam, Z. Eisenberg
- ENVR 375.** Rapid characterization of oil residues in the environment by Fourier-transform infrared spectroscopy. **C. Dhoonmoon**, M. Luu, C. Samuels, H.K. White
- ENVR 376.** Perchlorate and sulfate in arctic snow from the AD 1600 Huaynaputina (Peru) volcanic eruption. **J. Gibson**, A. Shea, J. Kennedy, J. Cole-Dai
- ENVR 377.** Removal of industrial dyes from aqueous solution with ionic liquids. **A. Hall-Terracciano**, R.E. Del Sesto
- ENVR 378.** Investigating the reactivity and growth of iron oxide nanoparticles using catechol. **N. Harper**, J. Voelz, R. Penn
- ENVR 379.** Photochemical Degradation and Relative Toxicity of Various Motor Oils. **L. Heidenreich**, **I. Parker**, P.L. Bann, M. Bertelli, C. Smylie, C. Pratt, W.H. Jeffery, **P.P. Benz**
- ENVR 380.** Development of organic solvent resistant hollow fiber nanofiltration via thermally induced phase separation. **J. Hou**, S. Jeon, J. Yun, H. Byun
- ENVR 381.** Multi-Analytical method of biocides from living chemical products using LC/MSMS. **J. Hyeong-Wook**, K. Hwang, J. Kwon, J. Moon
- ENVR 382.** Comparison of water quality and geomorphology changes of estuaries of the Natural Reserve Caño Boquilla in Mayagüez-Añasco, Puerto Rico. **E. Jusino-Jusino**, A.M. Gonzalez-Mederos, A. Navarro-Rodríguez, V. González
- ENVR 383.** Preparation of ion imprinted sorbent for selective removal of Cd(II). **Y. Kim**, H. Hong, J. Kim, H. Kwon
- ENVR 384.** Oxidation of chlorophenols by persulfate/heat activation. J. Son, C. Chen, S. Bae, S. Woo, **Y. Kim**



TECHNICAL PROGRAM

- ENVR 385.** Methylmercury removal on the surface of zero-valent iron particles. O. Lem, M. Abseit, G. Tokazhanov, Q. Ghulam, S. Han, **W. Lee**
- ENVR 386.** Crystallographic study of selectivity of Sr²⁺ ion in presence of competing cation as Na⁺ ion. **W. Lim**, H. Kim, D. Moon, J. Lee, O. Byambasuren
- ENVR 387.** Extraction and analysis of heavy metals from the soil in Alcorn State University kindergarten playground. **C. McCullum**
- ENVR 388.** Removal of hexavalent chromium from groundwater by stannous chloride reductive treatment. **D.T. Nguyen**, S. Sinha, P.K. Westerhoff
- ENVR 389.** Adsorption studies of the treatment of palm oil mill effluent (POME), using powdered defatted *Moringa oleifera* seed. **J.E. Osazuwa**
- ENVR 390.** Removal and stabilization of Cs⁺ using natural and synthetic zeolite. **M. Park**, J. Park, S. Kim, **H.Y. Jeong**
- ENVR 391.** Controlled release of persulfate and Fe²⁺ ions for contaminant treatment. **P. Pham**, R. Federico-Perez, Z. Xue
- ENVR 392.** Heavy metal remediation from aqueous solutions by new silica-immobilized-thiosemicarbazone materials. **E. Rush**, C.A. Hawkins, E.C. Lisic
- ENVR 393.** Dynamic behavior of mercury release during coal carbonization and iron ore sintering. **N. Tsubouchi**, J. Bud, Y. Mochizuki
- ENVR 394.** Selectively capturing tobacco specific nitrosamines by tailored activated carbon and graphene. C. Shi, X. Sun, Y. Wang, **J. Zhu**

Section A

Orange County Convention Center
West Hall C

Green Chemistry & the Environment

R. Luque, S. O. Obare, *Organizers*

4:00 - 6:00

- ENVR 395.** Bipyridine functionalized core-shell Ag@TiO₂ nanoparticle films for enhanced Raman spectroscopy: Applications for the detection of Cu(II) ions and film stability studies. F. Forato, S. Talebzadeh Farooji, N. Rousseau, J. Mevellec, B. Bujoli, D. Knight, **D. Wilson**, C. Queffelec, B. Humbert
- ENVR 396.** Removal of pharmaceutical compounds from water via cellulose acetate membranes embedded with the block-copolymer PEO-P4VP. **L.I. Penabad Peña**, M. Betancourt, J. Herrera, E. Nicolau
- ENVR 397.** Controlled Release Pellets embedded in Polyvinyl Acetate (PVAc) to release and Model KMnO₄ within different Soil Media. **M. Lamssali**, S. Luster-Teasley, **D. Deng**



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- ENVR 398.** Utilizing hydrotropes to increase flow battery storage densities. **Y. Cheng**, R. Hickey, C. Gorski
- ENVR 399.** Bioremoval of sulfur compounds from synthetic fuels using modified clays. **S.A. Shahrear**
- ENVR 400.** Microwave-assisted Knoevenagel-Doebner reaction: An efficient method for phenolic acids synthesis. **L. Mouterde**, F. Allais
- ENVR 401.** Demonstration of a novel nanopore biopolymer adsorbent for removal of Cadmium and Nitrate pollutants from water. **A. Esmailian**, A. Mahdavi Mazdeh, H. Ghafourian, K.E. O'Shea
- ENVR 402.** Simultaneous purification of PM and NO_x over 3DOM Fe-Mn oxide catalysts. **J. Tan**, J. Liu, Z. Zhao
- ENVR 403.** Sulfidogenic wastewater treatment with iron sulfide sludge oxidation and recycle process. **D. Deng**
- ENVR 404.** Citric juices-mediated synthesis of tellurium nanoparticles with antimicrobial and anticancer properties. **B. Zhang**, D. Medina, W. Tien-Street, X. Huang, A. Vernet, A. Roy, T. Webster
- ENVR 405.** Understanding the catalytic activity of Pt/Ni core shell nanoparticles toward oximation reactions. **S.S. Albalawi**, S.O. Obare
- ENVR 406.** Green nanoparticles for the detection of pharmaceuticals in the environment. **A.C. Ross-Obare**
- ENVR 407.** Environmental remediation of perfluorooctanoic acid using a novel multi-electron transfer system. **T.S. Saeed**, S.O. Obare
- ENVR 408.** Novel selective electrochemical sensor for toxic organophosphorus pesticides. **J.S. Arachchilage**, S.O. Obare
- ENVR 409.** Ultraviolet disinfection of activated carbon and its use for microbiological decontamination. A. Semenov, T. Sakhno, **N. Barashkov**
- ENVR 410.** Selectively reduced graphite oxide/poly(vinyl alcohol)nanocomposites for electromagnetic interference shielding application. **S. Srivastava**, K. Manna
- ENVR 411.** Investigation of a VOC emission prediction model for an automotive cabin based on equilibrium adsorption theory. J. Zheng, **L. Tong**, W. Liu, X. Liu, P. Zhang
- ENVR 412.** Effect of physical and chemical modification for cation and anion removal by natural organic polymer. **B. An**, T. Kim
- ENVR 413.** Comparative study on removal of heavy metals from aqueous solutions by different sizes of alginate hydrogels. **A. Albertorio-Rosado**, C.M. Osorio-Cantillo
- ENVR 414.** Purification of Lactic Acid by Using a Cost-Effective Adsorbent: Studying of Adsorption Isotherm for Scale-up Production. **C. Naksa-Nguan**, S. Wongkasemjit, T. Chaisuwan
- ENVR 415.** Adsorption of small polarisable molecules (CCl₄ CHCl₃) on Starbon® materials. **A.S. Aljameel**, V. Budarin
- ENVR 416.** Enhancement of electrolysis-ozonation system on removal of nitrobenzene by graphene electrode. **Y. Xin**, **C. Zhao**, **W. Tuo**, J. Lei, W. Cewen



TECHNICAL PROGRAM

ENVR 417. Correlation study between particulate matter and PAH concentrations: Bio-monitoring of pine tree leaves. **S. Deprele, S. Cortez, R. Moran**

ENVR 418. Cycloaddition of carbon dioxide to epoxides catalyzed by ionic liquids. **R. Brower**, S.T. Shipman

ENVR 419. Magnetic graphene oxide supported zeolitic imidazolate frameworks for As(III) removal from fresh water. **M. Marcos**, R. Arrieta, D. Villagran

ENVR 420. Facile, inexpensive, and scalable approach enabled robust TiO₂-coating on stainless steel mesh for oil/water separation. **W. Deng**, Y. Li

ENVR 421. Effect of pH change on the efficacy of *Acacia senegal* as a coagulant for rubber processing effluent treatment. **C.O. Ize-Iyamu, O.K. Ize-Iyamu**, J.E. Ukpebor, M.U. Farouk, B.O. Isiaka, R.E. Owhoudue, E.E. Ukpebor

ENVR 422. Green Avengers: An Environmental Club Promoting Local and Global Citizenship. **E. Englich**, S. Foster, G. Bonomo, M.M. Gillett-Kunnath, K. Ruhlandt-Senge

ENVR 423. *Moringa oliefera* seed powder for rubber processing effluent treatment by physicochemical method. **C.O. Ize-Iyamu, O.K. Ize-Iyamu**, J.E. Ukpebor, E.E. Ukpebor

Section A

Orange County Convention Center
West Hall C

Innovative & Practical Approaches for the Treatment of Per- & Polyfluoroalkyl Substances (PFAS)

J. Choe, J. Liu, S. Vyas, Y. Wang, *Organizers*

4:00 - 6:00

ENVR 424. Hydrodefluorination of poly- and perfluoroarenes by zeolite supported Rh-based catalysts. **S. An**, J. Choe

ENVR 425. pH-dependent solvated electron degradation of perfluorooctanesulfonate. **V.M. Breslin**, W.A. Maza, P.A. DeSario, A. Epshteyn, J. Owirutsky, B.B. Pate

ENVR 426. Reactivity comparison of various short-chain PFAS for TiO₂ photocatalytic decomposition. **N. Chowdhury**, H. Choi

ENVR 427. Urine and Serum Biomarkers of Per- and Polyfluoroalkyl Substances (PFAS) and Fluorinated Alternatives for Human Exposure Assessment. **K. Kato**, K. Hubbard, J. Eng, A.M. Calafat

ENVR 428. Concept development for physical adsorption combined with chemical decomposition of PFAS on reactive activated carbon. **A.C. Parenky**, N. Gevaerd de Souza, H.H. Nguyen, J. Jeon, H. Choi

ENVR 429. UV/nitritotriacetic acid process as a novel strategy for efficient photoreductive degradation of perfluorooctanesulfonate. Z. Sun, **C. Zhang**, L. Xing, Q. Zhou, W. Dong, M.R. Hoffmann



TECHNICAL PROGRAM

ENVR 430. Removal and Degradation Mechanism of Perfluorooctanoic acid (PFOA) during Electrocoagulation. M. Kim, T. Kim, T. Kim, **K. Zoh**

Section A

Orange County Convention Center
West Hall C

Micro- & Nano-Plastics in the Environment: Detection, Characterization, Fate & Impact

S. R. Al-Abed, M. J. Gallagher, P. Potter, *Organizers*

4:00 - 6:00

ENVR 431. Spatial distribution of microplastics in water and sediments from an urbanized river, Taiwan. **C. Tien**, C.S. Chen

ENVR 432. Formation of microplastics under environmental stressors. **T.S. Hebner**, M.A. Maurer-Jones

ENVR 433. Towards an extraction of MPs from muddy marshy and estuarine sediments (Winyah Bay, SC). **T.J. Hanebuth**, S.M. Ladewig, S.L. Whitmire, J.C. Bruni

Section A

Orange County Convention Center
West Hall C

Nanotechnology at the Water-Agriculture-Energy Nexus

A. A. Keller, G. Lowry, C. Sabilov, J. C. White, Y. Yang, *Organizers*

4:00 - 6:00

ENVR 434. Impact of ZnO nanoparticles on wastewater nitrification: A molecular approach. **V. Kapoor**

ENVR 435. Novel nanomaterials for oxidation of anoxic waters. **K.R. McCormac**, M.J. Beazley

ENVR 436. Magnetically Recyclable In-Pd Catalysts for Nitrate Degradation. **S. Guo**, C. Powell, D. Villagran, M.S. Wong

ENVR 437. Mechanisms of Scalable and Biocompatible Foliar Delivery of Engineered Nanomaterials to Crops. **P. Hu**, J. An, M. Faulkner, H. Wu, Z. Li, X. Tian, J. Giraldo

ENVR 438. Coordination Complex Based Artificial Multilayered Bifunctional Photoelectrode for Overall Water Splitting. **D. Kim**, M. Gu, B. Kim

ENVR 439. Carbon nanomaterials transformation during the water and wastewater treatment system. **Y. Li**



TECHNICAL PROGRAM

ENVR 440. Synthesis and characterization of highly-fluorescent and multifaceted optical carbon dots from enokitake mushroom for Cr⁶⁺ detection and imaging applications. **M.R. Pacquiao**, M.G. de Luna, P. Paoprasert, N. Thongsai

ENVR 441. Nanoparticle-enabled integrated solar thermal membrane distillation system. **R. Tanvir**, P. Yi

Section A

Orange County Convention Center
West Hall C

Per- & Polyfluoroalkyl Substances in the Environment: From Legacy To Emerging Contaminants

K. A. Barzen-Hanson, C. I. Olivares, A. Robel, *Organizers*

4:00 - 6:00

ENVR 442. Quantitation of per- and polyfluoroalkyl ether compounds at trace levels by LC/MS/MS. **A. Petlick**, J. Boyle, L. Leung

ENVR 443. LC-MS/MS analysis of polyfluoroalkyl substances in environmental water samples. K. Organtini, K.J. Rosnack, G. Cleland, **D. Stevens**

ENVR 444. Analysis of perfluoroalkyl acids (PFAAs) in contaminated soils from Bennington, VT. **M.S. Aldoroty**, A.K. Mahony, D. Bond, J.B. Foley, T. Schroeder, L. MacManus-Spencer

ENVR 445. Occurrence of Per-and Polyfluoroalkyl Substances (PFAS) in Asan Lake area, Korea. **Y. Son**, Y. Lee, J. Lee, J. Lee, S. Kim, Y. Ko, K. Zoh

ENVR 446. Distribution of Per- and Polyfluorinated Alkyl Substances (PFAS) in Galveston Bay, TX. **Y. Liu**, A. Pavia, G. Walsh, L. Kuo, K. Chu, S. Yang, S. Yvon-Lewis, G. Gold-Bouchot, S. Sweet, N. Tolic, R. Chu, T. Wade, A. Knap

ENVR 447. Spatial and Temporal Distribution of Per- and Polyfluorinated Alkyl Substances (PFAS) in the Main Basin of Puget Sound, WA, USA. **L. Kuo**, Y. Liu, K.L. Noor, J. Strivens, J.M. Brandenberger, T. Wade, A. Knap

ENVR 448. Removal of short-chain to long-chain perfluoroalkyl substances from water using organosilica adsorbents. **K. Pike**, E. Stebel, H. Hartmann, M. Klonowski, P. Edmiston

ENVR 449. Comparison of radiolysis, TiO₂ photocatalysis and sonolysis of “GenX”. **D. Cui**, A. Abdullah, J.R. Peller, P.V. Kamat, S.P. Mezyk, K.E. O’Shea

ENVR 450. New composite photocatalyst for efficient adsorption and photodegradation of perfluorooctanoic acid from water under solar light. D. Zhao, **T. Xu**

ENVR 451. Degradation of medium chain length fluorinated alkanes by *Pseudomonas* sp. strain 273. **Y. Xie**, A. May, G. Chen, S. Campagna, F. Loeffler

Section A



TECHNICAL PROGRAM

Orange County Convention Center
West Hall C

Photocatalytic & Electrochemical Processes in Green Energy & Environmental Remediation: A Symposium in honor of Professor Krishnan Rajeshwar

D. D. Dionysiou, C. Janaky, V. K. Sharma, N. Wu, *Organizers*

4:00 - 6:00

ENVR 452. Withdrawn

ENVR 453. Effect of boron doping on structural, morphological and adsorptive properties of graphene. **M. Kaur**, M. Kaur, D. Singh

ENVR 454. Fabrication and adsorptive characteristics of ternary nanocomposite of bentonite clay with graphene oxide-MgFe₂O₄ for Ni (II) and Pb (II) ions. **N. Kaur**, M. Kaur

Section A

Orange County Convention Center
West Hall C

Photooxidation in Engineered and Natural Systems

D. D. Dionysiou, G. Li Puma, D. Minakata, K. E. O'Shea, W. Song, *Organizers*

4:00 - 6:00

ENVR 455. Incorporation of metal oxides into a polymer substrate for buoyant photocatalysts. **L. Ainembabazi**

ENVR 456. Removal of bisphenol F in water by UV/H₂O₂ advanced oxidation processes. **J.R. Balough**, P.A. Ruiz-Haas

ENVR 457. Molecular oxygen activation in directionally nitrogen-doped in-plane metal-free heterostructure for high engineering photocatalytic performance. **S. Dong**, C. Liu, Y. Chen

ENVR 458. Residual toxicity of triphenyltin hydroxide and its transformation products in UV-254 and UV-H₂O₂ processes. **M. Hopanna**, **K. He**, L.P. Jones, L.M. Blaney

ENVR 459. Enhanced pollutant degradation by UV-LED/chlorine compared with conventional low-pressure UV/chlorine. **X. Zou**, B. Xu

Section A

Orange County Convention Center
West Hall C



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

Research Experiences in Environmental Chemistry Projects for Undergraduate & Graduate Students

M. A. Benvenuto, E. Roberts-Kirchhoff, *Organizers*

4:00 - 6:00

ENVR 460. Effects of organic matter and nitrogen fertilizer on rice paddy soil in Gongan County, Hubei Province. **I. Akpu, M. De Palma, D. Junio, J. Ha**

ENVR 461. Extraction, analysis of nutrients and heavy metals in the soil of *Tetraena qatarense* (*Zygophyllum qatarense*) and its physicochemical properties. **N.A. Ba Omar, H. Nimir, H. Hassan, H. Al Easa**

ENVR 462. Influence of soil pH on potentially toxic element content near E-waste Recycling Facility in Lagos, Nigeria. **P.K. Galvan, O.H. Anselm, C.M. Davidson**

ENVR 463. Computational toxicology e-textbook: A tool for an undergraduate course to understand and use toxicological information to avoid risk. **K. Gonzalez Ponce, K. Martinez Mayorga**

ENVR 464. Arduino based sensors for detection of water based environmental pathogens. **A. Kahl**

ENVR 465. Approaching environmental chemistry awareness in undergraduate students and the community. **F. Ocasio Idorwatt, G. Hernandez, L.I. Santiago**

ENVR 466. Examining climate science argumentation strategies by deaf students. **A.D. Ross, T.E. Pagano**

ENVR 467. Groundnut shell waste for pharmaceutical wastewater treatment. **F.A. Amoo, O.O. Onawumi, R. AbdulKareem, A. Salaudeen, O. Olaniba**

ENVR 468. Relating Soil Geochemistry to Microbial Activity and Methylmercury Content in Creek Sediments. **E. Angell, G. Schwartz, S. Brooks**

ENVR 469. Bioaccumulation of heavy metals in the aquatic macrophyte *Lemna Minor* in a natural wetland. **M. Ramos, Y. Cortes Rosario, T.M. Ulloa Ponce, N.X. Cabán Gonzales, J. Rosa Santiago**

ENVR 470. Nitrogen-containing compounds and salts emitted in poultry farming. **R. Drover, C. Michael, T. Cress, P.J. Silva, A. Foote, P. van Rooy, D. Cocker, M.J. Nee, K. Purvis-Roberts**

ENVR 471. Determination of hydroxyl radical production from sulfide oxidation in aqueous systems. **S. Lombardo, W. Arnold**

ENVR 472. Development of capillary electrophoresis assay for presence of *Nosema sp.* in *Apis Mellifera* as part of a greater strategy for identification of biomarkers for honeybee disease. **A.E. Connolly-Spring, C. Pazzi, F.M. Akgun, C. Mayack, R. Broadrup, A. Macherone**

ENVR 473. Variation in sediment nutrient concentrations in an urban-mangrove ecosystem, Piñones, Puerto Rico. **J.L. Rivera Cruz, T. Barreto Velez, M.V. Santos-Crespo, T.A. Crowl, D. Ogurcak, J. Fourqurean, M. Ross, J. Meeder, S. Charles, J. Kominoski, J. Smoak, A. Chapple, M. Yu, A.E. Lugo**



TECHNICAL PROGRAM

ENVR 474. Determination of heavy metals in distinct ecological matrix of the biotopes near the “Cavernas del Rio de Camuy” National Park. M. Ramos, **J.W. Torres Ayende**, **J. Soto**, **N. Maldonado**, **N. Cortés**, **J. Hernández Rivera**, S. Figueroa Padilla, **P.N. Molina Cora**

ENVR 475. Role of non-covalent interactions on the transport and fate of pharmaceutical contaminants in the aquatic environment. **C. Walsh**, G. Dalla Pozza, M. Nadim, M. Subir

ENVR 476. Using Spent Coffee Grounds for Adsorption of Natural Organic Matter in Water Treatment. **A.L. Willis**, **C.A. Kayuha**, **K.T. Hoard**, J.D. Geis, **S. Youn**

Section A

Orange County Convention Center
West Hall C

Transdisciplinary Approaches to Sustainable Solutions at the Food-Energy-Water Nexus

J. L. Goldfarb, D. Kriner, *Organizers*

4:00 - 6:00

ENVR 477. Bromination and Chlorination Kinetics of Dichloroacetamide Herbicide Safeners. **M.V. Niedzwiecki**, M.E. McFadden, G.H. LeFevre, D.M. Cwiertny, J.D. Sivey

Section A

Orange County Convention Center
West Hall C

True Positives in EPA'S Non-Targeted Analysis Collaborative Trial (ENTACT)

C. Grulke, S. Newton, J. Sobus, E. M. Ulrich, A. J. Williams, *Organizers*

4:00 - 6:00

ENVR 478. Examination of true positives in ENTACT solutions using GCMS with data processed through TIC analysis and deconvolution. **M.S. Clifton**

Section A

Orange County Convention Center
West Hall C

Uptake & Transformation of Contaminants of Emerging Concern In Plants

B. Chefetz, J. Gan, G. H. LeFevre, *Organizers*



TECHNICAL PROGRAM

4:00 - 6:00

ENVR 479. Comparative study on aqueous remediation of trace hazardous chemicals by two different hydrophytes planted in floating treatment wetlands: A mesocosm study. **J. Hwang**, F.O. Hinz, P. Wilson

ENVR 480. Bioaccumulation of Cu by the aquatic macrophyte *Bacopa monnieri* exposed to Cu nanoparticles and ionic Cu(II). M. Ramos, **J.M. Jimenez Cruz**, A. Cordero, P.M. López Meléndez, M.G. Toledo del Valle

ENVR 481. Bioavailability of organic phosphorus compounds for *Microcystis aeruginosa*. **B. Duersch**

ENVR 482. Biodegradation of sulfonamides using microalgae. **J. Xiong**, M. Kurade, S. Govindwar, B. Jeon

ENVR 483. Herbicides in unexpected places: Exudation and non-target impact of aminopyralid and triclopyr following basal bark treatments and an immunoassay for rapid detection in soil. **P.L. Tomco**, G. Graziano, C.L. Nicolet, M.R. McCoy, S. Seefeldt

ENVR 484. Effect of magnesium uptake by *Oriza Sativa* from organic and inorganic fertilizer fields -comparative study. **V. Retnaswamy**

ENVR 485. Enhanced leaching of uranium from stable mineral forms by plants under phosphorus stress. **N. Edayilam**, D. Montgomery, N. Martinez, B.A. Powell, N. Tharayil

ENVR 486. Removal and degradation mechanism of sulfamethoxazole by *Ipomea aquatica* from aquatic system: A lab-scale phytoreactor study. **M. Kurade**, J. Xiong, S. Govindwar, D. Kang, B. Jeon

Section A

Orange County Convention Center
West Hall C

When Chemistry Meets Biology: Novel Solutions for Emerging Challenges in Pollutant Control, Remediation & Resource Recovery

X. Mao, Y. Men, C. M. Sales, S. Yi, W. Zhuang, *Organizers*

4:00 - 6:00

ENVR 487. Developing a sustainable zero-waste multi-process remediation technology involving chemical immobilization and phytoremediation to remove excess nutrients (nitrate and phosphate) from a sewage treatment plant (STP) effluent. **R. Moyles**, **J. Wessel**, J. Penoyer, H. Harrington, A. Hoyt, B. Groth, M. Corona, I. Gergi, S. Zamule, P. Das, D. Giacherio

ENVR 488. Microbial degradation of polycyclic aromatic hydrocarbons at ambient near-surface coastal conditions. **C.G. Lewis**, M.J. Beazley, A.D. Campiglia

ENVR 489. Cerium bioleaching from abandoned uranium mine wastes. **M. Soleimanifar**, L. Rodriguez Freire

ENVR 490. Potential of Reusing WTR, A Water Treatment By-Product, to Design Sustainable Remediation Techniques for Rochester, NY Communities. **J. Penoyer**, R. Moyles, H. Harrington, A. Hoyt, B. Groth, M. Corona, J. Wessel, I. Gergi, S. Zamule, D. Giacherio, P. Das



TECHNICAL PROGRAM

ENVR 491. Efficiency of organic manure and macro-nutrient in the remediation of diesel oil contaminated soil. **I. Ayodeji**

ENVR 492. Improving phosphate recovery from poultry litter extracts through chitosan and bentonite addition during struvite precipitation. **M.A. Fleming**, O. Ndalamda, C.R. Portner, L.M. Blaney

ENVR 493. Survivability of genetically engineered *Thermosynechococcus elongatus* BP1 in different temperature conditions. **O. Sacko**, **C. Barnes**, L.H. Greene, **J.W. Lee**

ENVR 494. Liquid amphiphilic polymer for enhanced airborne dust suppression. **T. Lee**, M. Kim, D.S. Knoff

Section B

Orange County Convention Center
Valencia Ballroom B-D - Theater 10

Opioids & Their Impact on the Environment

S. O. Obare, E. Schoffers, *Organizers, Presiding*

1:00 Introductory Remarks.

1:05 ENVR 495. Addiction and the environment: Making big picture connections. **E. Schoffers**

1:30 ENVR 496. Detection of opioids in urban wastewater over a two-year period using SPE and LC-MS/MS. **T.H. Boles**, S.B. Reynolds, F. Mahmoudi

1:55 ENVR 497. LC-MS/MS optimization for the analysis of opioid metabolites in wastewater. **R. Rushing**, D.A. Burgard

2:20 Intermission.

2:35 ENVR 498. Developing Intelligent Sensors for Fentanyl and Related Toxins. **S. Vasu**

3:05 ENVR 499. Occurance and Source Apportionment of Pharmaceutical and Personal Care Products in Water and Sediment Samples from the Potomac River Bays and Estuaries. **A. Leahigh**, T.B. Huff, R. Jones, G.D. Foster

3:30 ENVR 500. Assessment of environmental fentanyl contamination exposure and analytical detection for remediation of affected areas. **S. Willison**, J. Lipscomb

3:55 Discussion.

4:20 Closing Remarks.

Section C

Orange County Convention Center
Valencia Ballroom B-D - Theater 8

Applications & Implications of Nanomaterials & Their Toxic Effects



TECHNICAL PROGRAM

S. R. Kanel, R. O'Hara, *Organizers*
S. Hussain, N. Mallikarjuna, B. A. Manning, *Organizers, Presiding*

1:00 ENVR 501. Development of a carbon nanomaterial-based nanocomposite aerogel for the removal of organic compounds from water. B.S. Litts, M.K. Eddy, P.M. Zaretsky, N.N. Ferguson, A.B. Dichiara, **R.E. Rogers**

1:40 ENVR 502. Nanomaterials integrated membranes for organic pollutant degradation to toxic metal capture. **D. Bhattacharyya**, H. Wan, S. Islam, S. Hernandez, L. Ormsbee

2:20 ENVR 503. U(VI) removal using rhamnolipid stabilized iron oxide nanoparticles. **N. Sharma**, J. Fortner, D. Giammar

2:40 ENVR 504. Selective removal of iodide from water using reduced graphene oxide aerogel functionalized with Cu₂O/Cu. **J. Li**, X. Liu, **J.S. Zheng**

3:00 Intermission.

3:15 ENVR 505. Influence of organic ligands and environmental factors on metal sulfide nanoparticle precipitation. **A.G. Donaghue**, E.R. McKenzie

3:35 ENVR 506. Adsorption properties of Sb onto kaolin coated nano zero valent iron (K-nZVI) and its remediation capabilities of Sb contaminated soils. **D.D. Amarasiriwardena**, A.B. Hernandez

4:15 ENVR 507. Recent advancements of MXenes for environmental remediation and water treatment applications. **K.A. Mahmoud**

4:35 ENVR 508. Nanomaterials integration and development: Platform for utilization of earth-abundant materials and waste to value added products. **S. Verma**, R.S. Varma, M. Nadagouda

4:55 Closing Remarks.

Section D

Orange County Convention Center
Valencia Ballroom B-D - Theater 12

Photocatalytic & Electrochemical Processes in Green Energy & Environmental Remediation: A Symposium in honor of Professor Krishnan Rajeshwar

D. D. Dionysiou, V. K. Sharma, *Organizers*
C. Janaky, N. Wu, *Organizers, Presiding*

1:00 ENVR 509. Titania-silica mesoporous materials for photocatalytic degradation of organics. **R.T. Koodali**

1:30 ENVR 510. Visible light-driven photocatalytic activity of defective Ti-based perovskites for antibiotic decomposition. **C. Wang**, R. Hailili



TECHNICAL PROGRAM

2:00 ENVR 511. Mesoporous TiO₂-BiOBr microspheres with tailorable adsorption capacities for photodegradation of organic water pollutants: Probing adsorption-photocatalysis synergy by combining experiments and kinetic modeling. **W. Deng, B. Batchelor, A. Abdel-Wahab, Y. Li**

2:20 ENVR 512. Highly efficient performance and conversion pathway of photocatalytic CH₃SH oxidation on self-stabilized indirect Z-scheme g-C₃N₄/I³⁺-BiOI. **C. He, L. Hu, Y. Huang**

2:40 ENVR 513. Multicomponent Bismuth Vanadate Heterostructures for Visible Light-Activated Catalytic Degradation of Halogenated Organic Compounds.. **E.M. Zahran, M.R. Knecht, L.G. Bachas**

3:00 Intermission.

3:15 ENVR 514. Heterogeneous photocatalytic organic synthesis: State-of-the-art and future perspectives. **D.W. Bahnemann**

3:45 ENVR 515. Ferrite nanoparticles and their graphene nanocomposites as adsorbents and photocatalysts: Current status and future perspective. **M. Kaur, V.K. Sharma**

4:05 ENVR 516. Highly effective heterogeneous activation of peroxymonosulfate by Cu-doped LaFeO₃ for antibiotics sulfadiazine degradation. **Y. Rao, F. Han**

4:25 ENVR 517. Four decades of heterogeneous photocatalysis: Some trends and reflections. **K. Rajeshwar**

4:55 Closing Remarks.

Section E

Orange County Convention Center
Valencia Ballroom B-D - Theater 13

ACS Award for Creative Advances in Environmental Science & Technology

S. O. Obare, V. K. Sharma, *Organizers*
D. D. Dionysiou, *Presiding*

1:00 Introductory Remarks.

1:05 ENVR 518. Data science for water research. **J. Hering**

1:30 ENVR 519. Photolysis across scales: From molecules to space. **W. Arnold**

1:55 ENVR 520. Does GAC with chlorination produce safer drinking water? Comprehensive evaluation of chlorinated, brominated, iodinated, and nitrogenous DBPs at full scale plants. **S.D. Richardson, A. Cuthbertson, S.Y. Kimura, H.K. Liberatore, R. Summers, D. Knappe, B. Stanford, J. Maness, R. Mulhern, M. Selbes**

2:20 Intermission.

2:30 ENVR 521. Nanomaterials: Not the next asbestos. **M. Wiesner**



TECHNICAL PROGRAM

2:55 ENVR 522. Pilot-scale pyrolytic remediation of crude-oil contaminated soil in a continuously-fed reactor: treatment intensity tradeoffs. W. Song, J.E. Vidonish, P. Yu, C. Chu, B. Moorthy, B. Gao, K. Zygourakis, **P.J. Alvarez**

3:20 ENVR 523. New frontiers in plant uptake and transformation of emerging contaminants. **G.H. LeFevre**

3:45 Intermission.

3:55 ENVR 524. Award Address (ACS Award for Creative Advances in Environmental Science and Technology sponsored by the ACS and the ACS Division of Environmental Chemistry). Bringing plant science into environmental chemistry and engineering. **J.L. Schnoor**

4:40 Discussion.

Section F

Orange County Convention Center
Valencia Ballroom B-D - Theater 14

Photooxidation in Engineered and Natural Systems

New Insight into Materials & Novel Technologies for Photooxidation

D. D. Dionysiou, D. Minakata, *Organizers*
G. Li Puma, K. E. O'Shea, W. Song, *Organizers, Presiding*

1:00 Introductory Remarks.

1:05 ENVR 525. Recent research progresses on photocatalytic "memory" effect. **Q. Li**

1:35 ENVR 526. Degradation of ofloxacin by perylene diimide supramolecular nanofiber sunlight-driven photocatalysis. P. Chen, **L.M. Blaney**, G. Cagnetta, J. Huang, B. Wang, Y. Wang, S. Deng, G. Yu

2:00 ENVR 527. Humic acid coated iron oxide magnetic nanoparticles (HA-MNP) as potential photosensitizer for the oxidation and subsequent adsorption of arsenite. M. Rashid, **P. Pham**, Y. Cai, B.P. Rosen, D.D. Dionysiou, K.E. O'Shea

2:25 ENVR 528. Black TiO₂ with MoS₂ Layers Nanocomposite for Highly Enhanced Visible Light Photodegradation of Arsenic. **H.J. Shipley**, A. Balati, K. Nash

2:50 Intermission.

3:05 ENVR 529. Photocatalytic removal of metformin using poly(3,4-ethylenedioxythiophene) (PEDOT) polymer. **R. Kumar**, R. Fucina, J. Travas-Sejdic, L.P. Padhye

3:30 ENVR 530. Combination of Sunlight and Nitrite Increases Trichloronitromethane Formation from Wastewater Effluents. **J. Xu**, Z. Kralles, N. Dai

3:55 ENVR 531. Nanobubbles characterization and environmental application. **L. Wang**



TECHNICAL PROGRAM

4:20 Concluding Remarks.

Section G

Orange County Convention Center
Valencia Ballroom B-D - Theater 11

When Chemistry Meets Biology: Novel Solutions for Emerging Challenges in Pollutant Control, Remediation & Resource Recovery

C. M. Sales, W. Zhuang, *Organizers*
X. Mao, Y. Men, S. Yi, *Organizers, Presiding*
C. Sales, *Presiding*

1:00 Introductory Remarks.

1:05 ENVR 532. Distinctive capabilities of micropollutant biotransformation by comammox bacterium *Nitrospira inopinata*. Y. Yu, P. Han, L. Zhou, Z. Tian, Z. Li, L. Hou, M. Liu, Q. Wu, M. Wagner, Y. Men

1:25 ENVR 533. Characterization of the Proteolytic Enzymes of a Marine Bacterium, *Alteromonas* Through Metalloproteomics. M.G. Mazzotta, M. Saito, M. McIlvin, D. Moran

1:45 ENVR 534. Biocatalytic degradation of parabens mediated by cell surface displayed cutinase. B. Zhu, N. Wei

2:05 ENVR 535. Metabolic potential and biogeography of enzymes derived from wastewater microbial communities: Assessing the biotransformation of antibiotics. M.T. Zumstein, D.E. Helbling

2:25 ENVR 536. Vault Packaged Ligninolytic Enzymes as Nanoscale Environmental Bioremediation Agents. S.S. Kalra, A.G. Lothe, M. Wang, Y. Chen, V. Kickhoefer, L.H. Rome, P. Allard, S. Mahendra

2:55 Intermission.

3:25 ENVR 537. Identification of functional genes from *Dehalococcoides mccartyi* 195 using *Desulfovibrio vulgaris* Hildenborough as a heterologous expression host system. S. Yi, M. Sun, Y. Tang, G. Zane, J. Wall, W. Zhuang, L. Alvarez-Cohen

3:45 ENVR 538. New insight into the reactivity of Mn (III) in bisulfite/permanganate for organic compounds oxidation: The catalytic role of bisulfite and oxygen. S. Zhong, H.J. Zhang

4:05 ENVR 539. Biomimetic heterogeneous catalysts for chlorate reduction. C. Ren, J. Gao, J. Liu

4:25 ENVR 540. Biocementation of soils through calcium carbonate precipitation using microbial catalysis. R. Vilar, K. Ikuma

4:45 Concluding Remarks.

Elucidation of Mechanisms & Kinetics on Surfaces



TECHNICAL PROGRAM

Catalysis on Metal Interfaces with Metal Oxides

Sponsored by CATL, Cosponsored by ENFL, ENVR, INOR and PHYS

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

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WEDNESDAY MORNING

Section A

Orange County Convention Center
Valencia Ballroom B-D - Theater 9

Current Status of Environmental Research on Water Contaminants

S. Ahuja, B. G. Loganathan, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 ENVR 541. Expanding our understanding of pharmaceutical exposures in aquatic environments: Development of a new pharmaceutical method and its application to wastewater and surface water samples. **E.T. Furlong**, M.C. Noriega, C.J. Kanagy, J.A. Simmons, P.J. Phillips, S.R. Corsi, D.W. Kolpin

8:55 ENVR 542. Quantifying the occurrence, fate and implications of pharmaceutical mixtures in a temperate-region wastewater effluent-dominated stream. **H. Zhi**, G.H. LeFevre, D.W. Kolpin, S. Meppelink, L. Iwanowicz, E. Meade, R. Klaper, M.T. Meyer

9:15 ENVR 543. Rapid removal of pharmaceuticals from contaminated water using magnetized Douglas fir biochar. **A. Lijanage**, T. Mlsna

9:35 ENVR 544. Characteristics and mechanisms of catalytic ozonation with Fe-shaving-based catalyst in industrial wastewater advanced treatment. **X. Li**, H. Wang

9:55 Intermission.

10:10 ENVR 545. Fabrication of size controlled magnetic chitosan adsorbent via in-situ coprecipitation approach for the wastewater treatment. **S. Pu**, H. Ma, K. Wang

10:30 ENVR 546. Mechanistic insights into heterogeneous catalytic ozonation process: Adsorption versus oxidant generation. **Y. Yuan**, G. Xing, S. Garg, J. Ma, D. Waite

10:50 ENVR 547. Sorption of organic contaminants from water using surfactant modified fly ash: Performance comparison of anionic and cationic surfactant modifications. **H. Aslam**, S. Mushtaq



TECHNICAL PROGRAM

11:10 ENVR 548. Residual micro organic pollutants of the effluent from the typical textile wastewater treatment plants: A regional survey. F. Xue, **B. Tang**, L. Bin, J. Ye

11:30 ENVR 549. 3D porous superhydrophobic material for oil and water separation. **N. Baig**, T.A. Saleh

11:50 Closing Remarks.

Section B

Orange County Convention Center
Valencia Ballroom B-D - Theater 10

Green Chemistry & the Environment

R. Luque, S. O. Obare, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 ENVR 550. Diabetes as an environmental risk factor: A biological significance of metabolic inhibitors and their curcumin adducts. **B. Dayal**, M.A. Lea, A. Kulkarni

8:30 ENVR 551. Novel sustainable polymers: Bio-derivable replacements for isophthalic and terephthalic acid. **J.W. Comerford**, A. Pellis, T. Farmer, T. Comerford

8:55 ENVR 552. Chemo-enzymatic tools for the green synthesis of bio-based polyesters. **A. Pellis**, J.W. Comerford, T. Farmer

9:20 ENVR 553. Novel bio-silicified laccases catalyze 2,5-Dimethylfuran oxidation and stereoselective ring opening. A. Franco, A.M. Balu, A. Romero, **R. Luque**

9:45 Intermission.

10:00 ENVR 554. From levoglucosenone to high value synthons: A green access to (S)- γ -hydroxymethyl- α,β -butyrolactone and cyrene®. **L. Mouterde**, F. Allais, J.D. Stewart

10:20 ENVR 555. Tetramethyloxolane (TMO): an unusual ether which can replace hazardous hydrocarbon solvents. **F.P. Byrne**, T. Farmer, **A.J. Hunt**, J. Clark

10:40 ENVR 556. Bioethanol production from microcrystalline cellulose under self-sustainable reaction conditions. **F. Mauriello**, B. Gumina, C. Espro, S. Galvagno, R. Pietropaolo

11:00 ENVR 557. Synthesis and evaluation of antiradical and anti-UV properties of new biobased dimers derived from sinapic acid. **A.L. Flourat**, M.M. Mention, C. Peyrot, F. Allais

11:20 ENVR 558. Catalytic Hydrothermal Processing of Fatty Acids and Lipids over Ru/C without External Hydrogen Addition. **J. Zhang**, X. Huo, Y. Li, T.J. Strathmann

11:40 Closing Remarks.



TECHNICAL PROGRAM

Section C

Orange County Convention Center
Valencia Ballroom B-D - Theater 8

Uptake & Transformation of Contaminants of Emerging Concern In Plants

B. Chefetz, J. Gan, G. H. LeFevre, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 ENVR 559. Process-driven approach to evaluating risks of emerging contaminants in agroecosystems. **J. Gan**, Q. Fu, H. Sun, S. Dudley

8:25 ENVR 560. Mixture vs. individual uptake of psychoactive pharmaceuticals by tomato and cucumber plants. **B. Chefetz**, T. Malchi, M. Shenker

8:45 ENVR 561. Plant-driven processes influencing the accumulation of wastewater-derived organic contaminants. **J.A. Pedersen**, S. Nason, K. Karthikeyan, E.L. Miller

9:05 ENVR 562. New Insights to Plant Uptake and Translocation of Environmental Contaminants: Artificial Intelligence Approaches. M. Bagheri, X. He, H. Zhang, W. Liu, H. Shi, **J.G. Burken**

9:25 ENVR 563. Simulation for the fate of emerging trace organic contaminants during reuse of reclaimed wastewater in agriculture. **J. Tan**, Y. Yang

9:45 Intermission.

9:55 ENVR 564. Experimental and theoretical evidences for diastereomer- and enantiomer-specific accumulation and biotransformation of HBCD in maize. **S. Zhang**, H. Huang

10:15 ENVR 565. Metabolic demethylation and oxidation of caffeine during uptake by vegetables. Y. Chuang, Y. Li, R. Hammerschmidt, W. Zhang, S. Boyd, **H. Li**

10:35 ENVR 566. Impacts and biotransformation of CECs in crops under acute and chronic exposures. **S. Dudley**, C. Sun, M. McGinnis, J. Trumble, J. Gan

10:55 ENVR 567. Transformation of neonicotinoids in aqueous medium by a synergistic duckweed-microbe system. **C. Muerdter**, G.H. LeFevre

11:15 ENVR 568. Transfer and transformation mechanisms of pharmaceutical and personal care products in algae-based passive water treatment. **E. Passeport**, C. Larsen, E. Yu

11:35 ENVR 569. Plant uptake and transformation of pharmaceuticals in a novel treatment wetland configuration. **A. Perantoni**, D.L. Sedlak

11:55 Concluding Remarks.

Section D



TECHNICAL PROGRAM

Orange County Convention Center
Valencia Ballroom B-D - Theater 12

Electrochemical Water Treatment

J. Blotevogel, B. P. Chaplin, C. Schaefer, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 ENVR 570. Using electrons to clean the water: are electrochemical systems the future of water treatment? **J. Radjenovic**, N. Sergienko, E. Irtem, J. Albahaca Oliva, G. Florjan-Norra, L. Pires

8:35 ENVR 571. Recent developments and scale up of boron-doped diamond electrodes for water treatment. **D.J. Mazur**, T. Mathee, T. Christensen

8:55 ENVR 572. Simultaneous adsorption and electrochemical reduction of water contaminants using carbon-Ti₄O₇ composite reactive electrochemical membranes. **S. Almassi**, Z. Li, W. Xu, C. Pu, T. Zeng, B.P. Chaplin

9:15 ENVR 573. Decomposition of nitrosamines through electrochemically-mediated reduction on carbon xerogel electrodes. J.G. Thompson, X. Gao, **S. Toma**, K. Abad, S. Bhatnagar, J.R. Landon, K. Liu

9:35 ENVR 574. TiO₂ decorated electrospun nanofibers for electro-catalytic degradation of water pollutants. **J. Wu**, L. Ya Hsuan, C. Hou

9:55 Intermission.

10:15 ENVR 575. Degradation of sulfonamide antibiotics by electro-Fenton with heterogeneous iron catalysts. **T. Kim**, T. Kim, K. Zoh

10:35 ENVR 576. Cathodic reduction of nitrobenzene using TiO₂ nanotube electrodes with different morphologies. **A. Ahmadi**, T. Wu

10:55 ENVR 577. Modeling of effect of electrodeposition parameters of a graphite/PbO₂ anode on 2,4-dinitrophenol removal efficiency: Comparison between RSM and ANN. **P. Mandal**, A.K. Gupta, B.K. Dubey

11:15 ENVR 578. Bioelectrochemical Oxidation of Recalcitrant 1,4-Dioxane and Per- and Polyfluoroalkyl Substances in Mixed Contaminant Plumes. **N. Pica**, N. Johnson, Yu Miao, Y. Miao, J. Funkhouser, S. Mahendra, J. Blotevogel

11:35 ENVR 579. Bioelectrochemical reduction of perchlorate in contaminated groundwater. **A. Hanson**, C. Lamson, S.K. De Long, J. Blotevogel

Section E

Orange County Convention Center
Valencia Ballroom B-D - Theater 13

ACS Award for Creative Advances in Environmental Science & Technology



TECHNICAL PROGRAM

S. O. Obare, V. K. Sharma, *Organizers*
W. Arnold, *Presiding*

8:00 Introductory Remarks.

8:05 ENVR 580. Jerry Schnoor and impacts on phytoremediation research at a global scale. **J.G. Burken**

8:30 ENVR 581. Bioaugmentation and phytoremediation of dioxane in simulated groundwater. **R. Simmer**, J. Mathieu, P.J. Alvarez, J.L. Schnoor

8:55 ENVR 582. Understanding the toxicity of hydroxylated PCBs for plants: A transcriptomic analysis. **B. Van Aken**, S. Subramanian, R. Tehrani

9:20 ENVR 583. Non-Aroclor emissions from consumer products and the potential for inexpensive and effective remediation of airborne PCBs in Schools. **K.C. Hornbuckle**, J. Jahnke, M.K. Bannavti, C.L. Just

9:45 Intermission.

10:05 ENVR 584. Transformation of 1,1,1,3,8,10,10,10-octachlorodecane in air phase: promoted by phyto-genic volatile organic compounds (PVOCs) of pumpkin seedlings. **Y. Li**, J. Liu, J.L. Schnoor, G. Jiang

10:30 ENVR 585. Bioanalytical tools for the assessment of mixtures of organic micropollutants in water, sediment, biota and people. **B. Escher**

10:55 ENVR 586. Boosting lead adsorption on ultrathin iron oxychloride (FeOCl) nanosheets. **J. Luo**, M. Sun, J.C. Crittenden, M. Elimelech

11:20 ENVR 587. Growth of *Dehalococcoides mccartyi* and increased abundance of reductive dehalogenase genes in anaerobic PCB-contaminated sediment microcosms. J.M. Ewald, A. Martinez, J.L. Schnoor, K.C. Hornbuckle, **T. Mattes**

11:45 Discussion.

11:55 Closing Remarks.

Section F

Orange County Convention Center
Valencia Ballroom B-D - Theater 14

Innovations, Advances, and Sustainability in Additive Manufacturing for Electrochemical, Energy, and Environmental Applications

N. Aich, S. Rahaman, *Organizers, Presiding*

8:00 ENVR 588. 3D printed supercapacitors. **Y. Li**



TECHNICAL PROGRAM

8:25 ENVR 589. Additively manufactured electrodes for electrochemical energy storage and conversion. V. Beck, A. Ivanovskaya, S. Chandrasekaran, T. Weisgraber, B. Moran, S. Watts, D. Tortorelli, J. Biener, M. Stadermann, E. Duoss, **M. Worsley**

8:45 ENVR 590. Exploring 3D-printed water electrolyzers for economic and high-efficiency energy storage. **G. Yang**, S. Yu, Y. Dohrmann, F.A. List, S.S. Babu, J.B. Green, F. Zhang

9:05 ENVR 591. Advanced manufacturing of hierarchical multifunctional foams for environmental and energy applications. **K. Sierros**, I. Pecora, M.T. Arango

9:25 ENVR 592. Novel 3D printed composites for gas storage applications and sustainable materials. **M.R. Hartings**

9:45 ENVR 593. Opportunities for Expanding Membrane Functionality Through Additive Manufacturing. **W.A. Phillip**

10:05 Intermission.

10:15 ENVR 594. New additive manufacturing technologies using graphene based materials for flexible electronics. T. Morrison, X. Shen, **H.E. Naguib**

10:40 ENVR 595. Development of 3D-printed structured adsorbents for the recovery of renewable alcohols. **B. Claessens**, G. Baron, J. Cousin-Saint-Remi, J. Denayer

11:00 ENVR 596. Scalable 3D printed hydrogel-based biosensors for environmental applications. A.S. Finny, A. Othman, F. Mustafa, **E. Andreescu**

11:20 ENVR 597. Emissions and control of particulate matter and volatile organic compounds from desktop three-dimensional (3D) printers. **P. Azimi**, B. Stephens

11:40 ENVR 598. Withdrawn

Section G

Orange County Convention Center
Valencia Ballroom B-D - Theater 11

Innovative & Practical Approaches for the Treatment of Per- & Polyfluoroalkyl Substances (PFAS)

J. Choe, Y. Wang, *Organizers*
J. Liu, S. Vyas, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 ENVR 599. Treatment of per-and polyfluoroalkyl substance (PFAS) contaminated groundwater using an *in situ/ex situ* combined remedy. **M. Crimi**, T.M. Holsen, S. Mededovic Thagard, J. Guelfo, S. Woodard, N. Hagelin, D. Woodward, J. Heath

8:55 ENVR 600. PFAS impacts on wastewater and advanced water treatment for indirect potable reuse: A utility's perspective on the importance of source control. **D. Gonzalez**, C. Bott



TECHNICAL PROGRAM

9:25 ENVR 601. Defluorination of per- and polyfluoroalkyl substances (PFASs) with hydrated electron: Structural dependence and implications to PFAS remediation and management. M.J. Bentel, Y. Yu, L. Xu, B.M. Wong, Y. Men, **J. Liu**

9:45 ENVR 602. Investigating the application of non-equilibrium cold plasma technologies for the degradation of poly- and perfluoroalkyl substances in aqueous solutions. **C.M. Sales**, A. Fridman, A. Rabinovich, G. Fridman, **E.R. McKenzie**, R. Hammouri, M. Hadaya, I. Dragiev, T. Joyce

10:10 Intermission.

10:25 ENVR 603. Na_2SO_3 versus $\text{K}_4\text{Fe}(\text{CN})_6$ as photochemical sources of hydrated electrons for reduction of PFASs: pH and temperature effects. **W.A. Maza**, V.M. Breslin, P.A. DeSario, A. Epshteyn, J. Owrutsky, B.B. Pate

10:45 ENVR 604. Combination of nanofiltration and UV-sulfite as a novel treatment train for the removal and destruction of PFASs in AFFF-impacted groundwater. **G. McKay**, C. Liu, R. Tenorio, D. Jiang, J. Brown, H. Wright, C. Schaefer, C.P. Higgins, C. Bellona, T.J. Strathmann

11:05 ENVR 605. Absolute rate constant measurements for hydrated electron reductive destruction of aqueous perfluoroalkyl species in water. **L. Twight**, S.P. Mezyk

11:25 ENVR 606. Role of structure in the reductive defluorination of perfluoroalkyl substances. D.J. Van Hoomissen, **S. Vyas**

11:45 Closing Remarks.

Applications of Cheminformatics to Environmental Science

Sponsored by CINF, Cosponsored by ENVR

Activation of Light (C1-C4) Hydrocarbons: Theory & Experiments

Sponsored by CATL, Cosponsored by ENFL, ENVR, INOR and PHYS

Chemical Catalysis for Bioenergy Consortium: Addressing Deactivation during Biomass Conversion

Sponsored by CATL, Cosponsored by ENFL, ENVR and INOR

WEDNESDAY AFTERNOON

Section A

Orange County Convention Center
Valencia Ballroom B-D - Theater 9



TECHNICAL PROGRAM

Current Status of Environmental Research on Water Contaminants

S. Ahuja, B. G. Loganathan, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 **ENVR 607.** Reactivity of monochloramine with amino acids under wastewater conditions. **R. Shinh**, J. Gleason, S.P. Mezyk, K.P. Ishida

1:55 **ENVR 608.** Dichloramine reactivity with organic materials in wastewater. **E.D. Walker**, S.P. Mezyk, K.P. Ishida

2:15 **ENVR 609.** Kinetics of trichloramine reactions with organic species under AOP conditions. **L. Watts**, S.P. Mezyk

2:35 **ENVR 610.** Investigating hypochlorite radical kinetics with carcinogenic nitrosamines in waters. **A. Lechner**, S.P. Mezyk

2:55 Intermission.

3:10 **ENVR 611.** Withdrawn

3:30 **ENVR 612.** Kinetics of synthetic musks and phthalates with the persulfate and dichloride radical. **M. Vo Luong**, S.P. Mezyk

3:50 **ENVR 613.** Adsorption of saxitoxin onto powdered activated carbon: The influence of carbon type. **Y. Liu**, J.J. Lenhart

4:10 **ENVR 614.** Remediation of chlorinated alkanes by zero-valent Iron and vitamin B12. **N. Lapeyrouse**, C. Yestrebsky, G. Booth

4:30 **ENVR 615.** Role of ferrate and ferrate in activating ferrate by calcium sulfite for enhanced oxidation of organic contaminants. **X. Guan**

4:50 Closing Remarks.

Section B

Orange County Convention Center
Valencia Ballroom B-D - Theater 10

Green Chemistry & the Environment

R. Luque, S. O. Obare, *Organizers, Presiding*

1:00 Introductory Remarks.

1:05 **ENVR 616.** Tool to evaluate used electronic flows for the United States. **J.A. Glaser**, E. Sahle-Demessie, T. Richardson, C.C. Lee, C. Northeim, J. Petrusa, J. Larson, M. McGrath



TECHNICAL PROGRAM

1:35 ENVR 617. Renewable chemicals and materials from land, sea and air. **F.M. Kerton**, J.N. Murphy, J.L. Vidal, G. Margoutidis, S. MacQuarrie, K. Hawboldt

2:00 ENVR 618. NO₂ adsorption by recycled concrete aggregates and its application to control corrosion in steel reinforced concrete. S. Patel, E. Ariyachandra, **A. Orlov**, S. Peethamparan

2:25 ENVR 619. Pharmaceuticals and other emerging contaminants in sewage: An overview of current clean-up techniques, R&D approaches and needs. **V. Birke**, C. Schutt, H. Burmeier, F. Langschwager

2:50 Intermission.

3:05 ENVR 620. Introducing Green Chemistry into paint strippers. **B. Engendahl**, M. Beernaert, T. Fennelly

3:30 ENVR 621. State-of-the-art nanomaterials for environmental stewardship applications. **S. Hunyadi Murph**

3:55 ENVR 622. Biochemical transformations of iron and sulfur in a iron-dosed anaerobic wastewater treatment process with characterizaion and microbial community analyses. **D. Deng**

4:20 ENVR 623. Alkyl-Methyl-Imidazolium Ionic Liquids as Green Solvents for Epoxy Recycling. **R.L. Perez**, A.F. Ezzir, I.M. Warner

4:40 ENVR 624. Life cycle assessment of furfural-derived phthalic acid alternative (CBDA-2) for coating applications. **M. Ukey**, G. Pourhashem, Q.R. Chu

Section C

Orange County Convention Center
Valencia Ballroom B-D - Theater 8

Combined Biological-Chemical Reactions for Contaminant Transformation

J. Blotevogel, K. T. Finneran, S. Jin, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 ENVR 625. Application of zeolite as a biofilm carrier in wastewater treatment. N. Zalivina, C. Johnson, J. Kuhn, **S. Ergas**

1:55 ENVR 626. Enhanced groundwater contaminants degradation by microbes, electrodes, and “microelectrodes”. **S. Jin**, P. Fallgren

2:15 ENVR 627. Hybrid systems construction with silicon solar cell in microbial fuel cells and novel photoelectrochemical catalysis reactors. **G. Ren**, Y. Sun, A. Lu, H. Ding

2:35 ENVR 628. Compound-specific isotope analysis reveals the transformation processes of the insensitive munition component 2,4-dinitroanisole and its reaction products. **T.B. Hofstetter**, B. Ulrich, M.J. Berens, J. Spain, W. Arnold

2:55 ENVR 629. Sequential electrochemical and biological treatment train for chloronitrobenzene-contaminated water. **N. Pica**, S. Amiri, A. Hanson, T.B. Hofstetter, J. Blotevogel



TECHNICAL PROGRAM

3:15 ENVR 630. Combination of non-thermal plasma and biodegradation to simultaneously remove 1,4-dioxane and trichloroethane. Y. Xiong, R. Wandell, B.R. Locke, **Y. Tang**

3:35 ENVR 631. Treatment trains for dioxane and chlorinated volatile organic compounds influence microbial communities. Y. Miao, N.W. Johnson, K.N. Heck, P.B. Gedalanga, D.T. Adamson, C.J. Newell, M.S. Wong, **S. Mahendra**

3:55 Intermission.

4:05 ENVR 632. Combined persulfate chemical oxidation and bioremediation as in-situ strategies for AFFF and BTEX co-contaminant impacted sites. **C.I. Olivares**, E. Cook, E. Troyer, Y. Sun, S. Yi, D.L. Sedlak, L. Alvarez-Cohen

4:25 ENVR 633. Identification of microbial communities that exchange electrons with pyrogenic carbonaceous materials in engineered systems. **D.F. Call**, Q. Cheng

4:45 ENVR 634. Tailoring the reactivity of iron metal for *In Situ* Chemical Reduction (ISCR) via biological sulfate reduction process. S. Islam, A. Acosta, A. Redwan, K. Millerick, **W. Yan**

5:05 ENVR 635. Microbial ecological interactions in bioelectrochemical remediation of hydrocarbon-contaminated soils. **Z.J. Ren**, L. Lu, H. Wang, S. Jin, Y. Zuo

Section D

Orange County Convention Center
Valencia Ballroom B-D - Theater 12

Electrochemical Water Treatment

J. Blotevogel, B. P. Chaplin, C. Schaefer, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 ENVR 636. Electrochemical Technologies for Environmental Remediation: Fundamentals, Current Advances and New Trends. P. Villegas-Guzman, S. Oladejo Ganiyu, E. Vieira dos Santos, D. Ribeiro da Silva, **C.A. Martínez-Huitle**

2:05 ENVR 637. Bioelectrochemical denitrification: Limitations and scale up. **C. Castro**, K. Taha, D. Yeh

2:25 ENVR 638. Microbial Fuel Cell for Removal of Nitrate from the Effluent (Sidestream) of Aerobic Digestion. **H. Kassouf**, K. Orner, A. Garcia Parra, J.A. Cunningham

2:45 ENVR 639. Boron adsorption by aluminum hydroxide during electrocoagulation: experimental and modeling results. **M. Chen**, O. Dollar, K. Shafer-Peltier, S. Randtke, E.F. Peltier

3:05 ENVR 640. Fouling Characterization and Effectiveness of Countermeasures in Air-cathode Assisted Iron-Electrocoagulation (ACAIE). **A. Kumar**, S. Bandaru, M. Nahata, N. Hohman, A. Gadgil

3:25 Intermission.

3:45 ENVR 641. Air cathode assisted iron electrocoagulation: An effective and high-throughput arsenic remediation technology for contaminated groundwater in rural California. **D.A. Hernandez**, S. Bandaru, A. Gadgil



TECHNICAL PROGRAM

4:05 ENVR 642. Air cathode assisted iron-electrocoagulation for treating wastewater for emerging contaminants. **S. Bandaru**, J. Barazesh, C. Prasse, C.M. Van Genuchten, A. Gadgil

4:25 ENVR 643. Virus control using iron electrocoagulation: Distinguishing removal and inactivation. **S. Chellam**, K. Kim

4:45 ENVR 644. Low permeability zone remediation *via* coupling electrokinetic migration with *in situ* electrochemical degradation. **B. Liu**, G. Li, F. Zhang

5:05 ENVR 645. Mechanisms of bacteria inactivation at low applied potentials. **B.P. Chaplin**, I. Lin, S. Mehraeen

Section E

Orange County Convention Center
Valencia Ballroom B-D - Theater 13

True Positives in EPA'S Non-Targeted Analysis Collaborative Trial (ENTACT)

S. Newton, *Organizer*

C. Grulke, J. Sobus, E. M. Ulrich, A. J. Williams, *Organizers, Presiding*

S. Newton, *Presiding*

1:30 Introductory Remarks.

1:35 ENVR 646. What are the true positives? Mixture construction, sample tracking, and chemical-data linkages in support of the ENTACT project. **C. Grulke**, E.M. Ulrich, M. Strynar, J. Sobus, A.J. Williams, A. Richard

1:55 ENVR 647. EPA's Non-Targeted Analysis Collaborative Trial. **E.M. Ulrich**, J. Sobus, C. Grulke, A. Richard, S. Newton, M. Strynar, K. Mansouri, A.J. Williams

2:15 ENVR 648. CompTox chemicals dashboard: Data and tools to support chemical and environmental risk assessment and the ENTACT project. **A.J. Williams**, C. Grulke, A. McEachran, E. Schymanski, J. Sobus, E.M. Ulrich, A. Richard, J. Dunne, J. Edwards

2:35 ENVR 649. Challenges and methodologies in creating highly curated databases and libraries for the EPA ENTACT study. **T. Anumol**

2:55 Intermission.

3:15 ENVR 650. Using standard reference material dust and EPA's Non-Targeted Analysis Collaborative Trial (ENTACT) mixtures to evaluate methodology and applications of NTA to environmental samples. **S. Newton**, J. Sobus, E.M. Ulrich, R. Singh, A. Chao, J. McCord, S. Laughlin, M. Strynar

3:35 ENVR 651. Comprehensive, non-target environmental exposome sample characterization using GCxGC and high resolution time of flight mass spectrometry. L. Fell, J. Binkley, **T. Richards**

3:55 ENVR 652. Standards-free identification of small molecules using multi-feature matching. **J. Nunez**, D. Thomas, S. Colby, M. Tfaily, N. Tolic, T. Metz, J. Teegarden, R. Renslow

4:15 Panel Discussion.



TECHNICAL PROGRAM

4:55 Concluding Remarks.

Section F

Orange County Convention Center
Valencia Ballroom B-D - Theater 14

Innovations, Advances, and Sustainability in Additive Manufacturing for Electrochemical, Energy, and Environmental Applications

N. Aich, S. Rahaman, *Organizers, Presiding*

1:30 ENVR 653. 3D Printed Thin Film Composite Membranes. **J.R. McCutcheon**, M. Chowdhury

2:00 ENVR 654. Formulation of CO₂ solid adsorbents into practical contactors using 3D printing technique. S. Lawson, **F. Rezaei**

2:20 ENVR 655. Electrospun superhydrophobic and amphiphobic nanocomposite membranes with reduced graphene oxide in poly(vinylidene fluoride-co-hexafluoropropylene) for membrane distillation. **T. Chen**, N. Anwar, S. Rahaman

2:40 ENVR 656. Emissions from consumer level 3D printers and their potential health impacts. **Q. Zhang**, A. Davis, M. Black, R. Weber

3:00 ENVR 657. Innovative 3D printed materials for electrochemical wastewater treatment. O. Garcia-Rodriguez, E. Mousset, H. Olvera-Vargas, Z. Wang, F. Deng, **O. Lefebvre**

3:20 ENVR 658. Chitosan Beads Packed Photocatalytic Reactor: Sustainable Platform for Water Purification under Solar Light Irradiation. **Q. Zheng**, D. Shuai

3:40 Intermission.

3:50 ENVR 659. 3D printing of small device for analytical and environmental applications. L. Hu, **G. Jiang**

4:10 ENVR 660. Construction of three dimensional branched crystalline carbon nitride nanoneedle with accelerated charge collection and separation for Efficient photocatalysis. **Z. Zeng**, X. Quan

4:30 ENVR 661. Efficient photoelectrocatalytic O₂ reduction to H₂O₂ and photoelectron-Fenton pollutants degradation on a WO₃-FPC system. **F. Ye**, X. Quan

4:50 ENVR 662. PVDF blended PVDF-g-PEGMA ultrafiltration membrane: effect of PVDF-g-PEGMA synthesis time and non-woven PET fabric on membrane performance. **B. Liu**

5:10 ENVR 663. 3D printed graphene based hybrid aerogel for contaminant removal from water. **A. Masud**, A. Tabassum, C. Zhou, N. Aich

Section G

Orange County Convention Center
Valencia Ballroom B-D - Theater 11



TECHNICAL PROGRAM

Innovative & Practical Approaches for the Treatment of Per- & Polyfluoroalkyl Substances (PFAS)

J. Liu, S. Vyas, Y. Wang, *Organizers*
J. Choe, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 ENVR 664. Degradation of perfluoroalkyl substances (PFAS) in water by ultrasonic irradiation. **A. Abdullah**, N.S. Quinete, K.E. O'Shea

1:55 ENVR 665. Understanding the structure-activity relationship of emerging perfluoroether acids (PFEAs) by UV-generated hydrated electron. **M.J. Bentel**, Y. Yu, L. Xu, B.M. Wong, Y. Men, J. Liu

2:20 ENVR 666. Removal of perfluorooctane sulfonate (PFOS) from aqueous solution by reduced graphene oxide-iron nanohybrid. **A. Masud**, N.G. Chavez Soria, D.S. Aga, N. Aich

2:40 ENVR 667. New adsorptive photocatalyst for highly efficient adsorption and degradation of perfluorooctanoic acid (PFOA). **D. Zhao**, F. Li, W. Liu, Z. Wei

3:00 Intermission.

3:15 ENVR 668. Degradation of PFAS using the BOHP/UV process: Photocatalysis mechanisms and pilot study results. **E.L. Cates**, M. Qanbardazeh, D. Wang, M. Ateia, H. Torkzadeh

3:40 ENVR 669. Reactive electrochemical membrane (REM) for the oxidation of perfluoroalkyl compounds. **B.P. Chaplin**, H. Le

4:00 ENVR 670. Enhanced degradation of perfluorooctane sulfonate in a heterogeneous UV-electrochemical system. **Y. Su**, U. Rao, B.M. Wong, D.M. Cwiertyny, D. Jassby

4:20 ENVR 671. Transformation of 6:2 fluorotelomer sulfonate by activated peroxy monosulfate at conditions representative of in situ chemical oxidation. **Y. Zhang**, J. Liu, S. Ghoshal

4:40 ENVR 672. Reductive and oxidative decomposition of PFAS by using nZVI combined with oxidants: reaction pathways and mechanisms. **N. Gevaerd de Souza**, A.C. Parenky, H.H. Nguyen, J. Jeon, H. Choi

5:00 Closing Remarks.

Activation of Light (C1-C4) Hydrocarbons: Theory & Experiments

Sponsored by CATL, Cosponsored by ENFL, ENVR, INOR and PHYS

Applications of Cheminformatics to Environmental Science



TECHNICAL PROGRAM

Sponsored by CINF, Cosponsored by ENVR

Chemical Catalysis for Bioenergy Consortium: Addressing Deactivation during Biomass Conversion

Sponsored by CATL, Cosponsored by ENFL, ENVR and INOR

THURSDAY MORNING

Section A

Orange County Convention Center
Room W330A

Red Tide and Strategies for Detection, Remediation & Environmental Impact

M. Bourgeois, *Organizer, Presiding*

K. Hubbard, *Presiding*

8:00 Introductory Remarks.

8:05 ENVR 673. Complexity of nutrients and extreme events supporting harmful algal blooms: *Karenia brevis* as a case study. **P.M. Glibert**

8:25 ENVR 674. Fate and Effects of brevetoxins along the Florida Gulf coast. **R. Pierce**

8:45 ENVR 675. Climate Change Effects on Harmful Algal Blooms and Antibiotic Resistance in Microbes Affecting Seafood Safety and Contact Recreation: Development of Ecological Forecasts to Better Protect Human Health.. **G. Scott**, S. Chatterjee, J. Ferry, S. Putnam, M. Smith, P. Sandifer, B.W. Brooks

9:10 ENVR 676. Remediation of harmful algal blooms in South Florida. **S. Leatherman**

9:30 Intermission.

9:40 ENVR 677. Protecting environment and public health through innovation and citizen science. **T. Fanara**

10:00 ENVR 678. Brevetoxin is an effector of mammalian thioredoxin reductase (TrxR). **K.S. Rein**, A. Tuladhar, R.J. Hondal

10:20 ENVR 679. Differences in xanthophyll de-epoxidase activity in high and low toxic strains of *K. brevis*. **R. Colon**

10:40 Intermission.

10:50 ENVR 680. Rapid detection and enumeration of the red tide organism *Karenia brevis* in the Gulf of Mexico by mRNA amplification and ocean observing system data analysis. A. Hoagland, R. Currier, D. Nieuwkerk, K. Hubbard, **J. Paul**



TECHNICAL PROGRAM

11:10 ENVR 681. Red tide on the West Florida Shelf – an overview of developing technologies for mitigation. **V. Lovko**

11:30 ENVR 682. Development of Electrochemical Sensor for Phosphate Ion Determination in Environmental Water. **S. Sahu**, A. Prasad, M.R. Gartia

11:50 Concluding Remarks.

Section B

Orange County Convention Center
Room W331B

Green Chemistry & the Environment

R. Luque, S. O. Obare, *Organizers, Presiding*

8:00 ENVR 683. Principal components analysis for green process development. **K.C. Caflin**, E. Gauthier

8:20 ENVR 684. Multi-electron transfer System for the Reduction of Chromium. **T.S. Saeed**, S.O. Obare

8:40 ENVR 685. Toward a natural dispersant for crude oil spills: Okra (*Abelmoschus esculentus*) mucilage. J. Sardina, **D.I. Fox**

9:00 ENVR 686. Towards sustainable remediation in the 21st century: Defined mechanochemical reductive dehalogenation at room temperature in a ball mill. **V. Birke**, C. Schutt

9:20 ENVR 687. Role of ferrate in the valorization of biomass residues. S. Tulaphol, S. Yu, **W. Den**, N. Gridanurak

9:40 ENVR 688. Plant Mediated Synthesis of Silver Nanoparticles: Adsorption and Kinetic Studies. **N.E. Efiog**, S.E. Shaibu

10:00 Intermission.

10:15 ENVR 689. Trapping of electromagnetic waves in shielding materials fabricated through core@shell approach. **S. Srivastava**

10:35 ENVR 690. Promoting sustainable material for As(V) and As(III) removal in point-of-use water treatment. **H. Yang**, S. Xu, Y. Wang

10:55 ENVR 691. Speciation of rare earth elements and yttrium (REY) in coal fly ashes (CFAs) and implications for REY extractability. **P. Liu**, R. Huang, Y. Tang

11:15 ENVR 692. Core–Shell Nature of Nanoscale Zero-Valent Iron (nZVI) for Arsenate Removal: A Case of Structure–Activity Relationship. **A. Liu**

11:35 Concluding Remarks.

Section C



TECHNICAL PROGRAM

Orange County Convention Center
Room W331C

Aqueous Contaminant Separation, Resource Recovery & Clean Energy Generation by Electrochemical Processes

D. F. Call, O. Coronell, M. Hatzell, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 ENVR 693. Redox-modulated electrosorption platform technology for aqueous contaminant removal and resource recovery. **T. Hatton**

8:35 ENVR 694. Rationally selecting electrode materials for harvesting salinity gradient energy. **C. Gorski**, J. Fortunato

8:55 ENVR 695. Thermodynamics of electrosorption based separations. **M. Hatzell**, D. Moreno

9:15 ENVR 696. Role of location and abundance of fixed chemical charge in improving the performance of capacitive deionization systems. **R.D. Cusick**, S. Hand, M. del Cerro, K.C. Smith

9:35 ENVR 697. Electrically assisted sorption and desorption of per- and polyfluoroalkyl substances. **S. Zhu**, E. Hossen, D. Knappe, D.F. Call

9:55 Intermission.

10:10 ENVR 698. *In situ* dilatometry of phosphate anion electroadsorption mechanisms. D. Moreno, Y. Bootwala, Q. Gao, W. Tsai, N. Balke, M. Hatzell, **K.B. Hatzell**

10:30 ENVR 699. Effective operation of capacitive deionization using annexed membranes. **A. Omosebi**, X. Gao, J.R. Landon, K. Liu

10:50 ENVR 700. Modeling transport of P(V) ions across anion exchange membranes for nutrient recovery via electrochemical potential gradients in Donnan dialysis. **U. Shashvatt**, L.M. Blaney, A. Bobby

11:10 ENVR 701. Ion transport in charged polymers for electromembrane applications. **G.M. Geise**

11:30 ENVR 702. Beyond swelling degree: Counter-ion hydration and its effect on ion exchange membrane performance. **R.S. Kingsbury**, J. Wang, O. Coronell

11:50 Concluding Remarks.

Section D

Orange County Convention Center
Room W331D

Electrochemical Water Treatment



TECHNICAL PROGRAM

J. Blotevogel, B. P. Chaplin, C. Schaefer, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 ENVR 703. Understanding electric field and catalyst effects on rates of water splitting and ion concentrations in bipolar membranes. **J. Farrell**, R.J. Martinez, Y. Chen, D. Gervasio, J.C. Baygents

8:35 ENVR 704. Electrochemically Enhanced Separation Performance of Nanocarbon-based Membranes. **X. Quan**, X. Fan

8:55 ENVR 705. Anti-fouling electroconductive forward osmosis membranes: Electrochemical and chemical properties. **E. Nicolau**

9:15 ENVR 706. Water Softening using Membrane Capacitive Deionization: What Affects Selectivity? L. Wang, **S. Lin**

9:35 ENVR 707. Functionalized and self-assembled ion exchange coatings for capacitive deionization. A. Jain, J. Kim, K. Zuo, I.A. Said, S. Walker, Q. Li, **R. Verduzco**

9:55 Intermission.

10:10 ENVR 708. Integration of photovoltaic energy supply with membrane capacitive deionization (MCDI) for salt removal from brackish waters. C. Tan, C. He, W. Tang, P. Kovalsky, J. Fletcher, **T. Waite**

10:40 ENVR 709. Bromide ions: Specific removal and recovery by electrochemical desalination. **I. Cohen**, B. Shapira, E. Avraham, A. Soffer, D. Aurbach

11:00 ENVR 710. Feasibility of energy extraction from acidic wastewater by capacitive mixing with a molecular-sieving carbon cathode. **B. Shapira**, D. Aurbach, E. Avraham

11:20 ENVR 711. Selective removal of iodide and bromide from Shale Gas Produced Water using a novel electrochemical unit. **J.S. Zheng**, **J. Li**, X. Liu

11:40 ENVR 712. *In situ* electrochemical passivation of lead pipes in water distribution systems. **G.P. Lobo**, A. Gadgil, S. Bandaru

Section G

Orange County Convention Center
Room W340B

Innovative & Practical Approaches for the Treatment of Per- & Polyfluoroalkyl Substances (PFAS)

J. Choe, J. Liu, S. Vyas, *Organizers*
Y. Wang, *Organizer, Presiding*

8:45 Introductory Remarks.



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

8:50 ENVR 713. Holistic approaches designed for removing PFAS from contaminated environment. **Y. Liang**, W. Zhang, D. Zhang

9:15 ENVR 714. Examination of structure-activity relationship for cobalt-catalyzed defluorination of per- and polyfluoroalkyl substances. **T. Liu**, **S. Fernandez**, J. Liu

9:35 ENVR 715. Adsorption of per- and polyfluoroalkyl substances on functionalized mesoporous silica. **X. Min**, J. Huo, Q. Dong, Y. Wang

9:55 ENVR 716. Functionalized mineral adsorbents for the removal of perfluorinated chemicals. **Q. Dong**, J. Huo, X. Min, Y. Wang

10:15 Intermission.

10:30 ENVR 717. Thermo-responsive polymer hydrogel and pore functionalized membrane for temperature swing sorption and desorption of PFOA. **D. Bhattacharyya**, A. Saad, R. Mills, A. Aher

10:55 ENVR 718. Near-instant removal of poly- and perfluorinated alkyl substances by polyethylenimine-functionalized cellulose microcrystals. **M. Ateia**, M. Attia, N. Tharayil, F. Alexis, D.C. Whitehead, T. Karanfil

11:15 ENVR 719. Magnetic Nanocomposite Adsorbents for the Selective Capture and Removal of PFAS from Contaminated Water Systems. **M. Frazar**, T. Dziubla, J.Z. Hilt

11:35 ENVR 720. Perfluorooctanoic acid binding to heme-proteins and potential remediation by cyclodextrin extraction. **A. del Valle**, J. Betancourt, N.L. Perera, J. Miksovskya, K.E. O'Shea

11:55 Closing Remarks.

Chemical Catalysis for Bioenergy Consortium: Addressing Deactivation during Biomass Conversion

Sponsored by CATL, Cosponsored by ENFL, ENVR and INOR

Elucidation of Mechanisms & Kinetics on Surfaces

Sponsored by CATL, Cosponsored by ENFL, ENVR, INOR and PHYS

THURSDAY AFTERNOON

Activation of Light (C1-C4) Hydrocarbons: Theory & Experiments

Sponsored by CATL, Cosponsored by ENFL, ENVR, INOR and PHYS



TECHNICAL PROGRAM

Elucidation of Mechanisms & Kinetics on Surfaces

Sponsored by CATL, Cosponsored by ENFL, ENVR, INOR and PHYS

FLUO

Division of Fluorine Chemistry

O. Boltalina, *Program Chair*

SUNDAY MORNING

Section A

Orange County Convention Center
Room W304F

ACS Award for Creative Work in Fluorine Chemistry: Symposium in honor of Norio Shibata

O. V. Boltalina, D. O'Hagan, *Organizers*
T. Umemoto, *Organizer, Presiding*
S. Fustero Lardies, *Presiding*

8:30 FLUO 1. New nickel-mediated chemistry involving fluorinated ligands and substrates. **D.A. Vicic**, M.D. Kosobokov, T. Xue

8:55 FLUO 2. Late-stage fluorination with metal alkali fluoride. **V. Gouverneur**

9:20 FLUO 3. Oxidative trifluoromethylation and difluoromethylation of heteroarenes. **F. Qing**

9:45 FLUO 4. Generation and applications of fluorobenzyl anions. **H. Amii**

10:10 Intermission.

10:25 FLUO 5. Strategic incorporation of fluorine into bioactive compounds for medicinal chemistry and drug discovery: A progress report. **I. Ojima**

10:50 FLUO 6. Enamine catalyzed visible-light induced perfluoroalkylation. **T. Yajima**

11:15 FLUO 7. Selectively fluorinated motifs for bioactives discovery. **D. O'Hagan**

11:40 FLUO 8. Fluorine effects in asymmetric hydrogen atom transfer reactions. **D. Cahard**

SUNDAY AFTERNOON



TECHNICAL PROGRAM

Section A

Orange County Convention Center
Room W304F

ACS Award for Creative Work in Fluorine Chemistry: Symposium in honor of Norio Shibata

D. O'Hagan, T. Umemoto, *Organizers*
O. V. Boltalina, *Organizer, Presiding*
V. Gouverneur, *Presiding*

1:30 FLUO 9. Synthesis of novel fluorinated aliphatic amines. **P. Mykhailiuk**

1:55 FLUO 10. New insights into the enantioselective difluoromethylation. **F.R. Leroux**, C. Batisse, M. Céspedes Dávila, A. Panossian, G. Hanquet

2:20 FLUO 11. Fluoropyrroles. **G. Sandford**

2:45 FLUO 12. Strategies for the synthesis of simple mono- and trifluoromethylated scaffolds. **S. Fustero Lardies**

3:10 Intermission.

3:25 FLUO 13. Application of fluoro reagents beyond fluorination and trifluoromethylation. **T. Umemoto**

3:50 FLUO 14. Selectivity of different amine/HF reagents for synthesis of functionalized organic fluorine compounds. **G. Haufe**

4:15 FLUO 15. Preparation and reactions of tetrafluoro- λ^6 -sulfanyl containing polymers: Synthesis, photochemical, and physical properties. K. Bonetti, M. Deng, **J.T. Welch**

4:40 FLUO 16. Trifluoromethyl group as a bioisosteric replacement of aliphatic nitro group in CB₁ receptor positive allosteric modulators (PAMs). **M. Zanda**, I.R. Greig, C. Tseng, R. Ross

5:05 FLUO 17. Fluorine effects in catalysis and biomedicine. **R. Gilmour**

SUNDAY EVENING

Section A

Orange County Convention Center
Room W304G

ACS Award for Creative Work in Fluorine Chemistry: Symposium in honor of Norio Shibata

O. V. Boltalina, D. O'Hagan, T. Umemoto, *Organizers*

5:30 - 7:30



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

FLUO 18. Recent topics in fluorine chemistry at Central Glass. **H. Kobayashi**

FLUO 19. ^{19}F magnetic resonance probes for activity-based sensing of formaldehyde. K. Minder, J. Lange, J. Powell, L. Eltahir, J. Kelts, **J.O. Massing**

MONDAY MORNING

Section A

Orange County Convention Center
Room W304F

ACS Award for Creative Work in Fluorine Chemistry: Symposium in honor of Norio Shibata

O. V. Boltalina, T. Umemoto, *Organizers*
D. O'Hagan, *Organizer, Presiding*
G. Haufe, *Presiding*

8:30 FLUO 20. Activation of fluorinated alkanes und alkenes: From homogeneous to heterogeneous reactions and back. **T. Braun**, E. Kemnitz, M. Ahrens, G. Meißner, M. Talavera

8:55 FLUO 21. Spectroscopic and computational study of weak O–H...F hydrogen bonding in metal salt hydrates of the $\text{B}_{12}\text{F}_{12}^{2-}$ superweak anion. **S.H. Strauss**, M.R. Lacroix, Y. Liu, Y. Yang, J. Hetmanczyk

9:20 FLUO 22. Fluorination for control of molecular packing: Singlet fission in 1,3-diphenylisobenzofurans. J. Kaleta, E.A. Buchanan, M. Tan, J. Wen, B.E. Kahr, I. Císarová, Z. Havlas, **J. Michl**

9:45 FLUO 23. Fluoride removal by chitosan modified by ferrum ion adsorbents for groundwater treatment. **Y. Gao**, Z. Yuan, J. Liu

10:10 Intermission.

10:25 FLUO 24. Direct high-temperature trifluoromethylation of polycyclic aromatic hydrocarbons: New developments. **O.V. Boltalina**, N.J. DeWeerd, K. Rippy, B.J. Reeves, C. Brook, S.H. Strauss

10:50 FLUO 25. Sulfur [^{18}F]/[^{19}F]fluoride exchange of aryl fluorosulfate: Click chemistry and new agents for PET imaging. **Q. Zheng**, H. Xu, H. Wang, G. Yang, P. Wu, K.B. Sharpless

11:15 FLUO 26. General leaving group-assisted strategy for photoinduced fluoroalkylations using *N*-hydroxybenzimidoyl chloride esters. **Y. Wang**, W. Zhang, Q. Zhang, Z. Zou, Y. Pan

11:40 FLUO 27. New strategies in fluoroalkylselenolations. **T. Billard**

MONDAY AFTERNOON

Section A



TECHNICAL PROGRAM

Orange County Convention Center
Room W304F

ACS Award for Creative Work in Fluorine Chemistry: Symposium in honor of Norio Shibata

O. V. Boltalina, *Organizer*
D. O'Hagan, T. Umemoto, *Organizers, Presiding*
D. A. Vacic, *Presiding*

1:30 FLUO 28. Fluorinated sugars: Formulation of customized cannabis concentratesaluable building blocks and chiral tools in organic synthesis. **H. Koroniak**, M. Bilaska-Markowska, K. Koroniak-Szejn, J. Tomaszewska

1:55 FLUO 29. Difluoroallene chemistry: Versatile platform for syntheses of ring-fluorinated carbo- and heterocycles. **J. Ichikawa**

2:20 FLUO 30. Synthesis of (Z)-1,1,1,4,4,4-hexafluoro-2-butene and (E)-1,1,1,4,4,4-hexafluoro-2-butene by direct coupling of 2,2-dichloro-1,1,1-trifluoroethane. **X. Sun**

2:45 FLUO 31. Synthesis, stability, and reactivity of azidofluoroalkanes. **P. Beier**

3:10 Intermission.

3:25 FLUO 32. Our recent foray into fluorinations and fluoroalkylations. **S.G. Prakash**

3:50 FLUO 33. From C1 to C2: Pentafluoroethylation with Ruppert-Prakash reagent. **J. Hu**

4:15 FLUO 34. Some recollections of my research with fluorine chemistry. **N. Shibata**

Chemistry in Space: Future Directions

Sponsored by YCC, Cosponsored by AGFD, ANYL, BIOT, BMGT, CHAS, ENVR, FLUO, GEOC, HIST, I&EC, MEDI, POLY and PROF

GEOC

Division of Geochemistry

N. Kabengi, *Program Chair*

SUNDAY MORNING

Section A



TECHNICAL PROGRAM

Orange County Convention Center
Room W311G

Molecular Processes at Mineral-Water Interfaces: Predictions via Linking Theory & Experiments

Cosponsored by COLL
V. Starchenko, *Organizer*
J. Bracco, H. Wang, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 **GEOC 1.** Linked microcalorimetry and density functional theory study of cations exchange on quartz. H. Watts, N. Allen, J.D. Kubicki, **N. Kabengi**

9:05 **GEOC 2.** Relative permittivity in the electrical double layer from nonlinear optics. **F. Geiger**

9:25 **GEOC 3.** Chemo-mechanical fracture of silica in aqueous electrolyte solutions. **J.M. Rimsza**, R. Jones, L.J. Criscenti

9:55 **GEOC 4.** Kinetics and mechanisms of phenolic contaminant oxidation by environmentally-relevant manganese oxides. **E.L. Trainer**, M.A. Ginder-Vogel, C.K. Remucal

10:15 Intermission.

10:30 **GEOC 5.** Surface hydrophobicity and energetics at Mica-water interfaces. **A. Koishi**, S. Lee, P. Fenter, A. Fernandez-Martinez, L. Michot, I.C. Bourg

11:00 **GEOC 6.** Understanding molecular assembly on mica surfaces: Influence of buried hydroxyls. **A. Tuladhar**, M.D. Baer, B.A. Legg, Z. Chase, J. Tao, S. Zhang, Z. wang, C.J. Mundy, H. Wang, J.J. De Yoreo

11:20 **GEOC 7.** Subcritical nucleation clusters: Structure, energetics, populations, and fluctuations. **B. Legg**, M.D. Baer, C.J. Mundy, J.J. De Yoreo

11:50 **GEOC 8.** Heterogeneous $(Ca_x, Mg_{1-x})CO_3$ precipitation on organics. B. Cao, N. Deng, D. DePaolo, **Y. Hu**

12:10 **GEOC 9.** Cation sorption at the Barite (001): Water interface. **J. Bracco**, S. Lee, J. Stubbs, P.J. Eng, A. Kommu, P. Fenter, J.D. Kubicki, A.G. Stack

Section B

Orange County Convention Center
Room W311F

Understanding Shale-Gas-Fluid Interactions for Water & Energy

J. R. Bargar, A. Hakala, A. D. Jew, C. Lopano, *Organizers*
Q. Li, M. Y. Stuckman, *Organizers, Presiding*

8:30 Introductory Remarks.



TECHNICAL PROGRAM

8:35 GEOC 10. Characterizing and quantifying CO₂-fluid-shale interactions and pore changes. **S. Sanguinito**, A. Goodman, B. Kutchko, S. Natesakhawat, D. Crandall, P. Cvetic

9:05 GEOC 11. Transport of alkaline earth metals in natural and synthetic produced water through porous media. **Z. Ye**, V. Prigiobbe

9:25 GEOC 12. Experimental study of barite scaling in Marcellus shale during a simulated injection and shut-in period of hydraulic fracturing. **W. Xiong**, J. Moore, M.Y. Stuckman, A. Hakala, D. Crandall, C. Lopano

9:45 GEOC 13. Geochemical alteration of shale fractures and the bordering rock matrix. **H. Deng**, M. Voltolini, M.C. Cheshire, **S. Molins**, C. Steefel, D. DePaolo, J. Ajo-Franklin, A.G. Stack, L. Anovitz

10:15 Intermission.

10:30 GEOC 14. Influence of slickwater additives on fate of residual fracturing fluids and flowback composition in shale gas reservoirs. **B. Ellis**

11:00 GEOC 15. Alteration depths from the shale surface into the matrix. **Q. Li**, A.D. Jew, A. Kohli, G.E. Brown, K. Maher, J.R. Bargar

11:20 GEOC 16. Isotopic fingerprinting of produced water from Utica and Point Pleasant Shale. **W.D. Burgos**, T. Tasker, N.R. Warner

11:40 GEOC 17. Radium removal from dilute and high ionic strength solution using barium sulfate (BaSO₄): Comparison of experimental results and molecular simulations. **A. Gusa**, H. Alkhashab, R.D. Vidic, J. Flora

Carbon Dioxide Conversion & Utilization

CO₂ Hydrogenation to Fuels & Chemicals

Sponsored by ENFL, Cosponsored by CATL, COMP and GEOC

New Frontiers in the Confluence of Experimental Thermodynamics, Structural Investigations & Theory/Computation

Experimental Thermodynamics

Sponsored by PHYS, Cosponsored by GEOC

SUNDAY AFTERNOON

Section A

Orange County Convention Center
Room W311G



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

Molecular Processes at Mineral-Water Interfaces: Predictions via Linking Theory & Experiments

Cosponsored by COLL
V. Starchenko, *Organizer*
J. Bracco, H. Wang, *Organizers, Presiding*

1:45 Introductory Remarks.

1:50 **GEOC 18.** Linking microscopy and metadynamics simulations to understand gibbsite dissolution at high pH. **K. Rosso**, X. Zhang, Z. Shen, A.G. Stack, S.N. Kerisit, S. Zhang, J. Tao, J.J. De Yoreo

2:30 **GEOC 19.** DFT + thermodynamics prediction of MAI_{12} keggin heteroatom reactivity and substitution. **J.L. Bjorklund**, J.W. Bennett, T. Forbes, S.E. Mason

2:50 **GEOC 20.** Validating molecular dynamics simulations of the Al_2O_3 /water interface with specular and nonspecular X-ray reflectivity. **K. Letchworth-Weaver**, K. Harmon, M.K. Chan, G.A. Galli, P. Fenter

3:20 **GEOC 21.** Size-dependent adsorption and hydrolysis of polyphosphates on aluminum oxides. **B. Wan**, R. Huang, Y. Tang

3:40 Intermission.

4:00 **GEOC 22.** Ion adsorption and perturbations of solvent structure at mineral-aqueous interfaces. **E. Borguet**

4:30 **GEOC 23.** Using DFT, molecular dynamics, and thermodynamics modelling, to connect with experimental information about Al_2O_3 -water interface structure and reactivity. **A. Abbaspour Tamijani**, **W. Marquardt**, **S.E. Mason**

4:50 **GEOC 24.** Surface chemistry of silica-coated magnetic nanoparticles. **S. Goberna-Ferron**, A. Fernandez-Martinez, L.L. Charlet, J. Greneche

5:10 **GEOC 25.** EXAFS analysis for the interaction of molybdate ($Mo(VI)O_4^{2-}$) with hematite and magnetite. **J. Zhang**, V.S. Coker, S. Shaw

Section B

Orange County Convention Center
Room W311F

Understanding Shale-Gas-Fluid Interactions for Water & Energy

J. R. Bargar, A. Hakala, A. D. Jew, C. Lopano, *Organizers*
Q. Li, M. Y. Stuckman, *Organizers, Presiding*

1:30 **GEOC 26.** Detection of antibiotic and metal resistance genes in deep shale microbial community members. **J. Luek**, C. Murphy, K. Wrighton, P. Mouser

1:50 **GEOC 27.** Genomic insights into microbial processes in Permian Basin produced waters. **D. Lipus**, K. Tinker, D. Ross, D. Gulliver



TECHNICAL PROGRAM

2:10 GEOC 28. Microbial (de)halogenation pathways in hydraulically fractured natural-gas wells in the Appalachian Basin. **M.V. Volker**, R.A. Daly, K. Wrighton, P. Mouser

2:30 GEOC 29. Degradation of phosphonate-based scale inhibitors by Fe-bearing phyllosilicates under energy-related subsurface environmental conditions. L. Zhang, **Y. Jun**

2:50 GEOC 30. Nanogeochemistry of CH₄-CO₂-H₂O in unconventional oil/gas reservoirs. **Y. Wang**

3:20 Intermission.

3:35 GEOC 31. Molecular simulation of the multicomponent interaction in kerogen nanopore. **T.A. Ho**, Y. Wang, L.J. Criscenti, A. Ilgen

3:55 GEOC 32. Recovering the oil trapped in organic pores of shales by surfactant mixtures. **H. Dehghanpour**, A. Habibi

4:15 GEOC 33. Evaluation of wettability and EOR potential of organic-rich shales. **H. Dehghanpour**, M. Yassin

4:35 GEOC 34. Impact of pore connectivity on two-phase relative permeability in shale formations. **D. Davudov**, R.G. Moghanloo, Y. Zhang, A. Mabadeje

Carbon Dioxide Conversion & Utilization

CO₂ Conversion to Carbonates

Sponsored by ENFL, Cosponsored by CATL, COMP and GEOC

New Frontiers in the Confluence of Experimental Thermodynamics, Structural Investigations & Theory/Computation

Experimental Thermodynamics

Sponsored by PHYS, Cosponsored by GEOC

MONDAY MORNING

Section A

Orange County Convention Center
Room W311G

Molecular Processes at Mineral-Water Interfaces: Predictions via Linking Theory & Experiments

Cosponsored by COLL
V. Starchenko, *Organizer*
J. Bracco, H. Wang, *Organizers, Presiding*



TECHNICAL PROGRAM

8:00 Introductory Remarks.

8:05 **GEOC 35.** Fate of As during the Interactions between metal-substituted iron oxides and Fe(II). **H. Liu**, X. Lu, E. Flynn, J.G. Catalano

8:25 **GEOC 36.** Reduction of Magnetite by Polysulfide and its effect on reductive immobilization of Chromate. **J.S. Zheng**, X. Liu, J. Li, C. Xu

8:45 **GEOC 37.** Colloidal transport of hexavalent chromium in groundwater. M. Bhattacharya, **A. Singh**

9:05 **GEOC 38.** Oxidation of 17 β -estradiol by Fe(II)-activated nontronite. **R.E. Washington**, D.R. Griffith, C. Hutchinson, A. Ilgen

Section A

Orange County Convention Center
Room W311G

General Geochemistry

N. Kabengi, *Organizer, Presiding*

10:00 Introductory Remarks.

10:05 **GEOC 39.** Distribution of biomarker in enugu shale, anambra basin nigeria: Implication on hydrocarbon potential. **A.K. Adeyemi**, T.A. Adedosu, G. Ogungbesan, J. Onyeocha

10:25 **GEOC 40.** Fate of ferrihydrite-associated organic carbon during Fe reduction: adsorption versus coprecipitation. **L. Han**, K. Sun, B. Xing

10:45 **GEOC 41.** Impact of NOM and oxyanions on aggregation of amorphous iron hydroxides. **S. Yeo**, D. Lawler, L.E. Katz

11:05 Intermission .

11:20 **GEOC 42.** Reductive immobilization of Cr(VI) by Polysulfide-reduced Maghemite. **X. Liu**, J. Li, J.S. Zheng, C. Xu

11:40 **GEOC 43.** Insights to catagenesis reactions from molecular mass balance in hydrous pyrolysis. **W.C. Hockaday**, T. Longbottom, O. Craven

Section B

Orange County Convention Center
Room W311F

2019 Geochemistry Division Medal Symposium in Honor of Everett Shock



TECHNICAL PROGRAM

Cosponsored by PROF†
A. Anbar, S. N. Kerisit, *Organizers, Presiding*

8:30 Introductory Remarks .

8:35 GEOC 44. Calorimetric determination of microbial activity in low-energy environments. **J. Amend**, J. Feyhl-Buska, F. Wu, A. Robador, V. Orphan, S. Finkel

8:55 GEOC 45. Thermodynamic properties of organic compounds at high temperatures and pressures and the stability of organic carbon in deep crustal rocks. **L. Richard**

9:15 GEOC 46. Chemical and metabolic landscape of seawater-basalt interaction. **T. Ely**, E. Shock

9:35 GEOC 47. Hydrothermal fluids: Are they best served cold? **V.P. Milesi**, E. Shock

9:55 Intermission .

10:00 GEOC 48. Host rock influences metal abundance in terrestrial hot springs. **B. St Clair**, A. Cox

10:20 GEOC 49. Metal speciation and bioavailability in biologically relevant fluids via estimation of metal-ligand stability constants. **A. Prasad**, E. Shock

10:40 GEOC 50. Goethite surface inhibition of the dehydration of *cis*-1,2-cyclohexanediol at 200°C. **C.F. Estrada**, C. Bockisch, K. Fecteau, I.R. Gould, H.E. Hartnett, K. Robinson, L. Williams, E. Shock

11:00 Intermission.

11:05 GEOC 51. hydrothermal solar system: Enceladus as an example of Everett Shock's legacy. **C. Glein**

11:25 GEOC 52. Organic compounds as tracers of temperature and pH in geologic systems. **K. Robinson**, C. Bockisch, I.R. Gould, K. Fecteau, E. Shock

11:45 GEOC 53. Hydrogen dependent carbon reduction: The physiology of the last universal common ancestor, Luca. **W. Martin**

12:05 GEOC 54. Tracking potential sources of carbon in surface expressions of terrestrial subsurface ecosystems. **D. Meyer-Dombard**, D. Cardace, M.R. Osburn, E. Shock

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Sponsored by PROF, Cosponsored by AGFD, ANYL, BIOL, BIOT, CARB, CELL, CHED, CMA, COLL, COMP, ENVR, GEOC, I&EC, MEDI, MPPG, NUCL, ORGN, PHYS, PMSE, POLY, PRES, WCC and YCC

Carbon Dioxide Conversion & Utilization



TECHNICAL PROGRAM

CO2 Capture & Separation

Sponsored by ENFL, Cosponsored by CATL, COMP and GEOC

MONDAY AFTERNOON

Section B

Orange County Convention Center
Room W311F

2019 Geochemistry Division Medal Symposium

Cosponsored by PROF
N. Kabengi, S. N. Kerisit, *Organizers, Presiding*

2:30 Introductory Remarks .

2:40 GEOC 55. Using geochemical insights to illuminate deep subsurface microbiology. **M.R. Osburn**, C. Casar, T. Flynn, B. Kruger

3:10 GEOC 56. Organic geochemistry of Earth's upper mantle. **D.A. Sverjensky**

3:40 GEOC 57. Origin of organic-rich vent fluids at the Pescadero Basin hydrothermal field. **J. McDermott**

4:10 GEOC 58. Geomicrobiology: Chemists learning from geologists. C. Bockisch, Z. Yang, H.E. Hartnett, L. Williams, E. Shock, **I.R. Gould**

4:40 GEOC 59. Geobiochemistry and planetary habitability. **E. Shock**, G. Boyer, P. Canovas, J. Dick

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Sponsored by PROF, Cosponsored by AGFD, ANYL, BIOL, BIOT, CARB, CELL, CHED, CMA, COLL, COMP, ENVR, GEOC, I&EC, MEDI, MPPG, NUCL, ORGN, PHYS, PMSE, POLY, PRES, WCC and YCC

Chemistry in Space: Future Directions

Sponsored by YCC, Cosponsored by AGFD, ANYL, BIOT, BMGT, CHAS, ENVR, FLUO, GEOC, HIST, I&EC, MEDI, POLY and PROF

Carbon Dioxide Conversion & Utilization

CO2 as an Oxidant



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

Sponsored by ENFL, Cosponsored by CATL, COMP and GEOC

New Frontiers in the Confluence of Experimental Thermodynamics, Structural Investigations & Theory/Computation

Experimental Thermodynamics & Theory/Computation

Sponsored by PHYS, Cosponsored by GEOC

Undergraduate Research Posters

Geochemistry

Sponsored by CHED, Cosponsored by GEOC and SOCED

MONDAY EVENING

Section A

Orange County Convention Center
West Hall C

Sci-Mix

N. Kabengi, *Organizer*

8:00 - 10:00

11, 34, 40-41, 49. See previous listings.

76, 78, 86, 106, 111, 127, 138, 151, 154. See subsequent listings.

TUESDAY MORNING

Section A

Orange County Convention Center
Room W311G

Chemical Transport & Remediation in Mining Legacy Sites



TECHNICAL PROGRAM

J. M. Blake, J. M. Cerrato, K. Walton-Day, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 GEOC 60. Mobilization, methylation and exposure of mercury from artisanal and small-scale gold mining in Madre de Dios, Peru. **H. Hsu-Kim**, S. Diringer, C. Weinhouse, A. Berky, M. Marani, E. Ortiz, W. Pan

9:05 GEOC 61. Uranium, arsenic and iron speciation in acid mine drainage environments. **J. Lezama Pacheco**

9:35 GEOC 62. Metagenomics study of acidic pit lakes in the Iberian Pyrite Belt, Spain. **W.D. Burgos**, D. Munoz

9:55 GEOC 63. Biogeochemistry of the treatment of mining-impacted water in mining legacy sites: integrating aqueous phase and solid phase analyses to elucidate efficiencies and mechanisms. **S.R. Al-Abed**, P. Pinto, P. Potter, J. McKernan

10:15 Intermission.

10:30 GEOC 64. Biogeochemical and reactive transport modeling as an integrative tool for simulation and forecasting of contaminant chemistry, transport, and remediation. **P.A. O'Day**, E. Reinoso-Maset, S. Helmrich

11:00 GEOC 65. Hydrological-geochemical controls over uranium mobility in unsaturated zone sediments. **J.R. Bargar**, S. Roycroft, K. Boye, V. Noel, R. Johnson, Z. Perzan

11:30 GEOC 66. Potential of arsenic sulfide and uranium phosphate minerals for passive remediation and natural attenuation in mining environments. P. Le Pape, L. Fernandez-Rojo, L. Stetten, A. Adra, A. Mangeret, F. Battaglia, L. Olivi, J.R. Bargar, C. Cazala, C. Casiot, **G. Morin**

Section B

Orange County Convention Center
Room W311F

Planetary & Meteoritic Chemistry

Cosponsored by ANYL and PHYS
S. Singletary, Y. Tang, *Organizers*
D. Kao, J. D. Kubicki, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 GEOC 67. Widespread presence of Fe-Mg amorphous silicates in the early solar system: Evidence from the matrices of the most pristine asteroidal meteorites. **N.M. Abreu**, K. Howard

9:05 GEOC 68. Phase Transitions in MgSiO₃ Post-perovskite in super-Earth Mantles. **R.M. Wentzcovitch**

9:35 GEOC 69. Constraints on the heavy elements abundances in the interiors of Saturn and Jupiter. **B. Militzer**, S. Wahl, W. Hubbard

10:05 Intermission.



TECHNICAL PROGRAM

10:20 GEOC 70. New insights into Mars surface geochemistry from orbiters and rovers. **J. Wray**

10:50 GEOC 71. Carbonate identification in Tyrrhena Terra on Mars and potential habitability of the region. **Y. Liu**

11:05 GEOC 72. Organic matter in 3.5-billion-year-old mudstones from an ancient lake in Gale Crater, Mars. **J.L. Eigenbrode**, R.E. Summons, A. Steele, C. Freissinet, M. Millan, P.R. Mahaffy, B. Sutter, A. McAdam, H. Franz, P.D. Archer

Carbon Dioxide Conversion & Utilization

Electrocatalysis

Sponsored by ENFL, Cosponsored by CATL, COMP and GEOC

Carbon Dioxide Conversion & Utilization

Electrocatalysis

Sponsored by ENFL, Cosponsored by CATL, COMP and GEOC

New Frontiers in the Confluence of Experimental Thermodynamics, Structural Investigations & Theory/Computation

Experimental Thermodynamics

Sponsored by PHYS, Cosponsored by GEOC

TUESDAY AFTERNOON

Section A

Orange County Convention Center
Room W311G

Chemical Transport & Remediation in Mining Legacy Sites

J. M. Blake, J. M. Cerrato, K. Walton-Day, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 GEOC 73. Application of non-traditional isotope measurements to studies of mine-wastes and remediation systems. **D. Blowes**, C. Ptacek, H. Shrimpton, J. Buis, R. Parigi, J. Jamieson-Hanes, J. Eagling, H. Veeramani, R. Amos



TECHNICAL PROGRAM

2:05 GEOC 74. Faro Waste Rock Project: Integration of synchrotron-based spectroscopic techniques with field and laboratory measurements to characterize sulfide oxidation rates and mechanisms of gas transport in waste-rock dumps. **Z. Bao**, D. Blowes, C. Ptacek, J. Bain, S. Holland, Y. Finrock, D. Wilson, W. Wilson

2:25 GEOC 75. Spectroscopic investigation of uranium binding onto functionalized electrospun polymers. **M. Shaikh**, A. Ali, D.M. Cwiertny, T. Forbes, A.J. Haes, J.M. Cerrato

2:45 GEOC 76. Vapor deposited gold nanofilm electrode for electrochemical detection of arsenite. **T. Casuse**, A. Benavidez, L. Tsui, J. Plumley, J.M. Cerrato, F. Garzon

3:05 GEOC 77. Effects of carboxylic, phenolic, and carbonyl functional groups on uranium reactivity under laboratory conditions. **C.A. Velasco**, J. Gonzalez-Estrella, K. Artyushkova, J.M. Cerrato

3:25 GEOC 78. Investigation of the effect of microbial processes on arsenic stability in sediments from Cheyenne River, South Dakota, USA. **C. DeVore**, L. Rodriguez Freire, J. Gonzalez-Estrella, N. Villa, A. Ali, C. Ducheneaux, K. Artyushkova, J.M. Cerrato

3:45 Intermission.

4:00 GEOC 79. Geochemical and geological assessment of areas susceptible to occurrence and persistence of uranium, arsenic, molybdenum, and selenium related to mining in the Texas Gulf Coast. **J. Blake**, D.B. Yager, K. Walton-Day, T.J. Gallegos, V. Stengel, D. Humberson, A. Teeple, K. Becher

4:30 GEOC 80. Understanding background conditions as a first step in developing remediation goals. **K.A. Radloff**, T.S. Bowers

4:50 GEOC 81. Geochemical monitoring and modeling of water chemistry changes to North Fork of Clear Creek following remediation of acid mine drainage inputs. **E. Lloyd**, J. Meyer, J. Murphy, K. Smith, J.F. Ranville

5:10 GEOC 82. Uranium accumulation in cells of *Brassica juncea*: Effect of calcium in carbonate solutions. **E. El Hayek**, A. Brearley, T. Howard, P. Hudson, C. Torres, S. Cabaniss, A. Ali, J.M. Cerrato

Section B

Orange County Convention Center
Room W311F

Planetary & Meteoritic Chemistry

Cosponsored by ANYL and PHYS
D. Kao, J. D. Kubicki, *Organizers*
S. Singletary, Y. Tang, *Organizers, Presiding*

2:00 Introductory Remarks.

2:05 GEOC 83. Theoretical chemical kinetics as a tool for exploring the chemistry of planetary atmospheres. **S.J. Klippenstein**

2:35 GEOC 84. Withdrawn



TECHNICAL PROGRAM

2:50 GEOC 85. Calculation of kinetic rate constants by high-level *ab initio* quantum chemical methods for astrochemistry and planetary sciences. **S.R. Barua**, P. Romani

3:05 GEOC 86. Search for self-sustaining chemical systems capable of Darwinian evolution. **S.D. Domagal-Goldman**

3:35 Intermission.

3:50 GEOC 87. Avoiding "false negatives" in the search for life on other worlds: Lessons from ancient Earth. **A. Anbar**

4:20 GEOC 88. Synthesis, characterization, and potential prebiotic chemistry of metal phosphites. **H.L. Abbott-Lyon**, M.A. Pasek

4:35 GEOC 89. Density functional theory modeling of C and H isotopic fractionation of adsorbed organic compounds. **J.D. Kubicki**, A. Fox, J. Boettger, H. Watts, K. Freeman

4:50 GEOC 90. Study chirality of amino acids with density functional theory. **D. Kao**, S.D. Domagal-Goldman

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Sponsored by PROF, Cosponsored by ENVR, GEOC, I&EC, MEDI, MPPG, NUCL, ORGN, PHYS, PMSE, POLY, WCC and YCC

Carbon Dioxide Conversion & Utilization

Photo, Electro & Plasma Catalysis

Sponsored by ENFL, Cosponsored by CATL, COMP and GEOC

WEDNESDAY MORNING

Section A

Orange County Convention Center
Room W311G

Chemical Transport & Remediation in Mining Legacy Sites

J. M. Blake, J. M. Cerrato, K. Walton-Day, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 GEOC 91. Geochemical and mineralogical characterization of legacy mine tailings to develop remediation strategies. **C. Ptacek**, D. Blowes, J. Bain, M. Moncur



TECHNICAL PROGRAM

8:35 GEOC 92. Drivers of and solutions for uranium plume persistence at DOE's Old Rifle, Colorado former uranium mill site. **K. Williams**, J. Christensen, C. Hobson, M. Rigali

9:05 GEOC 93. Water quality changes following remediation of abandoned draining mines using structural bulkheads, upper Animas River, and upper Arkansas River Watersheds, Colorado, USA. **K. Walton-Day**, M.A. Mast, R.L. Runkel

9:25 GEOC 94. Mechanisms of iron oxyhydroxide deposition in abandoned mine drainage (AMD). K.N. Ambruso, N.T. Fretz, E.K. Herman, **M.M. McGuire**

Section A

Orange County Convention Center
Room W311G

Nanoparticles in Nature: Detection, Characterization, Origin & Formation Mechanisms

Cosponsored by COLL
M. Baalousha, M. Mansor, J. Xu, *Organizers, Presiding*

10:00 Introductory Remarks.

10:05 GEOC 95. Optimization of an extraction method for copper oxide nanoparticles from soil. **G. Bland**, G. Lowry

10:25 GEOC 96. Fast multi-element quantification of nanoparticles in waste water sludge using single particle ICP-MS. **Y. Huang**, J. Nelson, A.A. Keller

10:45 GEOC 97. Monitoring titanium dioxide engineered nanoparticles in environmental systems. **M. Baalousha**

11:05 Intermission.

11:20 GEOC 98. Synthesis-based approaches towards characterization of the diversity of metal sulfide nanoparticles that can plausibly formed in nature. **M. Mansor**, D. Berti, C. Winkler, M. Murayama, M.F. Hochella, J. Xu

11:40 GEOC 99. Effect of redox cycles on the transformation of d-MnO₂ nanosheets to tunnel structured Mn oxide. **H. Jung**, Y. Tang

12:00 GEOC 100. Theoretical study on the reaction mechanisms of most stable Si₄C₄ cluster formation from Si₂C₂ clusters. **X.F. Duan**, J. Lutz, L. Burggraf

Section B

Orange County Convention Center
Room W311F

Environmental Interfaces under Nano-scale Confinement

Cosponsored by COLL
A. Knight, *Organizer*
A. Ilgen, *Organizer, Presiding*
L. Anovitz, *Presiding*



TECHNICAL PROGRAM

8:30 Introductory Remarks.

8:35 **GEOC 101.** Relationships between water confined within synthetic nanotubes and nanoporous geologic media. **T. Forbes**

9:05 **GEOC 102.** Role of H₂O structure and mobility in controlling reactivity in adsorbed H₂O films. **J. Loring**, Q. Miller, R. Placencia-Gomez, E.S. Ilton, O. Qafoku, C.J. Thompson, D.A. Dixon, K. Rosso

9:25 **GEOC 103.** Dendritic oxide growth in zero-valent iron nanofilms revealed by atom probe tomography. **F. Geiger**

9:45 **GEOC 104.** Withdrawn

10:15 Intermission.

10:35 **GEOC 105.** Neutron spectroscopy of water molecules under ultra-confinement. **A.I. Kolesnikov**, L. Anovitz, N. Choudhury, G. Ehlers, C. Hoffmann, P. Kent, M. Krzystyniak, E. Mamontov, A.A. Podlesnyak, T.R. Prisk, G.F. Reiter, G. Romanelli, A. Seel, X. Wang, D. Wesolowski

11:05 **GEOC 106.** Insights into anomalous ion hydration and mineral transformation kinetics under nanoconfinement. **Q. Miller**, J.P. Kaszuba, H.T. Schaefer, S.N. Kerisit, M. Bowden, K. Rosso, B.P. McGrail

11:25 **GEOC 107.** Coordination chemistry of copper in nanoscale confinement. **A. Knight**, P. Ilani-Kashkouli, N. Kabengi, A. Ilgen

Section C

Orange County Convention Center
Room W311H

Mineral Crystallization, Aggregation & Dissolution

C. Pearce, Z. Shen, X. Zhang, *Organizers, Presiding*

8:30 Introductory Remarks .

8:35 **GEOC 108.** Understanding the relationship between interfacial structure, interparticle forces and assembly dynamics during growth of crystals by oriented attachment. **J.J. De Yoreo**, L. Liu, G. Zhu, M.L. Sushko, X. Zhang, S.N. Kerisit, J.A. Soltis, K. Rosso

9:05 **GEOC 109.** Nanocrystals as chemical building blocks. **H. Cölfen**

9:35 **GEOC 110.** Formation and aggregation of lead phosphate particles: Implications for lead immobilization in water supply systems. J. Zhao, D. Giammar, J.D. Pasteris, C. Dai, Y. Bae, **Y. Hu**

9:55 **GEOC 111.** Size and facet controlled synthesis of Hematite nanoparticles and crystal growth mechanisms. **M. Zong**, X. Zhang, X. Huang, Z. wang, X. Lu, K. Ross

10:15 Intermission.



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

10:35 GEOC 112. Iron oxides in reactive systems: Aggregation, growth, and dissolution. **R. Penn**, J. Voelz, N.D. Burrows, J.A. Soltis, A.M. Vindedahl, J.H. Strehlau, C. Johnston, W. Arnold

11:05 GEOC 113. Understanding the driving forces for particle-based crystallization through theory and simulations. **M.L. Sushko**, K. Rosso, X. Zhang, J.J. De Yoreo, Z. Shen, S.N. Kerisit

11:35 GEOC 114. Real-time analysis of boehmite aggregation: (U)SAXS/WAXS. **L. Anovitz**, A. Krzysko, E. Nakouzi, X. Zhang, J. Ilavsky, M. Frith, I. Kuzmenko, K. Weigandt, J. Weston

12:05 Concluding Remarks.

Carbon Dioxide Conversion & Utilization

CO₂ Capture & Conversion

Sponsored by ENFL, Cosponsored by CATL, COMP and GEOC

New Frontiers in the Confluence of Experimental Thermodynamics, Structural Investigations & Theory/Computation

Theory/Computation & Structural Investigations

Sponsored by PHYS, Cosponsored by GEOC

WEDNESDAY AFTERNOON

Section A

Orange County Convention Center
Room W311G

Microbial Interactions in Natural, Geological Processes & their Application in Remediation of Contaminants

E. Chung, Y. Han, B. Jeon, M. Kurade, D. Tsang, *Organizers, Presiding*

2:00 Introductory Remarks .

2:05 GEOC 115. Effect of different conductive materials on direct electron exchange in syntrophic methanogenesis. H. Kang, S. Lee, **H. Park**

2:40 GEOC 116. Reductive transformation of contaminants by abiotic and biotic interactions. S. Bae, G. Tokazhanov, O. Lem, M. Babaa, G. Lee, **W. Lee**



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

3:15 GEOC 117. Mineral defects enhance microbial reduction of goethite. **L. Notini**, J. Byrne, E.J. Tomaszewski, D. Latta, Z. Zhou, M. Scherer, A. Kappler

3:40 GEOC 118. Effects of ferrihydrite impurities on the microbially-mediated redox cycling of uranium and iron. K. Belli, P. Van Cappellen, **M. Taillefert**

4:05 Intermission.

4:25 GEOC 119. *In-situ* phytoremediation of textile effluent using *Vetiveria zizanioides* in constructed wetland/phytobeds. V. Chandanshive, S. Kadam, M. Kurade, B. Jeon, J. Jadhav, **S.P. Govindwar**

5:00 GEOC 120. Impact of arsenic on microbial metal reduction. S. Owings, G. McNamee, J. Beckler, **M. Taillefert**

5:25 GEOC 121. Formation and redox reactivity of ferrihydrite-organic carbon-calcium co-precipitates. D. Adhikari, T.D. Sowers, J. Stuckey, X. Wang, D.L. Sparks, **Y. Yang**

Section B

Orange County Convention Center
Room W311F

Environmental Interfaces under Nano-scale Confinement

A. Ilgen, *Organizer*

A. Knight, *Organizer, Presiding*

N. Kabengi, *Presiding*

1:15 Introductory Remarks.

1:20 GEOC 122. Nanogeochemistry of radionuclide reaction and migration in subsurface environments. **Y. Wang**

1:50 GEOC 123. Using lanthanides to probe the interfacial chemistry of nano-scale pores. **A. Ilgen**, L. Loera, A. Knight, K. Leung

2:10 GEOC 124. Impact of nanoporosity on the behavior of water and aqueous solutions. **D. Cole**, A. Striolo, S. Gautam

2:40 Intermission.

3:00 GEOC 125. Calcite and barite mineral precipitation in (nano)porous media. **A.G. Stack**, M.C. Cheshire, H. Wang, V. Starchenko, H. Deng, K. Page, L. Anovitz

3:30 GEOC 126. Confined water dynamics in diatomite. **C.A. Colla**, K. Nakajima, J. Kerr, H. Li, P. Zarzycki, R. Castro, M.P. Augustine, T. Tokunaga, B. Gilbert

4:00 GEOC 127. Influence of octahedral cation distribution in montmorillonite on interlayer hydrogen counter-ion retention strength by DFT simulation. **Y. Li**, C. Schulthess, K. Co, S. Sahoo, P. Alpay

4:20 GEOC 128. The Glass transition of a one dimensional Water string in Cordierite. **P. Ben Ishai**



TECHNICAL PROGRAM

Section C

Orange County Convention Center
Room W311H

Mineral Crystallization, Aggregation & Dissolution

C. Pearce, Z. Shen, X. Zhang, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 **GEOC 129.** Energetics and the role of defects in Fe(II)-catalyzed goethite recrystallization from molecular simulations. **K. Rosso**, P. Zarzycki

2:05 **GEOC 130.** Resolving atom exchange fronts in the Fe(II)-catalyzed recrystallization of Fe(III) (hydr)oxides using isotopic mapping probes. **S. Taylor**, J. Liu, X. Zhang, B.W. Arey, L. Kovarik, J.B. Cliff, D.K. Schreiber, D.E. Perea, K. Rosso

2:25 **GEOC 131.** Fe(II) inhibits Fe(II)-goethite electron transfer. **L. Notini**, D. Latta, A. Neumann, C. Pearce, M. Sassi, K. Rosso, M. Scherer

2:45 Intermission.

3:05 **GEOC 132.** Adsorption and incorporation of actinides during iron oxyhydroxide formation, crystallisation and transformation. **S. Shaw**, L.T. Townsend, E.H. Winstanley, K.F. Smith, J.S. Weatherill, K. Morris

3:35 **GEOC 133.** Investigating solid transformation of β -FeOOH to iron oxides by in situ transmission electron microscopy. **X. Zhang**, Y. He, L. Kovarik, M. Bowden, M. Engelhard, Y. Du, L. Liu, C. Wang, J.J. De Yoreo, K. Rosso

4:05 **GEOC 134.** Zinc release and reimmobilization during Fe(II)-catalyzed ferrihydrite transformation. **J. Yan**, J.G. Catalano, H. Chen, K. Wang

4:25 **GEOC 135.** Understanding nanorod dissolution mechanisms by liquid phase electron microscopy: The case of β -FeOOH. **L. Liu**, X. Zhang, E. Nakouzi, L. Kovarik, M. Sassi, K. Rosso, J. De Yoreo

4:45 Concluding Remarks.

New Frontiers in the Confluence of Experimental Thermodynamics, Structural Investigations & Theory/Computation

Thermodynamics of Material Synthesis & Structural Investigations

Sponsored by PHYS, Cosponsored by GEOC



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

New Frontiers in the Confluence of Experimental Thermodynamics, Structural Investigations & Theory/Computation

Thermodynamics of Organic, Bioorganic & Physiological Systems

Sponsored by PHYS, Cosponsored by GEOC

WEDNESDAY EVENING

Section A

Orange County Convention Center
West Hall C

General Geochemistry

N. Kabengi, *Organizer*

6:00 - 8:00

GEOC 136. Concentrations and occurrence modes of some potentially valuable elements in high-aluminium coals from Yanzishan mine, Datong Coalfield, Shanxi Province, China: in comparison to the Junger Coalfield and the Ningwu Coalfield.. **Y. Yuan**, S. Tang

GEOC 137. Redox interfaces of the proximal Permian Cutler Formation, western Colorado: Implications for metal reactivity. **D. Hullaster**, A. Elwood Madden, G.S. Soreghan, K. Dee

GEOC 138. Contribution of electroactive ligands to the iron-binding ligand pool in the eastern tropical South Pacific: Results from GEOTRACES GP16. **G.A. Browning**, K.N. Buck

GEOC 139. Rapid characterization of strata in the Delaware Basin by FTIR modelling. **J. Grant**, C. Xiao, G. Torrez

GEOC 140. Variation of air radiation dose rates inside cabin flights between Singapore and Tokyo, Japan by North Korea's nuclear test in September 2017. **H. Katsura**

GEOC 141. Ion Pair Chromatographic Separation of V^V , V^{IV} , and V^{III} Ions in Sulfidic Waters. S. Weston, M. Medina, **T.P. Vorlicek**

GEOC 142. In situ Synthesis of 3D Nanostructured CoAl-LDH on Boehmite Surface: Improved Arsenate Removal and Investigation of the Removal Mechanisms. S. Lee, K. Jung, B. Chang, **Y. Lee**

GEOC 143. Biogeochemical interactions of mercury with wildfire ash derived-dissolved organic matter. **M. Tsui**, P. Ku, R.A. Dahlgren, A.T. Chow

GEOC 144. Analysis of dissolved organic matter percolated from periphyton in the everglades and the interaction between percolated dissolved organic matter and mercury. **A. Anjuman**, Y. Cai



TECHNICAL PROGRAM

GEOC 145. Characteristics of Heavy metal adsorption of Zeolite and Bentonite with pH Variation. J. Kim, **J. Seo**, J. Kim, Y. Kim, S. Woo, C. Lee

GEOC 146. Adsorption characteristics of As, Cu, and Cd using precipitates from Dalseong Mine, Korea. J. Kim, **J. Seo**, Y. Kim, C. Lee, S. Woo

GEOC 147. Assessment of cement for its potential to remedy contaminant plumes induced by CO₂ leakage from underground storages. **J. Park**, M. Park, S. Kim, **H.Y. Jeong**

GEOC 148. Drifting plastics as outstanding sources of serious ocean pollution. K. Amemiya, H. Kimukai, **K. Koizumi**, B. Kwon, **K. Saïdo**, K. Kim, T. Sato, T. Hiaki, S. Mentese

Section A

Orange County Convention Center
West Hall C

Hydrocarbon/Water/Mineral Interactions in the Subsurface

Cosponsored by COLL
G. M. Bowers, N. Loganathan, J. Loring, G. Rother, *Organizers*

6:00 - 8:00

GEOC 149. Probing supercritical methane adsorption and dynamics by ¹³C MAS NMR: Influence of hydrophobicity and layer charge on methane-smectite interactions at ~1 km depth. **G.M. Bowers**, E. Walter, R.K. Larsen, S. Burton, D.W. Hoyt, R.J. Kirkpatrick

GEOC 150. Effect of cations on the intercalation of supercritical methane in smectite interlayers using grand canonical molecular dynamics simulations. **N. Loganathan**, G.M. Bowers, O. Yazaydin, R.J. Kirkpatrick

Section A

Orange County Convention Center
West Hall C

Mineral Crystallization, Aggregation & Dissolution

C. Pearce, Z. Shen, X. Zhang, *Organizers*

6:00 - 8:00

GEOC 151. New technique for removing oxyanions from aqueous solution by coprecipitation with barite. **K. Tokunaga**, Y. Takahashi, N. Kozai

Section A

Orange County Convention Center
West Hall C



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

Molecular Processes at Mineral-Water Interfaces: Predictions via Linking Theory & Experiments

Cosponsored by COLL

J. Bracco, V. Starchenko, H. Wang, *Organizers*

6:00 - 8:00

GEOC 152. Smectite nanopore and interfacial water dynamics in the presence of carbohydrates. **S.E. Kelch**, B. Lanson, L. Aristilde, E. Ferrage, L. Charlet

Section A

Orange County Convention Center
West Hall C

Planetary & Meteoritic Chemistry

D. Kao, J. D. Kubicki, S. Singletary, Y. Tang, *Organizers*

6:00 - 8:00

GEOC 153. Characterization of the Dyngjusandur Alluvial Plain in Iceland with an analogue of a Mars Instrumentation Suite. **G.K. Tan**, T. Cantrell, M.L. Cable, E.S. Amador, E. Rader, A.M. Stockton

GEOC 154. Suite of geochemical and spatial analogues for planetary life detection. **C.M. Novak**

GEOC 155. Field Exploration and Life Detection Sampling via Planetary Analogue Research (FELDSPAR): Microbial population and distribution at the Dyngjusandur, Iceland alluvial plain in 2016. **S. Sutton**, A.M. Stockton, M.L. Cable, T. Cantrell, Z. Duca, W.D. Geppert, D. Cullen

THURSDAY MORNING

Section A

Orange County Convention Center
Room W231A

Mineral Crystallization, Aggregation & Dissolution

C. Pearce, Z. Shen, X. Zhang, *Organizers, Presiding*

8:30 Introductory Remarks .

8:35 GEOC 156. Unique mechanisms of molecular modifiers in pathological mineralization. **J.D. Rimer**



TECHNICAL PROGRAM

9:05 GEOC 157. Energy barriers to calcium phosphate mineralization in confined collagen spaces. **Y. Jun**, D. Kim, B. Lee, S. Thomopoulos

9:35 GEOC 158. Smectite clay minerals: Templates for the crystallisation of green rust. **R. Collins**, A. Jones

9:55 GEOC 159. Decreased nucleation rate and nucleus crystallinity of CaCO_3 on quartz with sulfate incorporation. **Y. Zhu**, Q. Li, D. Kim, Y. Min, B. Lee, Y. Jun

10:15 Intermission.

10:35 GEOC 160. Using electron and ion microscopy to reveal the role of iron metabolizing bacteria in biomineralization. **J. Byrne**, A. Kappler

11:05 GEOC 161. Secondary minerals derived microbial oxidation sulfides. **X. Lu**

11:35 GEOC 162. Ion solvation and pairing in concentrated solutions: Structure, dynamics and reactivity. **H. Wang**, D. Semrouni, T.R. Graham, K. Page, E. Mamontov, A.G. Stack, C. Pearce

11:55 GEOC 163. Chloride ion solvation, dynamics and ion-pairing interactions in concentrated aqueous solutions: Combined computational simulation and neutron diffraction with isotopic substitution. **N. Rampal**, H. Wang, A.G. Stack, D. Biriukov, J. Neufeind

12:15 Concluding Remarks.

Section B

Orange County Convention Center
Valencia Ballroom A

Hydrocarbon/Water/Mineral Interactions in the Subsurface

G. M. Bowers, N. Loganathan, J. Loring, G. Rother, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 GEOC 164. Supercritical fluid interactions with porous materials: Magnetic resonance techniques. **E. Walter**, D.W. Hoyt, S. Burton, J. Loring, R.J. Kirkpatrick, G.M. Bowers

9:05 GEOC 165. Chemical trapping of CO_2 by smectite clays. **G.M. Bowers**, H.T. Schaefer, J. Loring, E. Walter, S. Cunniff, R.K. Larsen, S. Burton, D.W. Hoyt, R.J. Kirkpatrick

9:25 GEOC 166. Effects of F^- for OH^- substitution on clay hydrophobicity and the intercalation of H_2O and CO_2 using grand canonical molecular dynamics simulations. **N. Loganathan**, G.M. Bowers, O. Yazaydin, R.J. Kirkpatrick

9:45 GEOC 167. Molecular simulation studies of H_2O - CO_2 and H_2O - CO_2 - CH_4 mixtures in montmorillonite clay interlayers. Q. Rao, **Y. Leng**

10:15 Intermission.



TECHNICAL PROGRAM

10:30 GEOC 168. ^{13}C NMR spectroscopy and computational molecular dynamics modeling of fluids in shales and clays. **R.J. Kirkpatrick**, G.M. Bowers, N. Loganathan, O. Yazaydin, H.T. Schaefer, J. Loring, D.W. Hoyt, S. Burton, E. Walter

11:00 GEOC 169. Reactivity of C-O-H fluids in nanoporous regimes. **D. Cole**, A. Striolo, C.H. Turner

11:30 GEOC 170. Enhanced ion adsorption on gibbsite nanoparticles and the formation of gibbsite nano-aggregates from simulated compaction and dewatering. **L.J. Criscenti**, T.A. Ho, J.A. Greathouse, Y. Wang

New Frontiers in the Confluence of Experimental Thermodynamics, Structural Investigations & Theory/Computation

Experimental Thermodynamics of Interfacial Phenomena

Sponsored by PHYS, Cosponsored by GEOC

THURSDAY AFTERNOON

Section B

Orange County Convention Center
Valencia Ballroom A

Hydrocarbon/Water/Mineral Interactions in the Subsurface

G. M. Bowers, N. Loganathan, J. Loring, G. Rother, *Organizers, Presiding*

1:30 GEOC 171. Chemical effects on fracture in calcite single crystals and in carbonate-rich shale. **A. Ilgen**

2:00 GEOC 172. Wormhole formation in fractured media: control via reaction rate and flow regime. **V. Starchenko**, A. Ladd

2:20 GEOC 173. Nonlinear tracers and in situ computing: Subsurface sensing with chemical waves. **T. Dewers**, J. Heath, R. Jensen, K. Kuhlman

2:50 Intermission.

3:00 GEOC 174. Prediction of barium and strontium concentrations in produced water using major ion concentrations. **M. Veisi**, D. Whittemore, S. Alimoradi, E.F. Peltier

3:20 GEOC 175. Role of soil chemical processes in petroleum hydrocarbon bioremediation. **D. Peak**, J. Hamilton, D. Bulmer, S.D. Siciliano

3:40 GEOC 176. Structure property hazard relationships for a novel remediation amendment. **D. Bulmer**, P. Mussone, S.D. Siciliano, D. Peak

4:00 GEOC 177. Thermodynamics of nanoparticles: Organics interaction. **L. Wu**, A. Navrotsky, X. Guo



TECHNICAL PROGRAM

4:20 Concluding Remarks.

HIST

Division of the History of Chemistry

N. Tsarevsky, *Program Chair*

SUNDAY MORNING

Section A

Orange County Convention Center
Room W308C

Tutorial & General Papers

N. V. Tsarevsky, *Organizer, Presiding*

8:20 HIST 1. International places of the periodic table. **C.J. Giunta**, J.L. Marshall

8:50 HIST 2. Analytical chemistry and the Olympic games: Fighting to catch the cheaters. **A.R. Roerdink**

9:20 HIST 3. Analysis of plant-derived materials: The early years. **N.V. Tsarevsky**

9:50 Intermission.

10:00 HIST 4. Rise and fall of melting point: A brief history of once important analytical technique. **V. Dragojlovic**

10:30 HIST 5. William Duane, his radium cow, and the radiation chemistry of water. **R.L. Hudson**

11:00 HIST 6. Vladimir Vasil'evich Markovnikov: His rule and legacy. **D.E. Lewis**

11:30 HIST 7. Seeing red: A brief history of red pigments through the ages. **E. Bosch**

SUNDAY AFTERNOON

Section A

Orange County Convention Center
Room W308C



TECHNICAL PROGRAM

Archaeological Chemistry

Metals & Related Metallic Compounds

M. Orna, S. C. Rasmussen, *Organizers, Presiding*

1:00 Introductory Remarks.

1:10 HIST 8. Metals chemistry for the classroom, K-16: A tutorial on low-melting alloys. **A. Rogers**, T. Tieu Ngo, C. Blackwell, W. Arce, C. Baker, M.A. Benvenuto

2:25 HIST 9. Metals of archaeological interest: pedagogical perspectives and possibilities. P.J. Smith, **M. Orna**

3:10 Intermission.

3:30 HIST 10. Material matter: Exploring ancient pigments in the classroom. **H. Becker**, T. Rutkowski, G. Ersan, V. Imbruce, P. Smart, M.D. Poliks, L. Piper

4:15 HIST 11. Examination of a series of Japanese 100-mon coins by energy dispersive X-ray fluorescence spectrometry. **T. Tieu Ngo**, W. Arce, M.A. Benvenuto

MONDAY MORNING

Section A

Orange County Convention Center
Room W308C

Archaeological Chemistry

Glasses, Ceramics & Organic Materials

S. C. Rasmussen, *Organizer*
M. Orna, *Organizer, Presiding*

8:05 Introductory Remarks.

8:15 HIST 12. Development of chemical glassware: Evaluating historical narratives via chemical archaeological data. **S.C. Rasmussen**

8:45 HIST 13. XRF investigation on the green lead glass excavated from Wanggung-ri site at Iksan and sarira bottles. **C.H. Do**, G. Kim, B. Yu, J. Song

9:15 HIST 14. Investigating the medieval European glass trade through elemental analysis. **L. Adlington**, I.C. Freestone



TECHNICAL PROGRAM

9:45 HIST 15. Changes in the body, glaze, and enamel composition of early Meissen porcelain during 1723-ca. 1740. **N. Zumbulyadis**, V. Van Thienen, A. Bezur

10:15 Intermission.

10:30 HIST 16. Analysis of fossilized resin (amber) by carbon-13 nuclear magnetic resonance spectroscopy in solution: A worldwide survey. **J.B. Lambert**, T.A. Contreras, T. Nguyen, J.A. Santiago-Blay

11:00 HIST 17. Metabolomics analysis and its application to biomolecular archaeology of wine. **K. Duffy**, P. van Dommelen, U. Sommer, H. Loney

11:30 HIST 18. Geochemical analysis of ancient and modern soil health in Antigua, West Indies. **A.R. Tricarico**, E.C. Wells

Creating a Common Language for Chemistry: IUPAC's Past, Present & Future Roles

Sponsored by CINF, Cosponsored by HIST

MONDAY AFTERNOON

Section A

Orange County Convention Center
Room W308C

Archaeological Chemistry

Color in Archaeology & Pedagogy

M. Orna, *Organizer*

S. C. Rasmussen, *Organizer, Presiding*

1:15 Introductory Remarks.

1:25 HIST 19. Archaeological shades of purple from flora and fauna. **Z. Koren**

2:10 HIST 20. FTIR spectroscopy and medieval pigments: A long-term love affair. **P.L. Lang**, H.F. Noneman

2:40 HIST 21. Archaeological blue pigments: Problem children from the get-go. **M. Orna**

3:10 Intermission.

3:25 HIST 22. Color as trace evidence in archaeological materials science and forensic investigations. **I. Kakoulli**

3:55 HIST 23. Discovering hidden layers with X-ray vision: New applications of pXRF to rock art studies. **K.L. Steelman**, V. Roberts, C. Boyd



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

4:25 HIST 24. *Ars pigmentorum*: Roman painters and their knowledge of the chemical and physical properties of pigments. **H. Becker**

4:55 HIST 25. At the heart of the madder: Experiments in dye bath chemistry with prehistoric dye plants and alchemical texts. **M.L. LaBerge**

Chemistry in Space: Future Directions

Sponsored by YCC, Cosponsored by AGFD, ANYL, BIOT, BMGT, CHAS, ENVR, FLUO, GEOC, HIST, I&EC, MEDI, POLY and PROF

Creating a Common Language for Chemistry: IUPAC's Past, Present & Future Roles

Sponsored by CINF, Cosponsored by HIST

MONDAY EVENING

Section A

Orange County Convention Center
West Hall C

Sci-Mix

N. V. Tsarevsky, *Organizer*

8:00 - 10:00

1-2, 13-14, 17-19, 22, 25. See previous listings.

34, 37, 40-41, 43-44, 46-47. See subsequent listings.

TUESDAY MORNING

Section A

Orange County Convention Center
Room W308C

Pioneers of Magnetic Resonance



TECHNICAL PROGRAM

V. V. Mainz, *Organizer*
E. T. Strom, *Organizer, Presiding*

8:25 Introductory Remarks.

8:30 HIST 26. Yevgenii Konstantinovich Zavoiskii and the battle for EPR. **D.E. Lewis**

9:00 HIST 27. Samuel Isaac Weissman: Pioneer of chemical applications of EPR and the way he was. **J.R. Norris**

9:30 HIST 28. George K. Fraenkel: Neglected EPR pioneer. **J.H. Freed**

10:00 Intermission.

10:15 HIST 29. Harden M. McConnell: The life of a giant in magnetic resonance. **L.J. Berliner**

10:45 HIST 30. R. Linn Belford: A journey from understanding EPR spectra to multifrequency high field EPR. **A. Smirnov**

11:15 HIST 31. Spin relaxation and the history of EPR. **G.R. Eaton**, S. Eaton

TUESDAY AFTERNOON

Section A

Orange County Convention Center
Room W308C

Pioneers of Magnetic Resonance

E. T. Strom, *Organizer*
V. V. Mainz, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 HIST 32. Purcell and Bloch: The discovery and early developments in NMR. **V.V. Mainz**

1:35 HIST 33. H. S. Gutowsky and the use of NMR in chemistry. **H.N. Cheng**

2:05 HIST 34. Multi-pronged bite of NMR. **P. Laszlo**

2:35 HIST 35. Donald E. Woessner: Master of NMR relaxation effects. **E.T. Strom**

3:05 Intermission.

3:20 HIST 36. John Stewart Waugh and high-resolution NMR in solids. **R.G. Griffin**

3:50 HIST 37. Sixty years (and counting) of magic-angle spinning for NMR. **J.F. Schaefer**



TECHNICAL PROGRAM

4:20 HIST 38. Bid for immortality: A thirty-year race and rivalry between Paul Lauterbur and Raymond Damadian for the invention of MRI. M.A. Meyers, **E.T. Strom**

WEDNESDAY MORNING

Section A

Orange County Convention Center
Room W308C

Tutorial & General Papers

N. V. Tsarevsky, *Organizer, Presiding*

8:45 HIST 39. Life of John Lee Comstock: Chemist or plagiarist? **W.P. Palmer**

9:15 HIST 40. Gamma Sigma Epsilon: 100 Years of promoting excellence in chemistry. **G.R. Boyce**

9:45 HIST 41. Vanadium: Chemistry and history. **M. Mendoza, I. Villavicencio**, C. Hahn

10:15 Intermission.

10:30 HIST 42. Kingsville and uranium: A history of the South Texas uranium belt. C. Hahn, **J.T. Medina**

11:00 HIST 43. American nuclear chemist: Glenn Seaborg. C. Hahn, **D. Rodriguez**

11:30 HIST 44. Dorothy Hodgkin: The woman who revolutionized crystallographic investigations. **C. Chi, R. Garcia**, C. Hahn

WEDNESDAY AFTERNOON

Section A

Orange County Convention Center
Room W308C

Tutorial & General Papers

N. V. Tsarevsky, *Organizer, Presiding*

12:45 HIST 45. Clendenin, WV: The birth of the petrochemical industry. **M.W. Fultz, D. Stone**

1:15 HIST 46. Nobel-prize-winning science deniers: Albert Einstein. **S. Powell**, T.J. Fuhrer

1:45 HIST 47. Nobel-prize-winning science deniers: Paul Dirac. **T.J. Fuhrer**



I&EC

Division of Industrial & Engineering Chemistry

C. Abney and R. Mayes, *Program Chairs*

SUNDAY MORNING

Section A

Orange County Convention Center
Room W224E

ACS Award in Separations Science & Technology: Symposium in Honor of Sheng Dai

D. Jiang, S. M. Mahurin, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 I&EC 1. Role of separations in sustainability. **R.D. Rogers**

8:25 I&EC 2. Simulations of separation media and processes. **D. Jiang**

8:45 I&EC 3. Porous Metal-Organic Frameworks for gas separation and purification. **B. Chen**

9:05 I&EC 4. CO₂ separation by crystallization of guanidinium carbonates. **R. Custelcean**, N.J. Williams, K. Garrabrant, C. Seipp, F. Brethome

9:25 I&EC 5. Pore space partitioning and engineering of Metal-Organic Framework materials. **P. Feng**, X. Bu

9:45 Intermission.

10:00 I&EC 6. Hybrid membranes for CO₂ separation. **S.M. Mahurin**

10:20 I&EC 7. Selective Separation of C₄ Olefins with ionic materials. **H. Xing**

10:50 I&EC 8. Oriented assembly of functional mesoporous materials on interface. **D. Zhao**

11:20 I&EC 9. Anion receptor modified soft materials. **J.L. Sessler**

11:40 I&EC 10. Functionalized mesoporous materials for separation and other applications. **J. Liu**



TECHNICAL PROGRAM

Section B

Orange County Convention Center
Room W224F

I&EC Fellow: Symposium in honor of Nicholas Peppas

K. Matyjaszewski, *Organizer*
S. K. Mallapragada, *Organizer, Presiding*

8:00 Introductory Remarks.

8:10 I&EC 11. Diffusion in glassy and rubbery polymers: A rich field of chemical engineering problems. **N. Peppas**

8:50 I&EC 12. Biofabrication strategies for complex tissue regeneration. **A. Mikos**, S.M. Bittner, L.A. Diaz Gomez

9:30 Intermission.

9:45 I&EC 13. Hybrid Materials by ATRP. **K. Matyjaszewski**

10:25 I&EC 14. Crystallization pathways for protein crystals and colloidal assemblies. **S.C. Glotzer**, S. Lee, E. Teich, M. Engel, J. Glaser

Mechano- & Tribochemistry & Catalysis

Sponsored by CATL, Cosponsored by I&EC

Symposium in Honor of Chuck Peden's Research Career: Catalysis for Energy & the Environment

Sponsored by CATL, Cosponsored by ENFL, ENVR, I&EC and PHYS

SUNDAY AFTERNOON

Section A

Orange County Convention Center
Room W224E

ACS Award in Separations Science & Technology: Symposium in Honor of Sheng Dai

D. Jiang, S. M. Mahurin, *Organizers*
R. D. Rogers, J. Yu, *Presiding*



TECHNICAL PROGRAM

1:30 I&EC 15. Construction of highly efficient and recyclable metal-organic framework catalysts for artemisinin production. **H. Zhou, L. Feng**

1:50 I&EC 16. Structured growth of metal-organic frameworks from insoluble precursors. **K.S. Walton**

2:10 I&EC 17. Meta-organic frameworks for artificial photosynthesis. **W. Lin**

2:30 I&EC 18. Construction of zeolitic nanoporous functional materials and their emerging applications. **J. Yu**

3:00 I&EC 19. Diphosphonate–modified hydroxyapatites: synthesis and characterization. **S. Alexandratos, M. Finkenbergh, E. Amin, E. Naito**

3:20 Intermission.

3:35 I&EC 20. CO oxidation on single atom Pt1/CeO2. **Y. Wang**

3:55 I&EC 21. Novel NH₃ separation and recovery process based on ionic liquids. **H. Dong, S. Zhang**

4:25 I&EC 22. Carbon molecular sieve membranes - change agents for demanding gas separations. **W.J. Koros**

4:45 I&EC 23. Award Address (ACS Award in Separations Science and Technology sponsored by the Waters Corporation). Separation driven by functional materials. **S. Dai**

Section B

Orange County Convention Center
Room W224F

I&EC Fellow: Symposium in honor of Nicholas Peppas

S. K. Mallapragada, *Organizer*
K. Matyjaszewski, *Organizer, Presiding*

1:30 I&EC 24. Understanding and overcoming biological barriers for drug delivery. **S. Mitragotri**

2:10 I&EC 25. Clicking polymer networks together: Approaches to form smart, functional polymers from click chemistry. **C. Bowman**

2:50 I&EC 26. Lessons in biomaterials translation: Shifting tides in regenerative medicine. **J. Elisseeff**

3:30 Intermission.

3:45 I&EC 27. Molecular Simulation Design Framework (MoSDeF): An open-source software environment for computational screening of soft matterSystems. **P.T. Cummings**

4:25 I&EC 28. Self-assembly pathways for metamaterials design. **S.K. Mallapragada**

5:05 Concluding Remarks.



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

Mechano- & Tribochemistry & Catalysis

Sponsored by CATL, Cosponsored by I&EC

Symposium in Honor of Chuck Peden's Research Career: Catalysis for Energy & the Environment

Sponsored by CATL, Cosponsored by ENFL, ENVR, I&EC and PHYS

MONDAY MORNING

Section A

Orange County Convention Center
Room W224E

2019 ACS Sustainable Chemistry & Engineering Lectureship Awards: Symposium in Honor of Paul Dauenhauer

Cosponsored by CELL⁺
A. R. Teixeira, *Organizer*
O. Abdelrahman, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 I&EC 29. From biomass to chemicals: C-C bond formation using heterogeneous catalysts. **R.F. Lobo**

8:25 I&EC 30. Isosorbide and glucarodilactone-based polyethers and poly(ester-thioethers) via ring-opening and photoinitiated thiol-ene polymerization. **T.M. Reineke**

8:45 I&EC 31. Continuous synthesis of metastable zeolite crystals. **A.R. Teixeira**

9:05 I&EC 32. Industrial talk by former Dauenhauer student. **M. Mettler**

9:25 Intermission.

9:45 I&EC 33. Predicting molecular adsorption entropies in confined environments. **O. Abdelrahman**, P. Dauenhauer

10:05 I&EC 34. Toluene hydroalkylation as a platform for high performance polyesters. **J. Guzman**

10:25 I&EC 35. Non-oxidative conversion of methane to value-added chemicals. H. Toraman, K. Alexopoulos, **D.G. Vlachos**

10:45 I&EC 36. Microscopic view of observable trends in reactor performance during the hydrodeoxygenation of carboxylic acids. J. Gopeesingh, **J. Bond**

11:05 Intermission.



TECHNICAL PROGRAM

11:20 I&EC 37. At the frontier of renewable chemicals from biomass. **P.J. Dauenhauer**

Section B

Orange County Convention Center
Room W224F

I&EC Fellow: Symposium in honor of Pete Nickias

D. G. Barton, *Organizer, Presiding*
S. S. Dhingra, *Presiding*

8:00 Introductory Remarks.

8:05 I&EC 38. Experimental and theoretical mechanistic insights into the oxidative coupling of methane with soft oxidants. **T.J. Marks**, M. Neurock, T. Lohr, S. Liu, S. Udyavara

8:45 I&EC 39. Selective conversion of methane to light olefin feedstocks via catalytic sulfochlorination. **K.F. Hirsekorn**, P.N. Nickias, M.H. McAdon, W.J. Tenn

9:10 I&EC 40. Mechanistic features of catalytic alkene polymerization as revealed by chromophore-quench labeling. **C.R. Landis**

9:35 Intermission.

9:50 I&EC 41. Exploring metal-organic frameworks (MOFs) for catalysis and separation. **S.T. Nguyen**

10:15 I&EC 42. Discovery of rare earth catalyst for the selective dehydration of phenol. **D.G. Barton**

10:40 I&EC 43. Hydrocarbon separations in Metal-Organic frameworks. J.E. Bachman, M. Kapelewski, M. Gonzalez, D.A. Reed, D.E. Jaramillo, H.Z. Jiang, J. Oktawiec, E.D. Bloch, Z.R. Herm, J. Mason, P.J. Milner, W.L. Queen, M.R. Hudson, B.M. Wiers, C.M. Brown, **J.R. Long**

11:05 I&EC 44. Kinetics of zinc carboxylate catalyzed production of carbamates as non-phosgene isocyanate intermediates. **E.M. Calverley**

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Sponsored by PROF, Cosponsored by AGFD, ANYL, BIOL, BIOT, CARB, CELL, CHED, CMA, COLL, COMP, ENVR, GEOC, I&EC, MEDI, MPPG, NUCL, ORGN, PHYS, PMSE, POLY, PRES, WCC and YCC

Symposium in Honor of Chuck Peden's Research Career: Catalysis for Energy & the Environment

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TECHNICAL PROGRAM

Industrial Innovations in Polymer Science

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Celebrating 50 Years of ExxonMobil's Corporate Strategic Research Laboratories: A View Forward from a Retrospective

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Celebrating 50 Years of ExxonMobil's Corporate Strategic Research Laboratories: A View Forward from a Retrospective

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MONDAY AFTERNOON

Section A

Orange County Convention Center
Room W224E

2019 ACS Sustainable Chemistry & Engineering Lectureship Awards: Symposium in Honor of Kevin Wu

Cosponsored by CELL[†]

B. Hwang, *Organizer, Presiding*

1:30 I&EC 45. 2D chalcogenides for solar fuels: Defect engineering in SnS₂ and MoS₂ for enhanced CO₂ conversion efficiency and product selectivity. **L. Chen**, I. Shown, Y. Huang, H. Du, H. Lien, K. Chen

1:50 I&EC 46. Highly durable electrocatalysts for fuel cells. D. Chung, S.W. Jun, J. Yoo, H. Kwon, T. Hyeon, **Y. Sung**

2:10 I&EC 47. *Synthesis and modification of mesoporous nanomaterials for catalysis and forensic separations.* **B.G. Trewyn**

2:30 I&EC 48. Encapsulation of multiple catalysts into metal-organic frameworks. **C. Tsung**

2:50 I&EC 49. Mesoporous acid catalysts for high-efficient reaction processes. **J. Huang**

3:10 Intermission.

3:30 I&EC 50. Biomass conversion to fuel and chemicals over solid acid catalysts. **C. Sakdaronnarong**, P. Posoknistakul, N. Laosiripojana



TECHNICAL PROGRAM

3:50 I&EC 51. Catalytic depolymerization of cellulose and chitin. **A. Fukuoka**

4:10 I&EC 52. Heterogeneous catalysis in deoxydehydration reaction for the production of biomass-derived chemicals. **K. Tomishige**, Y. Nakagawa, M. Tamura

4:30 I&EC 53. Catalytic production of hexane-1,2,5,6-tetrol from bio-renewable levoglucosan in water. S.H. Krishna, M. de Bruyn, Z.R. Schmidt, B.M. Weckhuysen, J.A. Dumesic, **G.W. Huber**

4:50 I&EC 54. Functional nanoporous materials for lignocellulosic biomass conversion and chemical engineering applications. **K.C. Wu**

Section B

Orange County Convention Center
Room W224F

I&EC Fellow: Symposium in honor of Pete Nickias

D. G. Barton, *Organizer*

E. M. Calverley, K. F. Hirsekorn, *Presiding*

1:30 Introductory Remarks.

1:35 I&EC 55. Chemical industry dynamics and the Implications for Innovation and technology development. **B.R. Maughon**

2:15 I&EC 56. Organocatalytic polymerization: Generation of new gene delivery agents. **R.M. Waymouth**

2:40 I&EC 57. Looking for the silver lining. **C.L. Tway**, M. Syed, A. Kulkarni, V. Santos Castro, V.J. Sussman, J.C. McKeen, C. Todd

3:05 I&EC 58. Ethylene Oxide catalyst and process technology development. **S.S. Dhingra**

3:30 Intermission.

3:45 I&EC 59. Colloidal quantum dot downconverters for colorful and energy efficient solid state lighting. L. Hamachi, H. Yang, I. Rreza, I. Jen-La Plante, E. Chan, **J.S. Owen**

4:10 I&EC 60. Industrial problem solving using advanced analytical techniques and expertise. **W.V. Konze**

4:35 I&EC 61. Catalysis at Dow: vignettes in the application of catalysts towards products. **P.N. Nickias**

5:00 Concluding Remarks.

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

Sponsored by PROF, Cosponsored by AGFD, ANYL, BIOL, BIOT, CARB, CELL, CHED, CMA, COLL, COMP, ENVR, GEOC, I&EC, MEDI, MPPG, NUCL, ORGN, PHYS, PMSE, POLY, PRES, WCC and YCC

Chemistry in Space: Future Directions

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Symposium in Honor of Chuck Peden's Research Career: Catalysis for Energy & the Environment

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TUESDAY MORNING

Section A

Orange County Convention Center
Room W224E

Critical Materials: Rare Earth Elements

T. E. Albrecht-Schmitt, *Organizer*
G. A. Fugate, *Organizer, Presiding*
M. R. Healy, *Presiding*



TECHNICAL PROGRAM

8:00 Introductory Remarks.

8:05 I&EC 62. 1,10-phenanthroline carboxamide ligands for lanthanide separation: Diluent effect. **M.A. Simonnet**, T. Kobayashi, S. Suzuki, T. Yaita

8:25 I&EC 63. Mining e-waste through felicitous choice of processing parameters. C. Frankiewicz, B.S. Chang, **M.M. Thuo**

8:45 I&EC 64. Recycling REE with agriculture wastes. **D.W. Reed**, V. Thompson, Y. Fujita, H. Jin, Y. Jiao, J. Fisher, M. Crain-Zamora, K. Scalzone, J. Sutherland

9:05 Intermission.

9:20 I&EC 65. Accelerated development of substitutes for rare-earth permanent magnets. **T. Lograsso**

9:40 I&EC 66. Wrinkled mesoporous carbon (WMC) for the selective extraction of thorium and rare earth elements. **A.T. Brown**, Z. Wang, K. Tan, Y.J. Chabal, K.J. Balkus

10:00 I&EC 67. Critical materials recycling: Reuse materials or recover rare earth elements. **C.C. Nlebedim**, K. Gandha, H. Khazdozian, D. Prodius, P. Paranthaman

10:20 Intermission.

10:35 I&EC 68. Atmospheric chemistry of lanthanoids in Houston, Texas: Quantifying rare earths to apportion petroleum refining and African dust impacts on ambient airborne particulate matter. **S. Chellam**

10:55 I&EC 69. Ionic liquid processes for the extraction of rare earth elements from coal. **K.R. Di Bona**, C.M. Hill, G. Gurau, R.D. Rogers

11:15 I&EC 70. Coupled hydrothermal extraction and ligand-associated media sorption for REE recovery from coal fly ash. **T.M. Dittrich**, M. Dardona, J. Hovey, M.J. Allen, S.K. Mohanty, A. Migdisov, H. Boukhalfa

11:35 I&EC 71. Analytical procedure for precise detection of rare earth elements in coal and coal-related materials. **A.C. Strzelecki**, Z. Li, H. Boukhalfa, E. Kluk, G. Woldegabriel

11:55 Concluding Remarks.

Section B

Orange County Convention Center
Room W224F

I&EC International Fellow: Symposium in honor of Tom Baker

G. G. Stanley, *Organizer, Presiding*
A. D. Sutton, *Presiding*

8:00 I&EC 72. Theory can't be that wrong: Resolving the discrepancies to describe the reaction pathways leading to magnesium triborane. **T. Autrey**, A.J. Karkamkar, M. Bowden



TECHNICAL PROGRAM

8:25 I&EC 73. Advances and research challenges in materials research for renewable energy. **W. Tumas**

8:50 I&EC 74. Aerobic alcohol oxidation catalyzed by vanadium in solution and on a surface. **S.L. Scott**, B. Wigington, A. Serrano

9:15 I&EC 75. New metal catalysts for Polyurethane elastomer applications. **R. Keaton**, N. Wilmot, R. Duggal, P. Margl, D.R. Romer

9:40 Intermission.

10:00 I&EC 76. Water-tolerant olefin metathesis: Challenges and opportunities. A. Goudreault, D. Walden, C. Michel, S. Steinmann, V.R. Jensen, **D. Fogg**

10:25 I&EC 77. Some new efforts in the homogeneous catalytic hydrogenation of polar C=O bonds. **J.C. Gordon**, P. Dub

10:50 I&EC 78. Mechanistic studies on reactions of carbon dioxide and epoxides catalyzed by homogeneous iron- and boron-centered catalysts. **F.M. Kerton**, K.A. Andrea, D. Jagota

11:15 I&EC 79. Withdrawn

Exploring the Frontiers of Chemistry through NASA Research

Getting There: Advanced Materials for Space Travel

Sponsored by COMSCI, Cosponsored by ANYL, BIOL, BIOT, CELL, COLL, ENFL, I&EC, INOR, NUCL, PHYS, PMSE and POLY

ACS Sustainable Chemistry & Engineering: Symposium in honor of Dr. Silvia Vignolini

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GSSPC: Artificial Molecular Machines & the Next Generation of Molecular Control

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Light-Driven Chemistry: Photoelectrochemistry & Photocatalysis

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TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

Process Chemistry: New Developments in Pharmaceutical Process Development

Sponsored by ORGN, Cosponsored by I&EC

TUESDAY AFTERNOON

Section A

Orange County Convention Center
Room W224E

Critical Materials: Rare Earth Elements

G. A. Fugate, *Organizer*
T. E. Albrecht-Schmitt, *Organizer, Presiding*
E. Warzecha, *Presiding*

1:30 Introductory Remarks.

1:35 **I&EC 80.** Synthesis and spectroscopy study of Eu(III)-bearing nano-platelet gibbsite and boehmite. **Z. Wang**

1:55 **I&EC 81.** Electrochemical production of rare earth metals using room temperature ionic liquids. **D. Baek**, J. Mitchell, M. Case, R. Fox, R. Rodriguez, T. Lister

2:15 **I&EC 82.** Development of a biosorption process for recovery of rare earth metals. **Y. Jiao**, D. Park, H. Jin, A. Brewer, E. Chang, L. Lammers, D.W. Reed, Y. Fujita, J. Sutherland

2:35 Intermission.

2:55 **I&EC 83.** Investigative Studies toward the Extraction and Recovery of Praseodymium from Ionic Liquids Using Supercritical Carbon Dioxide. **R. Rodriguez**, R. Fox, D. Baek, M. Case, J. Mitchell

3:15 **I&EC 84.** Selective recovery of rare earth elements from e-waste with supported membrane solvent extraction. **S.Z. Islam**, V.G. Deshmane, P. Gangavarapu, R. Bhave, J. Klaehn

3:35 **I&EC 85.** Recovery of the rare earth elements (REE) from coal fly ash via the combination of physical separation and chemical extraction methods. **Y. Soong**, R. Lin, M.Y. Stuckman, B. Howard, C. Lopano, E.J. Granite

3:55 Intermission.

4:15 **I&EC 86.** New unsymmetrical diglycolamide extractants for lanthanide ion complexation. **B.G. Tokheim**, T.L. Hanson, D.S. Stankowski, M.G. Kroeger, M.S. Lindemann

4:35 **I&EC 87.** Advancement of lanthanide extraction through preorganized ligand design and coordination site studies. **M.R. Healy**, D. Stamberg, C.A. Albisser, B.A. Moyer, I. Popovs, S. Jansone-Popova

4:55 **I&EC 88.** Applying 'green chemistry' and 'circular economy' principles in recycling of rare earth elements from e-waste. **D. Prodius**, K. Gandha, C.C. Nlebedim



TECHNICAL PROGRAM

5:15 Concluding Remarks.

Section B

Orange County Convention Center
West Hall F3

ACS Award in Industrial Chemistry: Symposium in Honor of Guy R. Humphrey

Cosponsored by ORGN
S. M. Silverman, *Organizer*
K. R. Campos, *Presiding*

1:00 Introductory Remarks.

1:10 **I&EC 89.** New stereoselective, catalytic fluorination reactions. **E.N. Jacobsen**

1:50 **I&EC 90.** Unexpected transformations in heterocyclic chemistry. **E.J. Grabowski**

2:30 **I&EC 91.** Novel photoredox reactions. **D.W. MacMillan**

3:10 Intermission.

3:20 **I&EC 92.** Driving scientific excellence at Merck Process Research & Development through Academic-Industry collaborations. **R. Ruck**

4:00 **I&EC 93. Award Address** (ACS Award in Industrial Chemistry sponsored by the ACS Division of Industrial and Engineering Chemistry). Innovation in sustainable API commercial route discovery and development: A personal perspective. **G.R. Humphrey**

Section C

Orange County Convention Center
Room W304F

I&EC International Fellow: Symposium in honor of Tom Baker

G. G. Stanley, *Organizer, Presiding*
A. D. Sutton, *Presiding*

1:30 **I&EC 94.** Novel phosphine ligands and operando NMR techniques for homogeneous catalysis. **C.R. Landis**

1:55 **I&EC 95.** Dehydrogenation of alcohols and amines: heterolytic C-H and N-H/O-H activation. **W.D. Jones, A. Olivares, S. Chakraborty, R. Xu, J. Yuwen, S.M. Bellows, M. Wilklow-Marnell**

2:20 **I&EC 96.** Cascade catalytic conversion of CO₂ to MeOH. W. Chu, B.T. Wang, Z. Culakova, **K.I. Goldberg**



TECHNICAL PROGRAM

2:45 I&EC 97. Catalytic arene hydrogenation: from a molecular Rh (CAAC) complex to Rh nanoparticles. **R. Bullock**, B.L. Tran, J. Fulton, J.C. Linehan, J. Lercher

3:10 Intermission.

3:30 I&EC 98. Inorganic chemistry and R. Thomas Baker: Some personal observations and reflections. **A.P. Sattelberger**, R.R. Langeslay, M. Delferro

3:55 I&EC 99. Mechanism of hydroamidation photocatalysis. S. Ruccolo, Y. Qin, C. Schnedermann, **D.G. Nocera**

4:20 I&EC 100. Highly active cationic Co(II) hydroformylation catalysts: watch out rhodium! **G.G. Stanley**, D.M. Hood, R. Johnson

4:45 I&EC 101. Selective reduction of CO₂ to CO by a molecular rhenium catalysts and attachment to carbon electrode surfaces.. **C.P. Kubiak**, A. Zhanaidarova

Exploring the Frontiers of Chemistry through NASA Research

Living There: Science for the Future of Manned Space Exploration

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LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

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GSSPC: Artificial Molecular Machines & the Next Generation of Molecular Control

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TECHNICAL PROGRAM

Light-Driven Chemistry: Photoelectrochemistry & Photocatalysis

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TUESDAY EVENING

Section A

Orange County Convention Center
West Hall C

I&EC General Posters

Cosponsored by CTA
C. W. Abney, R. T. Mayes, *Organizers*

8:00 - 10:00

I&EC 102. Analysis of solid circulation rate effects in the CFD simulation of solar hybridized dual fluidized bed system. **S. Lee**

I&EC 103. Computational analysis of 2MWe Oxy-CFB boiler for anthracite coals. **S. Lee**, Y. Gwak

I&EC 104. Process intensification of distillation separation technology. **X. Gao**, H. Li, X. Li

I&EC 105. Lithium separation from alkali metals through liquid-liquid extraction. **M.R. Healy**, I. Popovs, S. Jansone-Popova, B.A. Moyer

I&EC 106. Investigation of PdCeO_x solid solution catalysts for selective hydrogenation of acetylene. **S. Kim**, W. Jang

I&EC 107. Hydrophobization of cellulose nanofibers through silylation at different pH conditions of aqueous system. **H. Youn**, S. Yook, H. Park, S. Park

I&EC 108. Sidewalk development and research. **A. Plumber**

I&EC 109. Hydrolysis parameters on anatase white pigment via short sulfate process. **C. Tian**

I&EC 110. Calcination intensity on rutile titanium dioxide white pigment production via short sulfate process. **C. Tian**, Y. Zhang

I&EC 111. Development of new composite molten salt fluid with increased heat capacity. **D. Dolzhenkov**, R.T. Mayes, S. Dai

I&EC 112. Absorption and capture of CO₂ using amino acids and guanidine crystalizing agents. **K.A. Garrabrant**

I&EC 113. Preparation of ionogel films using water-soluble cellulose. **S. Lee**, J. Lee

I&EC 114. Investigation on catalyst coating techniques for the deoxygenation of palm oil over Pd/TiO₂ catalysts using microscale-based reactor. **Y. Sangsaeng**, N. Sirimungkalakul, T. Sornchamni, Y. Boonyongmaneerat, S. Jongpatiwut



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- I&EC 115.** Quantification of pigment-binder interface using smart blur and locally adaptive thresholding technique. **H. Lee**
- I&EC 116.** Ionic liquids containing double bond as electrolytes for electrochemical double layer capacitor. **C. Oh, J. Lee**
- I&EC 117.** Investigation of electrochemical reaction of Ionic liquid containing allyl and vinyl group. **C. Oh, J. Lee**
- I&EC 118.** Designing the next generation of hair dyes using cheminformatics. T.N. Williams, **G. Van Den Driessche**, H.S. Freeman, D. Fourches
- I&EC 119.** Preparation of N-doped carbon nanoparticle and their properties. **S. Lee, J. Lee**
- I&EC 120.** Trisulfonamide and *o*-sulfonamidophenol ligands as extractants for trivalent actinides from alkaline high-level waste. **O.W. Adedoyin**, E.V. Govor, A.N. Morozov, A.M. Mebel, I. Chakraborty, R.G. Raptis, K. Kavallieratos
- I&EC 121.** Phosphate conversion coating for galvanized steel with enhanced adhesion to PVC and PET films. **J. Baek**
- I&EC 122.** Effects of metatitanic acid structure for rutile TiO₂ pigment production via short sulfate process. **C. Tian**
- I&EC 123.** Anatase pigment production from low concentration industrial TiOSO₄ solution via short sulfate process. **C. Tian**
- I&EC 124.** Enhanced solar thermal evaporation of ethanol–water mixtures, through the use of porous media. **F. Canbazoglu**, P. Bandaru
- I&EC 125.** Development of automated air sampling system including CO₂ and moisture separation process for analysis of radioactive ⁸⁵Kr. **Y. Ko**, H. Kim, S. Choi, J. Lim, W. Lee
- I&EC 126.** Centralised versus decentralized food manufacture: A modelling tool for assessing alternative manufacturing scenarios. **A. Almena**, P. Fryer, S. Bakalis, E. Lopez-Quiroga
- I&EC 127.** Electrochemical fabrication of silicon nanostructure for application to anode material for lithium ion battery. J. Choi, **S. Jeong**
- I&EC 128.** Study on tall oil solubility for improved resource recovery in chemical pulping of wood. **I. Dogaris**, M. Lindström, G. Henriksson

Section B

Orange County Convention Center
West Hall C

Celebrating 50 Years of ExxonMobil's Corporate Strategic Research Laboratories

C. W. Abney, M. Afeworki, G. Cao, *Organizers*

8:00 - 10:00

ExxonMobil CSR Poster.



TECHNICAL PROGRAM

- I&EC 129.** Electrocatalytic oxidation of a surrogate for methane. **S. Liu**
- I&EC 130.** Aerobic partial oxidation of hydrocarbons to make building blocks and monomers. **P. Nandi**, V. Grankina, B. Dutta, S. Biswas, S. Raman, S.L. Suib
- I&EC 131.** Fundamental studies of Metal-Organic Frameworks and their application in CO₂ capture. **S.C. Weston**
- I&EC 132.** Borate-assisted liquid-phase selective oxidation of *n*-pentane. S. Aworinde, A. Lapkin, **K. Wang**
- I&EC 133.** Directed metal–organic framework nucleation at surfaces. **K. Colwell**, R. Torres-Gavosto, J. Falkowski, S.C. Weston, P.D. Ashby, J.R. Long
- I&EC 134.** Synthesis and modification of new polymers of intrinsic microporosity For liquid separations. **K. Thompson**, N. Bruno, R. Mathias, B. Hamlett, Y. Ma, R. Lively, M. Finn
- ExxonMobil CSR Poster.

WEDNESDAY MORNING

Section A

Orange County Convention Center
Room W224E

I&EC Early-Career Fellow: Symposium in honor of Carter Abney

L. R. Martin, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 I&EC 135. Chloride molten salts in concentrated solar applications. **R.T. Mayes**, J.M. Kurley, S.S. Raiman

8:25 I&EC 136. Understanding and controlling corrosion of materials in molten chloridesalt. **S.S. Raiman**, J. McMurray, C.W. Abney, R.T. Mayes

8:45 I&EC 137. First-principles prediction of the aqueous solubility of organic salts. **A. Ivanov**, N.J. Williams, R. Custelcean, B.A. Moyer, V. Bryantsev

9:05 Intermission.

9:25 I&EC 138. Predictive modeling of ion selectivity in liquid-liquid extraction. **V. Bryantsev**, N.J. Williams, B.A. Moyer

9:45 I&EC 139. Achieving high selectivity for anions using simple iminoguanidinium based receptors. **N.J. Williams**

10:05 I&EC 140. Tailoring ionic liquids for advanced separation. H. Luo, **S. Dai**



TECHNICAL PROGRAM

10:25 Intermission.

10:45 I&EC 141. Separations in high level waste treatment. **K.M. Taylor-Pashow**

11:05 I&EC 142. Chemistry of actinyl (VI) ions in alkaline solution. **R. Wilson**

11:25 I&EC 143. Design and application of an online reactive gas cell for safeguards measurements of UF₆. **L.R. Martin**,
L.D. Trowbridge, J.M. Richards, G.A. Fugate

Section B

Orange County Convention Center
Room W224F

I&EC International Fellow: Symposium in honor of Tom Baker

G. G. Stanley, *Organizer, Presiding*
A. D. Sutton, *Presiding*

8:00 I&EC 144. To B-E or not to B-E? The phosphinoboration reaction. S.J. Geier, C.M. Vogels, **S.A. Westcott**

8:25 I&EC 145. Surface structural-chemical characterization of a supported organovanadium(III) catalyst. D.M. Kaphan,
R.R. Langeslay, M. Ferrandon, G. Celik, C. Liu, A.P. Sattelberger, **M. Delferro**

8:50 I&EC 146. Measurements of trace level actinides in environmental samples. **S.K. Hanson**, W.J. Oldham, J.L. Miller

9:15 I&EC 147. Withdrawn

9:40 Intermission.

10:00 I&EC 148. Development of applications-focused testing for identification of peroxygen activators. **M.B. Abrams**

10:25 I&EC 149. Materials for display applications. **N.S. Radu**

10:50 I&EC 150. Hitting the Trifecta! Unpublished research highlights from industry, national lab and academia. **R. Baker**

Light-Driven Chemistry: Photoelectrochemistry & Photocatalysis

Sponsored by CATL, Cosponsored by COLL, ENFL, I&EC, INOR and PHYS

WEDNESDAY AFTERNOON

Section A

Orange County Convention Center
Room W224E



TECHNICAL PROGRAM

I&EC Early-Career Fellow: Symposium in honor of Carter Abney

L. R. Martin, *Organizer, Presiding*

1:30 I&EC 151. Task-specific design and functionalization of advanced porous organic polymers for water purification. **S. Ma**

1:50 I&EC 152. Synthesis and structure of the 11-ring zeolite EMM-17. **S.C. Weston**, K.G. Strohmaier, A.W. Burton, H.B. Vroman, B.K. Peterson, M.D. Shannon

2:10 I&EC 153. Structure-property relationships in the flexible zeolitic imidazolate framework EMM-36: Controlling the thermodynamic driving force for framework phase transformation. **J. Falkowski**, P. Ravikovitch, S. Weston, M. Abdulkarim, G. Muraro, E. Strohmaier

2:30 Intermission.

2:45 I&EC 154. Application of Metal-Organic Frameworks for environmental et energy purposes. **M. Carboni**

3:05 I&EC 155. Nanoscale metal-organic frameworks for cancer therapy. **W. Lin**

3:25 I&EC 156. Advanced catalysts for electrochemical conversion of essential small molecules in the atmosphere. **H. Zhu**

3:45 Intermission.

4:05 I&EC 157. Harnessing inorganic coordination complexes for novel chemical sensing technologies. **S. Liu**

4:25 I&EC 158. Massively parallel computations and kinetic modeling of polymerization reactions. **C.R. Landis**

4:45 I&EC 159. Blenders should only be used for drinks: the art and science of processing battery materials. **G. Veith**

5:05 I&EC 160. Exploration of emergence in polyamidoxime adsorbents by x-ray absorption spectroscopy. **C.W. Abney**, V. Bryantsev, S. Dai, L. Earl, A. Ivanov, S. Ma, R.T. Mayes, C. Do, Y. Wang

5:25 Concluding Remarks.

Section B

Orange County Convention Center
Room W224F

Second Annual Joint Symposium of the Separations Subdivisions

M. L. Dietz, *Organizer*

K. Phinney, *Organizer, Presiding*

1:30 Introductory Remarks.



TECHNICAL PROGRAM

1:35 I&EC 161. Withdrawn

2:00 I&EC 162. Improved profiling of sialylated *N*-linked glycans by HPAE-PAD. **S. Patil**, J. Rohrer

2:25 Intermission.

2:45 I&EC 163. Cupric oxide oxidation of lignin: Effects of reaction time. **R. Roy**, **B. Jadhav**, D.E. Raynie

3:10 I&EC 164. Development and optimization of a simple high performance liquid chromatography (HPLC) /evaporative light scattering detector (ELSD) method to determine Polysorbate 80 in a pharmaceutical formulation. **B. Mondal**, M. Kote, M. Patel

3:35 I&EC 165. Preparation of organo-silica sol-gel monoliths using "single-pot" approach for applications in capillary liquid chromatography. **Z. Zajickova**

4:00 Intermission.

4:20 I&EC 166. Recent progress in understanding ionic liquid-based metal ion extraction systems. **M.L. Dietz**

4:45 I&EC 167. Ionic liquid polyacrylamide gel electrophoresis for separation of egg white peptides. **M.C. Brands**, R. Pérez, P. Vidanapathirana, A. Grove, J.N. Losso, I.M. Warner

Light-Driven Chemistry: Photoelectrochemistry & Photocatalysis

Sponsored by CATL, Cosponsored by COLL, ENFL, I&EC, INOR and PHYS

THURSDAY MORNING

Section A

Orange County Convention Center
Room W224E

I&EC General Papers

Cosponsored by CTA
C. W. Abney, R. T. Mayes, *Organizers*
D. Dolzhenkov, *Presiding*

8:00 Introductory Remarks.

8:05 I&EC 168. Indolizine Dimer Derivatives: Novel high-effective corrosion inhibitor for acidizing in petroleum engineering. **Z. Yang**, F. Zhan, B. Hou, R. Wang, Z. Qu, Y. Wang

8:25 I&EC 169. Particle size control by ultrasound. S. Bhoi, **D. Sarkar**



TECHNICAL PROGRAM

8:45 I&EC 170. Exploration of natural polymers/silver nanoparticles composites as inhibitors for corrosion protection of industrial metals. **M.M. Solomon**, S.A. Umoren

9:05 I&EC 171. Novel working solvents system for alkylated anthraquinone and anthrahydroquinone: Applications in hydrogen peroxide synthesis. **B. Bai, X. Fang**, Q. Liu, W. Xie, L. Jia, H. Xu, Z. Song

9:25 I&EC 172. Coordination mechanism of organic multidentate ligands with lanthanides. **S. Suzuki**, T. Kobayashi, T. Yaita

9:45 I&EC 173. Nucleation behavior of *Ethyl vanillin* in three solvents from the metastable zone widths in cooling crystallization. **Y. Jing**, S. Xu, J. Wang, J. Gong

10:05 Intermission.

10:15 I&EC 174. Synthesis of pitch-based carbon fiber: Insights from ReaxFF based molecular dynamics simulations. **C. Jian**, N. Ferralis, T. Zhu, Y. Wang, J.C. Grossman

10:35 I&EC 175. Mechanochemical reaction pathways to enhance solvent-free synthesis of ZSM-5 zeolite. **M.H. Nada**, S.C. Larsen, E.G. Gillan

10:55 I&EC 176. One-pot synthesis and production of iron oxide nanoparticles embedded mesoporous graphitic carbon spheres in a single low-temperature carbonization strategy. **A.C. Dassanayake**, M. Jaroniec

11:15 I&EC 177. Pyrene-benzimidazole hybrids as novel blue emitters for organic light emitting diodes (OLEDs). **T.P. De Silva**, S.G. Youm, G. Sahasrabudhe, F.R. Fronczek, E.E. Nesterov, I.M. Warner

11:35 I&EC 178. Coarse-grained model of ionic liquids and CO₂ diffusion mechanism. **F. Huo**, J. Tong, X. Xie, S. Zhang

Section B

Orange County Convention Center
Room W224F

Second Annual Joint Symposium of the Separations Subdivisions

K. Phinney, *Organizer*
M. L. Dietz, *Organizer, Presiding*

8:00 I&EC 179. Determination of hydrophobic interaction energy through inclusion complex formation for the development of next-generation materials-application to separation sciences. **S. Pandey**, D. Lucas, B.E. Richter, D.E. Raynie

8:25 I&EC 180. Multi-stage continuous ALPHA process of isolating ultraclean lignins from woody biomass for material applications. **J. Ding, C.L. Fitzgerald**, M.C. Thies

8:50 Intermission.

9:10 I&EC 181. Universal approach to the screening of plant-based toxins from a variety of genus and species. **A. Schrell**, R.F. Williams, H. Cui



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

9:35 I&EC 182. Robust integrated workflow of phosphopeptide enrichment for monitoring kinase and phosphatase activities in drug efficacy modeling. **A. Lee**

10:00 I&EC 183. Enhancing the information content of single cell analysis on microfluidic devices using optical fiber bridges for the analysis of reactive nitrogen species and kinases in immune system cells. **C.T. Culbertson**

10:25 Concluding Remarks.

INOR

Division of Inorganic Chemistry

S. Koch and N. Radu, *Program Chairs*

SUNDAY MORNING

Section A

Orange County Convention Center
Room W221A

Undergraduate Research at the Frontiers of Inorganic Chemistry

Bioinorganic and Materials Chemistry

C. Nataro, E. C. Sylvester, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 INOR 1. DEPC modification of the Cu_A protein from *Thermus thermophilus*. **L.M. Hunsicker Wang**, T. Devlin, C. Hofman, Z. Acevedo, K. Kohler

8:55 INOR 2. Chemical modification of metal-ligating histidines in ETC proteins. **K.R. Hoke**, L.J. Buttram, M. Moeller, M. Weaver

9:15 INOR 3. Synthesis, structures, and biological activity of N-heterocyclic thione and selone complexes of silver. **D. Rabinovich**

9:35 Intermission.

9:50 INOR 4. Exploring how bipyridine platinum(II) complexes form non-covalent interactions in solution via aggregation and ultimately the related polymorphic phase changes in the solid-state. **J. Zahn**, R.E. Bachman



TECHNICAL PROGRAM

10:10 INOR 5. Rational strategies in the design of materials to exhibit triboluminescence. **D.E. Janzen**, M.S. Butler, N. Rabaey, M. Stamp, A. Wilke

10:30 INOR 6. Highly responsive liquid crystalline metalloporphyrin VOC sensors. **M.R. Ramsey**, A.L. Dorfner, J.E. Winklerek, J.C. Kranick, L.J. Tucker, J.L. O'Donnell

10:50 INOR 7. Creative exercises in inorganic chemistry: Discovering student misconceptions and promoting meaningful learning. **J. Shaw**

Section B

Orange County Convention Center
Room W224B

F. Albert Cotton Award in Synthetic Inorganic Chemistry: Symposium in Honor of Jeffrey R. Long

M. Dinca, *Organizer*
J. K. McCusker, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 INOR 8. Transition metal signaling: bioinorganic chemistry beyond active sites. **C.J. Chang**

9:00 INOR 9. History of materials development in lithium-ion batteries: From lab to market. **S.S. Kaye**

9:25 INOR 10. Controlling sensitivity to temperature in ^{59}Co NMR thermometers. M. Peña, T. Ozvat, **J. Zadrozny**

9:50 Intermission.

10:05 INOR 11. Using noncovalent interactions to control molecular magnetism and (photo)reactivity. **M.P. Shores**

10:30 INOR 12. Teaching halide double perovskites to absorb sunlight. A. Slavney, B. Connor, L. Leppert, J. Neaton, **H. Karunadasa**

10:55 INOR 13. Unusual geometric and electronic structures and reactivity in redox active ligand complexes of group 13. **L.A. Berben**, A. Arnold, T.M. Bass, T.J. Sherbow, E.J. Thompson

Section C

Orange County Convention Center
Room W224A

Harry Gray Award for Creative Work in Inorganic Chemistry by a Young Investigator: Symposium in Honor of Jillian L. Dempsey

E. M. Matson, *Organizer*
A. J. Miller, *Organizer, Presiding*



TECHNICAL PROGRAM

8:30 Introductory Remarks.

8:35 INOR 14. Robust catalysts for solar-driven water splitting. **H.B. Gray**

9:00 INOR 15. Excited-state proton-coupled electron transfer using inorganic and organic complexes. **E.R. Young**, A.N. Oldacre

9:25 INOR 16. Proton-coupled electron transfer and driving force: A complicated relationship. **S. Hammes-Schiffer**

9:50 INOR 17. Excited state oxidation of iodide ions in terionic assemblies. S.A. Wehlin, L. Troian-Gautier, **G.J. Meyer**

10:15 Intermission.

10:30 INOR 18. Cobalt catalysts with pendant hydrogen-bond donors for electrocatalytic CO₂ reduction. **S.C. Marinescu**, A. Chapovetsky

10:55 INOR 19. Bridging molecular and heterogeneous electrocatalysis through graphite conjugation. M. Jackson, S. Oh, C.J. Kaminsky, **Y. Surendranath**

11:20 INOR 20. Pd-Silyl cations for the catalytic activation of C–O bonds. **M.R. Gagne**

11:45 INOR 21. Electrocatalytic H₂ evolution mediated by a concerted electron proton transfer pathway with [Co₁₃C₂(CO)₂₄]⁴⁻. **L.A. Berben**, C.R. Carr, A. Taheri

Section D

Orange County Convention Center
Room W224C

ACS Award in Organometallic Chemistry: Symposium in Honor of Alan S. Goldman

M. Brookhart, J. F. Hartwig, *Organizers*
R. G. Bergman, K. I. Goldberg, *Organizers, Presiding*

9:00 Introductory Remarks.

9:05 INOR 22. Hydrogen binding and cleavage by an Fe(I) complex. **R. Bullock**, D. Prokopchuk, G.M. Chambers

9:25 INOR 23. Phosphinobenzylsilanes: Beware of their versatility! M. Corona-González, J. Zamora-Moreno, C. Cuevas-Chávez, **S. Sabo-Etienne**, V. Montiel-Palma

9:45 INOR 24. Late metal catalysts for the homopolymerization of ethylene and the copolymerization of ethylene with polar vinyl monomers. **M. Brookhart**, O. Daugulis, Z. Chen

10:05 INOR 25. Reductive epoxide opening catalyzed by titanocene and CpCr(CO)₃ with H₂ as the only stoichiometric reagent. **J.R. Norton**, C. Yao, T. Dahmen, A. Gansäuer

10:25 Intermission.



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

10:40 INOR 26. New strategies for the development of highly active and selective polymerization catalysts. **G.W. Coates**

11:00 INOR 27. Investigations in low coordinate iron chemistry. G.M. George, D. Pokhriyal, S.P. Heins, S.N. MacMillan, **P.T. Wolczanski**

11:20 INOR 28. Electronic structures and electrochemistry of boronated cyanometalates. **H.B. Gray**, B. McNicholas, E. Despagnet-Ayoub, D. Ngo

11:40 INOR 29. Cleaving C–H bonds with separated oxidants and bases. **J.M. Mayer**, J. Darcy, S. Kolmar, M. Ener-Goetz

Section E

Orange County Convention Center
Room W221C

Structure-Property Correlations in Functional Inorganic Materials

Intermetallics: design, growth, structure, and properties

J. A. Aitken, E. E. Rodriguez, *Organizers, Presiding*

8:30 INOR 30. Structure determination of low-carrier-density germanides adopting the $\text{Yb}_3\text{Rh}_4\text{Sn}_{13}$ structure type. **J. Chan**

9:00 INOR 31. Synthesis, crystal structures and physical properties of the quaternary solid solutions $\text{Ca}_{14-x}\text{RE}_x\text{MSb}_{11}$ (RE = La–Nd, Sm, Gd; M = Zn, Cd). **S. Baranets**, S.S. Bobev

9:20 INOR 32. Metal flux growth of new multinary metal silicide zintl phases. **G.N. Vasquez**, A. Huq, S.E. Lattner

9:40 INOR 33. Identifying an unanticipated origin of strength in Mo_2BC . A. Mansouri Tehrani, A. Lim, **J. Brgoch**

10:10 Intermission.

10:40 INOR 34. Hydride route to complex intermetallics. G. Bhaskar, T. Cox, V. Gvozdetzkyi, **Y.V. Zaikina**

11:10 INOR 35. Unprecedented violation Wiedemann-Franz law: A story of disobeying clathrate. **J. Wang**, K. Kovnir

11:30 INOR 36. Opportunities in quantum materials research using neutrons at ORNL. **C. dela Cruz**

12:00 INOR 37. Chemical principles of topological semimetals. **L.M. Schoop**

Section F

Orange County Convention Center
Room W224D

Through the Lens of Inorganic Chemistry: Understanding Heterogeneous Processes in Energy Conversion & Storage



TECHNICAL PROGRAM

S. Marinescu, J. Y. Yang, *Organizers*
V. Thoi, *Organizer, Presiding*

8:30 INOR 38. Electrocatalytic metal-organic frameworks. H. Noh, A. Peters, O.K. Farha, **J.T. Hupp**

9:00 INOR 39. Probing sulfur redox chemistry in supramolecular frameworks for energy storage applications. A. Baumann, D. Burns, **V. Thoi**

9:30 INOR 40. Proton-coupled electron transfer reactions at metal oxide/solution interfaces. **J.M. Mayer**, J. Peper, C. Wise, J. Castillo-Lora, S. Laga, R. Agarwal, N. Gentry, S. Hill

10:00 Intermission.

10:15 INOR 41. Photo- and electro- catalytic hydrogen generation by redox-active metal-organic frameworks. **H. Zhou**, L. Feng

10:45 INOR 42. Highly oxidized metal centers and metal-metal cooperativity in oxo clusters for water splitting. **T. Tilley**

11:15 INOR 43. Bonding, mechanism and kinetics of water oxidation over oxide catalysts. **R.J. Nielsen**, W.A. Goddard

Section G

Orange County Convention Center
Room W221D

Bioinorganic Chemistry: Proteins & Enzymes & Model Systems

S. A. Koch, *Organizer*
B. F. Shaw, *Presiding*

8:30 INOR 44. Modeling steps in the sMMO reaction cycle: Forming a diiron(IV) complex via acid-assisted O–O bond cleavage of a peroxodiiron(III) intermediate derived from O₂. **S. Banerjee**, A. Draksharapu, L. Que

8:50 INOR 45. Disruption of the anticancer activity of dirhodium(II) tetraacetate by amino acid methionine. **A. Enriquez Garcia**, F. Jalilehvand, C.S. Shemanko, B.S. Gelfand, H. Harris

9:10 INOR 46. HAT vs cPCET mechanisms for C–H bond activations by LCu(III)–OH, –OOR, and –O₂CR compounds. **M. Mandal**, C.E. Elwell, W.B. Tolman, C.J. Cramer

9:30 INOR 47. Assessing the substrate scope of the chelatase CfbA. **A.E. Schuelke**, M.D. Liptak

9:50 INOR 48. Designed artificial Iron proteins. **K.R. Miller**, A. Borovik

10:10 Intermission.

10:30 INOR 49. Structural and functional changes induced by alkyl RNO binding to myoglobin & hemoglobin. **V.E. Herrera**, S. Powell, K.Y. Prather, N.T. Nguyen, J.E. Yi, G.B. Richter-Addo



TECHNICAL PROGRAM

10:50 INOR 50. Synthesis and reactivity through protonation in synthetic molybdenum cofactor models. **H.H. Varnum**, R. Fair, S.J. Nieter Burgmayer

11:10 INOR 51. Mechanisms of HNO reactions with ferric heme proteins. Y. Shi, **Y. Zhang**

11:30 INOR 52. Insights into binding and degradation of heme by *Mycobacterium tuberculosis* MhuD. **B. Thakuri**, A. Graves, A. Chao, S.L. Johansen, C. Goulding, M.D. Liptak

11:50 INOR 53. Organometallic conjugates of selected kinesin-5 inhibitors - synthesis and impact of organometallic moiety on biological activities. **D. Plazuk**, A. Wieczorek, M. Lomzik, A. Blauz, B. Rychlik

12:10 INOR 54. Charge regulation in metalloprotein electron transfer. **B.F. Shaw**

Section H

Orange County Convention Center
Room W221E

Chemistry of Materials - Materials for Energy & Catalytic Applications

C. G. Lugmair, *Organizer*
C. Bartel, D. J. Xiao, *Presiding*

8:30 INOR 55. Time-dependent spectroscopies of triads with heterobinuclear units reveal long-lived charge transfer states. **A.D. Hill**, A.A. Stone, D. Cobani, L.P. Livernois, Q.P. Ashmore, H.J. Salzmann

8:50 INOR 56. CO₂ insertion into C–H bonds for carboxylic acid synthesis. **D.J. Xiao**, E. Chant, A. Yau, M. Kanan

9:10 INOR 57. Soluble metal-organic supercontainers (MOSCs) promote organic reactions “on water”. **P. Jampani**, H. Zhou, Z. Wang

9:30 INOR 58. Structural dynamics of bismuth cathodes during the electrochemical reduction of CO₂ in the presence of RTILs. **J. Rosenthal**

9:50 INOR 59. Withdrawn

10:10 INOR 60. Withdrawn

10:30 Intermission.

10:45 INOR 61. Oxyanion hydrogenation over binary metal phosphides. **L. Wei**

11:05 INOR 62. Probing the degradation chemistry and enhanced stability of 2D organolead halide perovskites. **B.R. Wygant**, C.B. Mullins, A. Dolocan, D.M. Abbott, Q. Vu, A. Ye

11:25 INOR 63. Doping effect on structures and properties of metal oxide semiconductor nanomaterials. **Z.J. Li**, A. Riley, S. hosseini, T.S. Zubkov



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

11:45 INOR 64. Computational identification of all-inorganic cesium chloride double perovskite solar absorbers. **C. Bartel**, C. Sutton, B.R. Goldsmith, A. Holder, C. Musgrave

12:05 INOR 65. Solid-state NMR approaches to lead halide perovskites. D. Kubicki, D. Prochowicz, A. Hofstetter, M. Graetzel, **L. Emsley**

Section I

Orange County Convention Center
Room W232A

Lanthanide & Actinide Chemistry

A. De Bettencourt Dias, *Organizer*
J. Monteiro, P. Roesky, *Presiding*

8:30 INOR 66. Ortho-nitrophenyl photolyzable ligands as cages for tb(III) and other lanthanides. **S. Sakhdari**, I. Chakraborty, J. Miksovská, K. Kavallieratos

8:50 INOR 67. Recent advances in dysprosium single-molecule magnet design: high-temperature magnetic blocking and magneto-structural correlations. **K.R. McClain**, C.A. Gould, K. Chakarawet, S.J. Teat, T.J. Groshens, J.R. Long, B.G. Harvey

9:10 INOR 68. Luminescent lanthanide complexes with high two-photon absorption cross-section and viscosity-dependent emission. **J. Monteiro**, N.R. Fetto, M.J. Tucker, A. De Bettencourt Dias

9:30 INOR 69. Homoleptic imidophosphorane cerium complexes: Potent thermodynamic reductants and stabilization of tetravalent oxidation state. **N.T. Rice**, J. Su, E.R. Batista, J. Bacsá, P. Yang, H.S. La Pierre

9:50 Intermission.

10:00 INOR 70. Main group element cages as building blocks for 4f-metal coordination clusters. **P.W. Roesky**

10:20 INOR 71. Thermal charge-transfer oxidation of alcohols by uranyl (VI) to α -hydroxyalkyl radicals and their isomerization to alkoxy radicals catalyzed by the uranyl–water complex. **X. Sun**, D. Kolling, S. Deskins, E. Adkins

10:40 INOR 72. Reaction of lanthanide acetates with molybdenum trioxide. **A.W. Apblett**, K. Alrashidi, M. Chehbouni

11:00 INOR 73. Family of thorium redox active complexes and reactivity. **S.S. Galley**, S.C. Bart

11:20 INOR 74. X-Ray spectroscopy studies into the electronic structure of Ce(III) and Ce(IV) coordination complexes. **L.M. Moreau**, E. Lapsheva, Y. Qiao, W.W. Lukens, E.J. Schelter, C. Booth

Section J

Orange County Convention Center
Room W232B

Main Group Chemistry



TECHNICAL PROGRAM

T. Hudnall, *Organizer*
R. J. Gilliard, *Presiding*

8:30 INOR 75. Unsymmetrical triazenyl radicals stabilized by *N*-heterocyclic carbenes: Synthesis and their formation mechanism. **J. Back**, E. Lee

8:50 INOR 76. New synthetic strategies in carbene–bismuth chemistry. G. Wang, L. Freeman, D. Dickie, **R.J. Gilliard**

9:10 INOR 77. Systematic studies of carbodicarbenes and *n*- heterocyclic carbenes in alkaline earth metal chemistry. **J.E. Walley**, R.J. Gilliard, J. Dutton, D. Wilson, G. Briener, G. Wang, D. Dickie

9:30 INOR 78. Decomposition of sulfur hexafluoride (SF₆) with metals dissolved in liquid ammonia. **H.L. Deubner**, D. Kraus

9:50 Intermission.

10:00 INOR 79. Nucleophilic activation of red phosphorus into soluble polyphosphide anions. **M. Jo**, A. Dragulescu-Andrasi, M. Shatruk

10:20 INOR 80. Dispiro-4-bromobenzylaminophosphazenes: Synthesize reactions, spectroscopic properties, crystal structures, biological and cytotoxic activities. **N. Guven Kuzey**, M. Ozgur, N. Asmafiliz, L. Acik, B. Aydin, T. Hokelek, M. Turk, N. Cerci

10:40 INOR 81. 1,2-benzoazaphospholes as transition metal surrogates. **M.F. Cain**, P.M. Miura-Akagi

11:00 INOR 82. Reduction reactions of P-Cl compounds with Mg(I) bromide. **J. Arras**, H. Schnoeckel

Computational Methods in Lanthanide & Actinide Chemistry

Sponsored by NUCL, Cosponsored by COMP and INOR

Innovative Chemistry & Materials for Electrochemical Energy Storage

Li-Ion & Na-Ion

Sponsored by ENFL, Cosponsored by CATL, INOR and PMSE

Elucidation of Mechanisms & Kinetics on Surfaces

Mechanisms on Surfaces: C-C Coupling, C-H & C-O Bond Manipulations

Sponsored by CATL, Cosponsored by ENFL, ENVR, INOR and PHYS



TECHNICAL PROGRAM

SUNDAY AFTERNOON

Section A

Orange County Convention Center
Room W221A

Undergraduate Research at the Frontiers of Inorganic Chemistry

Organometallics and Catalysis

C. Nataro, E. C. Sylvester, *Organizers*
R. J. Swails, *Presiding*

1:30 INOR 83. Electronic properties of ruthenium complexes containing asymmetric pH-dependent polypyridyl ligands. **K. Benson**, J. Stash, M. Bezpalko, W.S. Kassel, T. Dudley, J.J. Paul

1:50 INOR 84. Mechanistic insights into base-free transfer hydrogenation using air and water stable Cp*Ir catalysts. **A. Smith**, S. Ahmed, A.R. O'Connor, C. Goldberg, G.L. Heard

2:10 INOR 85. Mechanistic studies of alkene aziridination with a dinuclear silver catalyst. **C. Mak**, M.G. Campbell

2:30 Intermission.

2:45 INOR 86. Phosphine-directed C–H borylation: accessing ambiphilic phosphine boronates. **T.B. Clark**, S.E. Wright, S. Richardson-Solorzano, T.N. Stewart, W. Schumacher, K.C. Morris

3:05 INOR 87. Remote Oxidative Activation of a [Cp*Rh] Monohydride. **E. Boyd**, D. Lionetti, J.D. Blakemore

3:25 INOR 88. Synthesis and characterization of *trans*-Co^{III}(DMC) mono-phenylacetylide and bis-phenylacetylide. **B. Oxley**, B. Mash, M. Zeller, S.D. Banziger, T. Ren

3:45 INOR 89. Pyridinium substituted Pd-NHC complexes: Synthesis, structure, and catalytic activity. **R.J. Swails**, M. Sebold, S. Kariofillis, A. Conner, R. Cerbone, J. Luo, J. Corcoran

Section B

Orange County Convention Center
Room W224B

F. Albert Cotton Award in Synthetic Inorganic Chemistry: Symposium in Honor of Jeffrey R. Long

M. Dinca, J. K. McCusker, *Organizers*
J. D. Rinehart, *Presiding*

1:30 INOR 90. What do we actually know about charge transport in conductive 2D MOFs? **M. Dinca**, J. Dou, G. Skorupskii, R. Day, I. Stassen, T. Chen, L. Yang



TECHNICAL PROGRAM

1:55 INOR 91. Understanding and optimizing porosity in coordination cages. **E.D. Bloch**

2:20 INOR 92. Structural studies of small molecules adsorbed in MOFs. **C.M. Brown**

2:45 INOR 93. Use of model guided high throughput experimentation for the development of MCM-68. **S.C. Weston**, K. Strohmaier, H.B. Vroman, J.C. Vartuli, J.T. Ippoliti, A.J. Lobo, D.W. Lewis

3:10 Intermission.

3:25 INOR 94. Porous aromatic frameworks (PAFs). **G. Zhu**

3:50 INOR 95. Metal-organic phase-change materials for thermal energy storage. R. McGillicuddy, **J.A. Mason**

4:15 INOR 96. Creating an ideal interface to form defect-free mixed-matrix membranes with UiO-66-NH₂. Q. Qian, **Z.P. Smith**

4:40 INOR 97. Development of MOFs for commercial gas separation applications. **T. McDonald**, Z. Herm, C. Anderson, G. Wenz, J. Lim, L. Porter-Zasada

Section C

Orange County Convention Center
Room W224A

Harry Gray Award for Creative Work in Inorganic Chemistry by a Young Investigator: Symposium in Honor of Jillian L. Dempsey

A. J. Miller, *Organizer*

E. M. Matson, *Organizer, Presiding*

1:30 INOR 98. Intermediates in catalytic CO₂ and proton reduction investigated by pulse radiolysis. **E. Fujita**, M.Z. Ertem, D.C. Grills, D.E. Polyansky

1:55 INOR 99. Molecular cobalt catalysts for H₂ generation with redox activity and proton relays in the second coordination sphere. **K.L. Mulfort**, L. Kohler, J. Niklas, R.C. Johnson, M. Zeller, O. Poluektov

2:20 INOR 100. Electrons, holes, protons, and proteins. **J.R. Winkler**, H.B. Gray, B. Sanders, J. Shin, P.J. Kielb

2:45 INOR 101. Exploring non-covalent interactions for energy storage and water purification. **N. Elgrishi**

3:10 Intermission.

3:25 INOR 102. Outer-sphere effects on the ligand-field excited-state dynamics of Fe(II) polypyridyl complexes. J. Miller, **J.K. McCusker**

3:50 INOR 103. Thermodynamic considerations for hydrogenation of CO₂: factors that limit catalyst performance. **C.T. Saouma**



TECHNICAL PROGRAM

4:15 INOR 104. Heterometallic polyoxovanadate clusters as redox-reservoirs for multielectron small molecule activation. **E.M. Matson**

4:40 INOR 105. Concerted proton-electron transfer reactions in the Marcus inverted region. **J.M. Mayer**, G. Parada, Z. Goldsmith, S. Kolmar, B.P. Rimgard, L. Hammarstrom, S. Hammes-Schiffer

Section D

Orange County Convention Center
Room W224C

ACS Award in Organometallic Chemistry: Symposium in Honor of Alan S. Goldman

R. G. Bergman, K. I. Goldberg, J. F. Hartwig, *Organizers*
M. Brookhart, *Organizer, Presiding*
F. Hasanayn, *Presiding*

1:30 INOR 106. Tandem C-H activation and N-N activation during conversion of arenes and N₂ into anilines. **P.L. Holland**, S.F. McWilliams, D.L. Broere, C.J. Halliday, B.Q. Mercado

1:50 INOR 107. Photochemical C-H activation: An early story. **R. Eisenberg**

2:10 INOR 108. Anisotropy of solid state NMR Chemical Shift signal informs on the π character of M-alkyl σ -bond in d⁰metal alkyl complexes. **O.G. Eisenstein**, C. Raynaud, R.A. Andersen, C. Gordon, C. Coperet

2:30 INOR 109. Metal-alkoxide based mechanism for alcohol dehydrogenative coupling. M. Ataya, **F. Hasanayn**

2:50 INOR 110. Rhodium-catalyzed alkenylation of allylbenzenes via C–C bond cleavage. **F. Kakiuchi**

3:10 Intermission.

3:25 INOR 111. Metal complexes of unusual silicon ligands in bond activations and new chemical transformations. **T. Tilley**

3:45 INOR 112. Base metal-catalyzed synthesis of nitrogen containing compounds through hydrogen borrowing. **K. Hultsch**, L. Homberg, N. Hofmann

4:05 INOR 113. Walking an electronic and steric tightrope in C–H borylation. **M.R. Smith**

4:25 INOR 114. Organometallic radical chemistry: The quantitative prediction of radical combination efficiencies in geminate cage pairs and random collisional cage pairs. **D.R. Tyler**, J. Barry

4:45 INOR 115. Please pass the salt: Counter ion effects to enhance hydroaminoalkylation catalytic reactivity. **L. Schafer**

Section E

Orange County Convention Center
Room W221C



TECHNICAL PROGRAM

Structure-Property Correlations in Functional Inorganic Materials

Optical and magnetic materials

J. A. Aitken, E. E. Rodriguez, *Organizers, Presiding*

1:30 INOR 116. High luminescent multinary halides: Crystal chemistry, properties and applications. **B. Saparov**, A. Yangui, R. Rocanova, M. Du

2:00 INOR 117. Chemist's view on square-net based topological materials. **S. Klemenz**, S. Lei, L.M. Schoop

2:20 INOR 118. Direct observation of photoinduced self-trapped hole polaron formation in perovskites. **C. Liu**, H. Tsai, W. Nie, X. Zhang

2:40 INOR 119. Lone pairs in the halide perovskites, hidden and otherwise. **R. Seshadri**

3:10 Intermission.

3:40 INOR 120. Chemistry perspective to design novel magnetic semiconductors/semimetals. **W.T. Xie**, X. Gui

4:10 INOR 121. Magnetovolume effects in geometrically frustrated Laves phases. **J. Cooley**, E. Levin, R. Seshadri

4:30 INOR 122. Magnetic properties of novel rhenium-based double perovskites. **F. Yuan**, C.M. Thompson

4:50 INOR 123. PARADIM: A new national user facility for accelerating materials discovery. **W. Phelan**

Section F

Orange County Convention Center
Room W224D

Through the Lens of Inorganic Chemistry: Understanding Heterogeneous Processes in Energy Conversion & Storage

V. Thoi, J. Y. Yang, *Organizers*
S. Marinescu, *Organizer, Presiding*

1:30 INOR 124. Influence of solvent-surface interactions on heterogeneous catalysis in porous inorganic oxides. **S.L. Scott**

2:00 INOR 125. Conductive metal dithiolene frameworks for electrocatalytic H₂ production. **S.C. Marinescu**, C.A. Downes, K. Chen, A.J. Clough

2:30 INOR 126. Single-site versus single-ion catalysts in metal-organic frameworks. **O.K. Farha**

3:00 INOR 127. Rapid detection method for probing the local pH and product distribution during CO₂ reduction. **A. Co**



TECHNICAL PROGRAM

3:30 Intermission.

3:45 **INOR 128.** Oxygen-atom vacancies in polyoxovanadate-alkoxide clusters. B. Petel, A.A. Fertig, **E.M. Matson**

4:15 **INOR 129.** MOFs are not zeolites, or oxides, or metals, or any other solid catalysts. **M. Dinca**, C. Sun, C. Neuma, E. Metzger, R. Comito, M. Korzynski

4:45 **INOR 130.** Metallo-cyclam metal organic frameworks for CO₂ utilization. J. Zhu, J. Liu, D. Troya, A. Esker, **A.J. Morris**

Section G

Orange County Convention Center
Room W221D

ACS Award for Distinguished Service in the Advancement of Inorganic Chemistry: Symposium in Honor of Debbie C. Crans

Bioinorganic and Structural Aspects

B. Baruah, N. E. Levinger, M. Lim, *Organizers*
N. S. Radu, *Presiding*

1:30 Introduction.

1:35 **INOR 131.** Genome mining for citrate-derived siderophores. **A. Butler**, J.R. Carmichael

2:00 **INOR 132.** Iron-siderophore complexes as redox-reversible anchors in artificial metalloenzymes. D. Raines, J. Clarke, K. Wilson, **A. Duhme-Klair**

2:25 **INOR 133.** Copper(I)-dioxygen derived complexes; formation, stabilization and reactivity. **K.D. Karlin**

2:50 **INOR 134.** Binuclear Ga₈Ln₂ Metallacrowns and their optical properties. **V.L. Pecoraro**, J. Lutter, B. Lopez Bermudez, E. Salerno, S. Eliseeva, S. Petoud, G. Collet

3:15 Intermission.

3:30 **INOR 135.** Selenium incorporation as a selective probe of the electronic structure in the iron-molybdenum cofactor of nitrogenase. **S. DeBeer**

3:55 **INOR 136.** Unravelling the structure of phytate, a prevalent source of phosphorus. **K. Bowman-James**, S. Pramanik, M. Reinmuth, S. Kaur, V. Day

4:20 **INOR 137.** Further studies of the reaction of green vitriol with the lye of blood. **S.A. Koch**

4:45 **INOR 138.** In sickness and in health: Exploring relationships between plasma metal ions and the development of infectious diseases. **P. Carver**



TECHNICAL PROGRAM

5:10 INOR 569. Tungsten oxo alkoxide precursors for the deposition of WO_x films and nanostructures. **L. McElwee-White**

Section H

Orange County Convention Center
Room W221E

ACS Award in Inorganic Chemistry: Symposium in Honor of George Christou

A. S. Veige, *Organizer, Presiding*

1:30 INOR 140. Expanding the range of ligands that stabilize the rare-earth metals in new low oxidation states. **W.J. Evans**

1:50 INOR 141. Discovery, design and prediction of inorganic solids: structural diversity to applications. **M.G. Kanatzidis**

2:10 INOR 142. Vacuum deposition of biferrocene thin films: growth strategies for stability and tuneable magnetism. R. Leber, L. Wilson, P. Robaschik, M.S. Inkpen, D. Payne, N.J. Long, T. Albrecht, C. Hirjibehedin, **S. Heutz**

2:30 INOR 143. High-frequency EPR studies of exchange coupled single-molecule magnets: Possible routes to molecule-based quantum technologies. **S. Hill**, J. Marbey, M. Shiddiq, T.N. Nguyen, T. Ghosh, G. Christou

2:50 INOR 144. From molecular magnets to tons of plutonium. **A. Schake**

3:10 Intermission.

3:30 INOR 145. Influence of ligand conformation on the spin-state properties of iron(ii) complexes. **M. Halcrow**, K.E. Burrows, I. Capel Berdiell, R.E. Kulmaczewski

3:50 INOR 146. Molecular lego for spintronics and quantum information. **G. Aeppli**

4:10 INOR 147. Magnetic bistability: pancake bonding vs. sigma-hole bonding. **K. Preuss**

4:30 INOR 148. Switchable paramagnets and their integration into nanomaterials. **G.G. Morgan**

4:50 INOR 149. Complexes with mixed N/S coordination: A new approach to spin-crossover complexes. S. Yergeshbaeva, A. Arroyave, A. Dragulescu-Andrasi, O. Hietsoi, V. Stubbs, J. Hrudka, Ö. Üngör, **M. Shatruk**

5:10 INOR 150. Opto-spintronics: Photoisomerization-induced spin state switching at 300 K in photochrome cobalt-dioxolene thin films. **N. Frank**

Section I

Orange County Convention Center
Room W232A

Functional Metal Nanostructures for Biomedical Applications



TECHNICAL PROGRAM

X. Xia, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 INOR 151. Chiroplasmonic nanoassemblies: Intracellular localization of nanoparticle dimers by chirality reversal. **N. Kotov**, L. Xu, M. Sun, J. Bang, H. Kuang, S. Alben, C. Xu

1:55 INOR 152. Engineered nanoconstructs for intracellular imaging and targeting. **T.W. Odom**

2:15 INOR 153. Unravelling physiology on the nanoscale with renal clearable metal nanoparticles. **J. Zheng**

2:35 INOR 154. Plasmonic nanomaterial based optofluidic biosensors for next generation point-of-care immunoassays. **P. Chen**

2:55 INOR 155. Using gold nanoparticles for diagnostics and sensing in low cost devices. **K. Hamad-Schifferli**

3:15 Intermission.

3:25 INOR 156. Designing plasmonic nanoparticles for ultrasensitive biosensing. **M. Stevens**

3:45 INOR 157. Structure-relaxivity relationships of magnetic nanoparticles for MR imaging. **X. Chen**

4:05 INOR 158. Advanced nanomaterials for rapid microbial diagnostics. **A. Abbas**

4:25 INOR 159. Surface engineering of ultrasmall luminescent gold nanoparticles for ratiometric imaging. **J. Liu**, L. Gong, Y. Chen

Section J

Orange County Convention Center
Room W232B

National Fresenius Award: Symposium in Honor of Brandi Cossairt

B. M. Cossairt, *Organizer*

D. M. Heinekey, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 INOR 160. Magic in magic sized clusters. **J.S. Owen**

1:55 INOR 161. Quantum-cutting ytterbium-doped halide perovskites that show photoluminescence quantum yields approaching 200%. **D.R. Gamelin**

2:15 INOR 162. Hydrogen-atom transfer chemistry of pnictide, chalcogenide and other materials. **J.M. Mayer**, M. Delley, N. Dwarica, C. Wise



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

2:35 INOR 163. Surface-functionalized inorganic clusters as redox-noninnocent ligands for transition metals: Synthesis, characterization and reactivity studies. **A. Velian**, J. Kephart, A. Chirila, A. Boggiano

2:55 INOR 164. Catalyst immobilization on electrode surfaces *via* silica supports for artificial photosynthetic devices. **M.R. Norris**, S. Clair, D.P. Harrison

3:15 Intermission.

3:30 INOR 165. Phosphoric acid as a precursor to chemicals traditionally synthesized from white phosphorus. M. Geeson, S. Shepard, P. Rios, **C.C. Cummins**

3:50 INOR 166. Making bonds with copper and light. **J.C. Peters**

4:10 INOR 167. Insertion of molecular oxygen into palladium(II) and platinum(II) methyl bonds. H.E. Zeitler, **K.I. Goldberg**

4:30 INOR 168. Award Address (National Fresenius Award sponsored by the Phi Lambda Upsilon, The National Chemistry Honor Society). There's plenty of room in the middle: Tales of nanoscale synthesis from a molecule maker. **B.M. Cossairt**

Innovative Chemistry & Materials for Electrochemical Energy Storage

Li-Ion & Na-Ion

Sponsored by ENFL, Cosponsored by CATL, INOR and PMSE

Computational Methods in Lanthanide & Actinide Chemistry

Sponsored by NUCL, Cosponsored by COMP and INOR

Elucidation of Mechanisms & Kinetics on Surfaces

Reductions & Hydrogenations

Sponsored by CATL, Cosponsored by ENFL, ENVR, INOR and PHYS

SUNDAY EVENING

Section K

Orange County Convention Center
West Hall C



TECHNICAL PROGRAM

ACS Award for Distinguished Service in the Advancement of Inorganic Chemistry: Symposium in Honor of Debbie C. Crans

B. Baruah, N. E. Levinger, M. Lim, *Organizers*

5:30 - 7:30

INOR 169. Aqueous solution reactions of Zn^{2+} and Cd^{2+} with glycine. **Y.Z. Hamada**

INOR 170. Malic acid with molybdenum(vi) in aqueous solutions. **Y.Z. Hamada**

INOR 171. Enhancing cancer killing oncolytic viruses with vanadium-based phosphatase inhibitors. **H. Murakami**, D.C. Crans, M. Selman, A. Bergeron, J. Diallo

INOR 172. Kinetic studies of interpeptidic Cu(II) exchange from Cu(II) tri- and tetrapeptide complexes. **L. Zocchi**, M. Hartman, C. Buening, C. Hureau, D.C. Crans

INOR 173. Interaction of vanadium(V) catecholate complexes with a model membrane system. **J.T. Koehn**, S.M. Petry, C.M. Glover, A. Levina, P.A. Lay, D.C. Crans

INOR 174. Antibacterial and ^{195}Pt NMR spectroscopic studies with a novel mixed-metal binuclear ruthenium(II)-platinum(II) complex. **J.S. Clark**, L. Moody, L. Seymour, M. Davis, R. Johnson, J.G. Hurdle, W.L. Jarrett, D.G. VanDerveer, Y. Tse-Dinh, A. Holder

INOR 175. Insight into the molecular mechanism of action of the anti-cancer properties of a novel cobalt(III) complex with a thiosemicarbazone ligand. **D.L. Askew**, J.L. Bullock, S. Sandhaus, J.F. Arca, M. LeBlanc, C.E. Baxter, D.M. Washington, M.J. Celestine, F.A. Beckford, Y. Tse-Dinh, S.J. Beebe, W.L. Jarrett, A. Holder

INOR 176. Synthesis and characterization of vanadium catecholates for enhancement of oncolytic viruses. **V. Bachtell**, H. Murakami, J.T. Koehn, D.C. Crans

INOR 177. Utilizing rhenium as an anticancer agent: A review. **A. Haase**, E. Bauer, R. Reich, F.E. Kuehn, D.C. Crans

INOR 178. Production of efficient hydrogen through water splitting by controlling electron spin. **V. Singh**

Section K

Orange County Convention Center
West Hall C

ACS Award in Inorganic Chemistry: Symposium in Honor of George Christou

A. S. Veige, *Organizer*

5:30 - 7:30

INOR 179. Ultrathin multifunctional two-dimensional metal-organic framework nanosheets for efficient CO₂ catalytic. **S. Zhang**, **Y. Chen**



TECHNICAL PROGRAM

INOR 180. *Ab initio* computational thermochemistry of SF₅OOX (X=H, F an Cl). **J.A. Martinez**, G.P. Pieffet, V.P. Loret, C. Buendía

INOR 181. Synthesis, structure and magnetic properties of molecular Bi-Mn and Pb-Mn-oxo clusters. **E.B. Earlywine**, K.A. Abboud, G. Christou

INOR 182. Cobalt-manganese-oxide clusters as water oxidation catalysts. **P. Mahalay**, T. Ghosh, G. Maayan, K.A. Abboud, G. Christou

INOR 183. Synthesis and characterization of a new antiferromagnetic iron-oxo cluster with Me₂AsO₂⁻ ligands: a covalently-linked [Fe₆]₂ dimer. **K. Lee**, K.A. Abboud, G. Christou

INOR 184. Study of tri-*t*-butyl tin hydride complexes of transition metals towards activation of small molecules. **S. Etezadi**

Section K

Orange County Convention Center
West Hall C

Alfred Bader Award in Bioinorganic or Bioorganic Chemistry: Symposium in Honor of Joan B. Broderick

J. Betz, S. R. Smith, *Organizers*

5:30 - 7:30

INOR 185. Smuggled cargo: copper binding to riboflavin binding protein. **S.R. Smith**, C. Goodis, A. Hashem, N. Leonardo

INOR 186. Refining catalytic insights toward the chemical mechanism of *R. capsulatus* formate dehydrogenase via EPR spectroscopy. **B.R. Duffus**, T. Hartmann, C. Teutloff, S. Leimkühler

INOR 187. Probing the pH sensitivity in the mechanism of myoglobin compound II auto-reduction. K. Hill, **H.R. Williamson**

INOR 188. Probing a Possible Cation Binding Site in [FeFe]-hydrogenase maturation enzyme, HydE. **S. Impano**, E.M. Shepard, J. Betz, A. Pagnier, W. Broderick, J.B. Broderick

INOR 189. Insights into the universal radical SAM organometallic intermediate, Ω. **E.C. McDaniel**, H. Yang, A. Byer, W. Broderick, K. Yokoyama, B.M. Hoffman, J.B. Broderick

INOR 190. Development and optimization of a computationally engineered PFL-AE mutant for improved crystallization. **S. Hill**, D. Rinauro, E.C. McDaniel, J. Moody, J.B. Broderick

INOR 191. Paramagnetic intermediates in spore photoproduct lyase. **A. Pagnier**, E.M. Shepard, W. Broderick, J.B. Broderick

INOR 192. Radical SAM maquette chemistry: C_x₃C_x₂C peptide coordinated redox active [4Fe-4S] clusters. **E.M. Shepard**, A. Galambas, J. Miller, M. Jones, A. Pineda, H. Watts, E. McDaniel, V. Copie, R.K. Szilagy, J.B. Broderick

Section K



TECHNICAL PROGRAM

Orange County Convention Center
West Hall C

Bioinorganic Chemistry: DNA, RNA & Inorganic Drugs

S. A. Koch, *Organizer*

5:30 - 7:30

INOR 193. Dinuclear platinum(II) complex with switchable near-infrared emission as a probe of nuclease activity. **M. Gabr**, F. Pigge

INOR 194. Cationic Au(I) complexes with aryl-benzothiazoles and their antibacterial effect on gram-negative bacteria. **H.R. Ouattara**, J. Stenger, P.K. Mascharak

INOR 195. QM/MM MD simulations of zinc finger proteins and their reactivity with reducible sulfur and selenium compounds. **A. Dreab**, P.B. Lutz, C.A. Bayse

INOR 196. How does the chromate reduction product chromium(III) bind DNA? **S. Brown**, S.A. Woski, J.B. Vincent

INOR 197. Development and study of novel ruthenium complexes as potential light-activated anticancer prodrugs: determining which characteristics have the highest impact on toxicity.. **J.L. Gray**, J. Park, F. Qu, A. Harriston, S. Altman, Y. Kim, E.T. Papish

INOR 198. Fluorescence and post-synthetic reactivity mixed fluorinated subphthalocyanines. **K.J. McAuliffe**, R.L. Calandrino, E.R. Trivedi

INOR 199. BODIPY optical probes for pH-responsive imaging. **P.B. Tsitovich**, B.N. Animasaun, J. Jeouty, M. Henry

Section K

Orange County Convention Center
West Hall C

Bioinorganic Chemistry: Proteins & Enzymes & Model Systems

S. A. Koch, *Organizer*

5:30 - 7:30

INOR 200. Biomimetics of [Fe-Fe]-hydrogenase: Catalysts for proton reduction. **C.A. Mebi**

INOR 201. Investigating the effect of multiple interactions on the dimerization and oxygen stability of the fumarate nitrate reductase transcription factor in *E. coli* bacteria. **S. Kazmouz**, **J.E. Eastman**, L.J. Moore

INOR 202. Does metallothionein-3 alter the polymerization kinetics of actin? **C. Hachicho**, R.N. Austin, C. Vizcarra



TECHNICAL PROGRAM

- INOR 203.** Metal-organic frameworks for protein stabilization. **Y. Chen**
- INOR 204.** Synthesis and studies of a new pterindithiolene model of the molybdenum cofactor. **V. Berke**
- INOR 205.** Inorganic model complexes for hydrogen gas production. **L. Nyarko**, M. Foster, E. Gladhill, D. Rokhsana
- INOR 206.** Developing manganese-based biomimetic water oxidation catalysts for energy production. **M. Kayne**, H. Tran, J. Prakash
- INOR 207.** Investigating insulin monomer and hexamer formation with Langmuir monolayers, Brewster angle microscopy, and fluorescence microscopy. **K.E. Saulcy**, **S. Croslow**, B. Allen, D.C. Crans, A. Sostarecz
- INOR 208.** Synthetic model systems for alkene dioxygenase. **F.A. Chavez**, A. Banerjee, R. Loloee, W.W. Brennessel, V. Schünemann
- INOR 209.** Evaluating the effects ligand oxidation state plays on structure, electronic, and reactivity properties of DMSO Reductase mimics. **S.A. Dille**, P. Basu
- INOR 210.** Exchanging protein ligands to examine the impact of molybdenum coordination in periplasmic nitrate reductase from *Campylobacter jejuni*. **B. Mintmier**, J. McGarry, P. Basu
- INOR 211.** Synthesis of metal-organic framework material mimicking carbonic anhydrase enzyme. **S. Kaur**, B. Yan
- INOR 212.** Nitroxyl (HNO) complexes of ruthenium porphyrins. **J.R. Zink**, E.G. Abucayon, G.B. Richter-Addo
- INOR 213.** Studying beta amyloid oligomer formation using fluorescence anisotropy and atomic force microscopy. **E.K. Adams**, M.R. Mackiewicz
- INOR 214.** Synthesis and reactivity of nitrogenase model complexes with sulfur- and carbon-based coordination environments. **A.L. Speelman**, I. Coric, B.Q. Mercado, P.L. Holland

Section K

Orange County Convention Center
West Hall C

Coordination Chemistry: Characterization & Applications

A. Larsen, *Organizer*

5:30 - 7:30

- INOR 215.** Luminescent lanthanide complexes containing anionic bidentate oxygen ligand. **P.K. Yuen**, C. Lau, A. Yuen
- INOR 216.** Functionalization of azamacrocycles by appendage attachment of molecules with known antioxidant properties. **T.M. Schwartz**, K.N. Green



TECHNICAL PROGRAM

INOR 217. Ligand-centered reactivity of triaminoborane-bridged diphosphine complexes with Mo, W, and Cu: Borenum ions, luminescent properties, and phosphorus substituent effects. **K. Lee**, P. Lai, C. Kim, C.M. Donahue, M.M. Wymore, T.S. Teets, S.R. Daly

INOR 218. Sterically hindered cross-bridged tetraazamacrocycles. M.L. Whorton, T. Davis, **T.J. Hubin**

INOR 219. Pyridine linked bis cross-bridged tetraazamacrocycles. T.L. Fletcher, T.R. Tadlock, M. Ayala, A.G. Oliver, J.A. Krause, **T.J. Hubin**

INOR 220. Hexacoordinate silicon complexes for applications in organic electronics. **M. Kocherga**, T.A. Schmedake, M.G. Walter, Y. Zhang

INOR 221. Transition metal complexes with persistent and isolable borenum ions. **J.D. Culpepper**, S.R. Daly, K. Lee

INOR 222. Investigations of a hybrid (experimental, computational, iterative) technique for the reliable determination of rapid-exchange binding in redox-active ligand systems. S.R. Wolfe, T.A. Christensen, **N.A. Johnson**, J. Counts, G. Borth, C. Kingsley, Z.M. Heiden, M.F. Roll, **K.V. Waynant**, J.G. Moberly

INOR 223. First-row transition metal complexes supported by a redox-active NNP-type pincer ligand and their application to electrocatalytic CO₂ reduction. **K. Talukdar**, A. Issa, J.W. Jurss

Section K

Orange County Convention Center
West Hall C

Francis P. Garvan_John M.Olin Medal-Olin Medal: Symposium in Honor of Lisa McElwee-White

L. J. Murray, *Organizer*

5:30 - 7:30

INOR 224. Design and synthesis of WO₂L₂ precursors for chemical vapor deposition of WO_x films. **X. Su**, P. Panariti, L. McElwee-White

INOR 225. Influence of photochemistry of (η^3 -allyl)Ru(CO)₃X precursors on photoassisted chemical vapor deposition. **O.M. Hawkins**, C.R. Brewer, **N.C. Sheehan**, B. Salazar, A.V. Walker, L. McElwee-White

INOR 226. Ruthenium(II) carbonyl halide complexes as focused electron beam induced deposition precursors. **J. Yu**, S.J. Matsuda, R.M. Thorman, H. Fairbrother, L. McElwee-White

INOR 227. Synthesis and evaluation of fluorinated tungsten (VI) oxo-alkoxide complexes as precursors for the chemical vapor deposition of WO_x thin films. **N.C. Ou**, D.C. Bock, L. McElwee-White

INOR 228. Synthesis of Cu(I) and Au(I) isocyanide complexes as precursors for focused electron beam induced deposition. **T.B. Dunn**, W.G. Carden, L. McElwee-White

INOR 229. Synthesis and characterization of a tungsten nitrido tert-butoxide complex as a precursor for aerosol-assisted chemical vapor deposition of WO_xN_y films. **T. Kim**, M.M. Nolan, L. McElwee-White



TECHNICAL PROGRAM

Section K

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West Hall C

Functional Metal Nanostructures for Biomedical Applications

X. Xia, *Organizer*

5:30 - 7:30

INOR 230. Withdrawn

INOR 231. Wrinkled mesoporous silica (WMS) for drug delivery. **J. Lin**, K.J. Balkus

Section K

Orange County Convention Center
West Hall C

Harry Gray Award for Creative Work in Inorganic Chemistry by a Young Investigator: Symposium in Honor of Jillian L. Dempsey

E. M. Matson, A. J. Miller, *Organizers*

5:30 - 7:30

INOR 232. Investigation of the catalytic cycle of [FeFe] hydrogenase from *Desulfovibrio desulfuricans* (DdHydAB). **M. Sanchez**, J. Birrell, E. Reijerse, W. Lubitz, R.B. Dyer

INOR 233. Electrochemical and spectroscopic characterization of potassium chromate in acidic solutions for water purification. **C.M. Stern**, D. Hayes, N. Elgrishi

INOR 234. Determination of electroactive windows of tetrahedral supramolecular coordination cages for electrocatalyst encapsulation. **R. Bujol**, N. Elgrishi

Section K

Orange County Convention Center
West Hall C

Inorganic Spectroscopy

C. V. Popescu, *Organizer*

5:30 - 7:30



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

INOR 235. Infrared spectroscopic and theoretical studies of the metal sulfur oxide complexes. **R. Wei**, Y. Gong

INOR 236. Metal ion detection using ^{19}F -MRI. **L. Basal**, A. Moon

INOR 237. Highly efficient heteroleptic monovalent coinage metal phosphors for modern display, signage and lighting apps. **L.M. Harris**, R. Mitch, V. Nesterov, M.M. Ghimire, M.A. Omary

INOR 238. Computational/experimental study on metal cation- π sandwich adducts. **M.N. Ericson**, M.A. Omary

Section K

Orange County Convention Center
West Hall C

Nanoscience

Nanoscience

B. G. Trewyn, *Organizer*

5:30 - 7:30

INOR 239. Intercalation of gemcitabine into zirconium phosphate nanoparticles for effective anti-cancer nanotherapy. J.M. Little, A. López Cubero, A.M. García Vargas, **A. del Valle Pérez**, **M. Martínez**, **J. Colón**

INOR 240. Ambient bi-stable reversible crystalline-crystalline phase transition in two-dimensional gete flake. F. Zhou, **L. Gan**

INOR 241. Variability study of the synthesis and growth kinetics of surface modified ZnO quantum dots using LiOH. **B. Groce**, **D.M. McCall-Butler**, J. Loguerico, J.K. Davis-Gunn, D. Francis, A. Mena, B. Colon, A. Schrock, K.S. Molek, P. Benz

INOR 242. Synthesis of silver nanoparticles with capping agents with different anions. **K. Nemeth**, **B.J. Bellott**, J.J. Determan

INOR 243. Comparison of synthetic methods and physical properties of carbon nanotubes for applications in organic light emitting diode (OLED) technology. **R. Dohoney**, **N. Bagnall**, M.B. Jacobs

INOR 244. Synergistic effects of copper-vitamin C incorporated alumina nanocomposite hydrogels for burn wound healing. **T. Dassanayake Mudiyansele**, S. Huang

INOR 245. Synthesis and characterization of Fe-Mn oxide nanowires and their catalytic activities towards oxygen evolution reaction. **A. Cetin**, A.M. Önal, E. Nalbant Esenturk

INOR 246. Cation exchange reactions and zinc chalcogenide nanocrystals. **A. Akinmola**, N. Huszainey, H.D. Hall, J.M. Miller, P.G. Van Patten

Section K



TECHNICAL PROGRAM

Orange County Convention Center
West Hall C

Organometallic Chemistry: Catalysis

N. S. Radu, *Organizer*

5:30 - 7:30

INOR 247. Withdrawn

INOR 248. Nickel (II) *N,N*-chelates as precatalysts for the benzonitrile hydrogenation. **A.A. Rodríguez Vázquez**, J.J. Garcia

INOR 249. Catalytic amine dehydrogenation using Ru^{II} complexes: The effect of electron density of the metal center on catalysis. **E.E. Joslin**, C.R. Ghareeb, S. Bourgeois

INOR 250. Electropolymerization of MOF-based conductive polymers for microelectrode functionalization. **J.A. Cruz**, L. Cunci

INOR 251. Molybdenum-promoted dearomatization of pyridines. **J. Wilde**, J.T. Myers, W.D. Harman

INOR 252. Accessing chiral ambiphilic phosphine boronates by directed C-H borylation reactions. **W. Schumacher**, **T.N. Stewart**, S.E. Wright, S. Richardson-Solorzano, K.C. Morris, T.B. Clark

INOR 253. Reactive intermediates in silver-catalyzed nitrene transfer. **I. Golden**, C. Mak, M.G. Campbell

INOR 254. Efficient hydroboration of carbonyl compounds with iminophosphinite POCN pincer complexes of nickel. **K.A. Gudun**, M. Segizbayev, A.Y. Khalimon

INOR 255. Copper catalyzed regioselective N – alkynylation of pyrazoles and anticancer activity of ethynyl- pyrazoles. **M. Sau**

INOR 256. Hemilabile, unsymmetrical pyrrole-based PNN pincer and its Ni(II) and Pd(II) complexes: highly active catalysts for norbornene polymerization reactions. **S. Das**, G. Mani

INOR 257. DFT modeling of the complete catalytic cycle of methane-to-methanol via Earth-abundant late 3d bimetallic complexes. **A. Najafian**, T.R. Cundari

INOR 258. Computational analysis of proton-coupled electron transfer in molecular electrocatalysts containing tris(triazolyl)borate ligand. **A. Nazemi**, T.R. Cundari

INOR 259. Salen manganese (V) catalyzed hydroboration of carbonyls. **S. Vijamarri**, G. Du

INOR 260. DFT survey of the effects of d-electron count and metal identity on the activation and functionalization of C–H bonds for mid to late transition metals. **C. Moulder**, t.R. Cundari

INOR 261. Oxygen atom transfer by dioxo mo (VI) bis-amidate complexes. **J.M. Smith**, R.K. Thomson



TECHNICAL PROGRAM

INOR 262. Iridium catalyzed allylic fluorination: Scope, mechanism and applications to PET Imaging. **A.M. Sorlin**, J.C. Mixdorf, D. Dick, H.M. Nguyen

INOR 263. Catalytic hydrostannylation by electronically unsaturated complex containing platinum and tin, Pt(SnBu₃)(IPr)(H). **M.M. Gamage**, A. Koppaka, B. Captain

Section K

Orange County Convention Center
West Hall C

Structure-Property Correlations in Functional Inorganic Materials

J. A. Aitken, E. E. Rodriguez, *Organizers*

5:30 - 7:30

INOR 264. Synthesis, crystal structure and physicochemical characterization of lithium-containing sulfides. **J.A. Aitken**

INOR 265. Synthesis, crystal structures and physical properties of the quaternary solid solutions Ca_{14-x}RE_xMSb₁₁ (RE = La–Nd, Sm, Gd; M = Zn, Cd). **S. Baranets**, S.S. Bobev

INOR 266. Do weakly polar anions break inversion symmetry in racemates? **M.L. Nisbet**, K.R. Poepelmeier

INOR 267. *In situ* diffraction studies on the structure evolution of perovskite La_{1-x}Sr_xCoO_{3-δ} under chemical looping condition. **T. Li**, R. Jayathilake, D. Taylor, E.E. Rodriguez

INOR 268. Synthesis and thermoelectric properties of *p*-type Zn-doped Cu₅Sn₂Q₇ (Q = Se, Te). **C. Sturm**, T. Mori, H. Kleinke

INOR 269. Exploring flux conditions on the synthesis of novel solid state battery materials. **D. Sandoval**, J. Mora, A.M. Fry

INOR 270. Molecular Fe₂Se₆ trapped in a non-centrosymmetric framework of metal chalcogenide. C. Weng, C. Yang, J. Jang, **K. Hsu**

INOR 271. Materials with a twist: The search for ferrotoroidics. **T.J. Diethrich**, S. Gnewuch, E.E. Rodriguez

INOR 272. Tunable molecular fluorescence in multivariate metal organic frameworks. **W. Newsome**, F.J. Uribe-Romo

INOR 273. General hydrothermal synthesis of amine intercalated iron chalcogenides and effect on superconductivity and magnetism. **H. Zheng**, B. Wilfong, X. Zhou, E.E. Rodriguez

INOR 274. Thermal expansion and response to pressure of NaM^VF₆ (M = Nb, Ta) ReO₃-type fluorides. **A.J. Lloyd**, E.B. Masterson, A.P. Wilkinson

Section K



TECHNICAL PROGRAM

Orange County Convention Center
West Hall C

Undergraduate Research at the Frontiers of Inorganic Chemistry

Bioinorganic Chemistry

C. Nataro, E. C. Sylvester, *Organizers*

5:30 - 7:30

INOR 275. Understanding the factors governing oxygen atom transfer of manganese-oxo complexes . **E.G. Stewart-Jones**

INOR 276. Towards new vanadium enzymes. **O.M. Peduzzi**, A. Paredes, K.E. Madore, A.J. Reig, K.M. Buettner

INOR 277. Hydrolytic titanium mini-metalloenzymes. **A. Paredes**, O.M. Peduzzi, K.E. Madore, A.J. Reig, K.M. Buettner

INOR 278. Preparation and conformational analysis of peptide derivatives of a rigid, bimetallic ring system. **M.L. Phillip**, T.P. Curran, J.L. Stewart

INOR 279. Effect of pH on the reduction potential of cytochrome c_2 and its H42F mutant. **M. Weaver**, M. Moeller, K.R. Hoke

INOR 280. Effect of active-site alterations on the reduction potential of the Rieske protein. **L.J. Buttram**, K.R. Hoke

INOR 281. Synthesis, characterization and determination of a beta-sheet conformation in an organometallic complex. **T.T. Nguyen**, T.P. Curran, J.L. Stewart

INOR 282. Determination of the reduction potential of copper bound- riboflavin binding protein. **N. Leonardo**, S.R. Smith

INOR 283. Isothermal titration calorimetry (ITC) of vitamin B2 binding to apo- riboflavin binding protein. **A. Hashem**, S.R. Smith

INOR 284. Amino acid sequence analysis of riboflavin binding protein across species; in search of a copper binding site. **C. Goodis**, S.R. Smith

INOR 285. Enhancement of peroxidase activity in a hemin-based artificial enzyme. **K. Itamura**, K.E. Splan

INOR 286. Impact of Cu(I) on RING finger domain structure. **I. Eckart-Frank**, K.E. Splan

INOR 287. Synthesis and characterization of diiron complexes: Structural mimics of [FeFe]-hydrogenase. **K. Dague**, S.C. Silver

INOR 288. Systematic evaluation of copper binding and activation by *de novo Due Ferri* single chain proteins. **S.E. Worthington-Kirsch**, B. VanDyke, A.J. Reig



TECHNICAL PROGRAM

INOR 289. Hydrolytic activity of *Due Ferri* single chain proteins. **S. Hawkins, A. Huynh, A. Paredes, O.M. Peduzzi, K.M. Buettner, A.J. Reig**

INOR 290. Characterization of PnpC1C2, a “type II” hydroquinone ring-cleaving dioxygenase. **M.C. Maker, T.E. Machonkin**

INOR 291. Polymer-supported copper complexes towards mimicking particulate methane monooxygenase activity. **D. Navarro, V. Tafuri, H.L. Ordon, M.R. Radlauer**

INOR 292. Enzyme-like catalysis: Encasing a soluble methane monooxygenase model in a polymer scaffold for improved catalysis. **H.L. Ordon, V. Tafuri, D. Navarro, M.R. Radlauer**

INOR 293. Investigating amyloid beta peptide aggregation in the presence of copper and zinc. **R.P. Lullo, D.S. Nashed, K. Cummins, M.A. Havens, J.J. Keleher, D. Kissel**

INOR 294. Investigating dechlorination mechanisms using biomimetic model compounds. **C. Ye, K.M. Van Heuvelen**

INOR 295. First-row transition metal mimics of superoxide dismutase active sites. **J. Bovill, A. Dillon, M. Carroll**

INOR 296. How susceptible are fungi, yeasts and bacterias to the properties of organometallic compounds based on iron and/or molybdenum? **S.I. Pérez Lozada**

Section K

Orange County Convention Center
West Hall C

Undergraduate Research at the Frontiers of Inorganic Chemistry

Coordination Chemistry

C. Nataro, E. C. Sylvester, *Organizers*

5:30 - 7:30

INOR 297. Purifying natural gas using a polymer stabilized iron complex with alkyl phosphine ligands. **K.J. MacCulloch, J.W. Gohdes**

INOR 298. Transition metal complexes with 2-(2-pyridine)-1,3-dioxolane and 2-(2-pyridine N-oxide)-1,3-dioxolane. **K.A. Goerl, P. Baran**

INOR 299. Gold(III) complexes with 2-*tert*-butyl-1,10-phenanthroline or an *N*-(8-quinolinyl)amide synthesized for intramolecular C-H bond activations. **M. Hernandez, K. Rutter, M. Sleck, J.E. Thompson, H.R. Murphy, K. Saucedo Chavez, G. Donalson, A.L. Rheingold, D.R. Weinberg**

INOR 300. Synthesis and spectroscopic properties of dinitrosyl iron complex with, tris(*o*-methoxyphenyl)phosphine, tris(2-carboxyethyl)phosphine and tris(2-furyl phosphine). **T. Hoang, W.R. Sueme, M. Patao, L. Li**



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- INOR 301.** Characterization of iron(III) coordination complexes in a tripodal ligand environment. **D. Fernandez**, W.M. Ames, U.J. Williams
- INOR 302.** Optimizing the synthesis of a new tetradentate mixed donor ligand. **A.J. Reuter**, **S.A. Brunclik**, C.M. Seong, E.E. Marlier
- INOR 303.** Synthetic and computational investigation of cobalt silylene reactivity. **A.M. Conley**, J. Zhang, D.L. Kohen, M.T. Whited
- INOR 304.** Two novel Eu³⁺-Rhodamine-B derivative complexes as sensors to detect G-type nerve gas agents. **A. Rich**, E. Sinn, A. Venter, D.E. Wheeler, A. Weerasinghe
- INOR 305.** Amide protons as binding groups in a polypyridyl rhenium (I) sensor. **G. Kyro**, L.D. Schmitt, J. Ainsworth, A.J. Lees
- INOR 306.** Coordination of 2-methoxy-6-methylpyridine N-oxide with 3d metals. **A. Montgomery**, P. Baran
- INOR 307.** Synthesis and characterization of heteroleptic alkaline earth metal silyl amides. **C. Nicholson**, M.S. Cousins, M.M. Gillett-Kunnath, K. Ruhlandt-Senge
- INOR 308.** TCNE attachment to iron dinitrosyl complexes containing bis(diphenylphosphine) derivatives: potential as anti-tumor agents. **D.A. Velarde**, R. Bourland, L. Li
- INOR 309.** Synthesis, characterization, and coordination studies of novel bismuth compounds. **M. Vonden Steinen**, B. Wilson, Y. Takahashi, T. Ngo, D.G. Allis, M.M. Gillett-Kunnath, K. Ruhlandt-Senge
- INOR 310.** Closer look at the synthesis and characterization of alkaline earth metal heteroleptic tetraarylborate pyrazolates. **A. Clements**, J.J. Woods, C.M. Lavin, M.S. Cousins, K. La, D.G. Allis, M.M. Gillett-Kunnath, K. Ruhlandt-Senge
- INOR 311.** Exploration of a two-electron reservoir electrocatalyst to facilitate the two-electron reduction of carbon dioxide. **A. Sosa-Parada**, H. Plummer, G.A. Felton
- INOR 312.** Tuning of an iron-centered compound for carbon dioxide activation. **H. Plummer**, A. Sosa-Parada, G.A. Felton
- INOR 313.** Design and synthesis of porphyrins with liquid crystalline properties. **A.L. Dorfner**, M.R. Ramsey, J.E. Winklerek, C.J. Timony, S.J. Wallace, M.E. Zick, L.J. Tucker, J.L. O'Donnell
- INOR 314.** Synthesis of yttrium complexes supported by tridentate ketoiminate ligands. J.M. Fritsch, **A.S. Butler**
- INOR 315.** Preparation of manganese complexes of amine bis(phenolate) ligands. **N. McCutcheon**, B. Wile
- INOR 316.** Exploration of non-symmetrical amine bis(phenolate) ligands using a combined synthetic and computational approach. **N.M. Braunscheidel**, T.M. Perrine, B. Wile
- INOR 317.** Synthesis and characterization of ruthenium complexes bearing tris(pyrazolyl)methane or terpyridine as a tridentate ligand. **R. Lash**, C.R. Turlington
- INOR 318.** Experimental and computational investigation of the solvatochromism of [Mo(diimine)Cl₄]⁻ compounds. **S. Helland**, P. Hutchison, A. Chang, W.T. Eckenhoff



TECHNICAL PROGRAM

INOR 319. Redox Active Al(III) complexes: Electron donating ligands to improve charge transfer. **A. Smith**, A. Arnold, L.A. Berben

INOR 320. Temperature and solvent dependent kinetics and quantum yields of [Fe-Fe] hydrogenase model complexes. **B.J. Jolly**, C.F. Works

INOR 321. Investigation of the ligand properties necessary for effective cobalt-based nitrate reduction. **J.P. Madriaga**, H. Kwon, D. Ashley, E. Jakubikova

INOR 322. Synthesis of [O, O, N, O] Ligands for Application in Polymerization. **K.E. Myers**, A. Anderson-Wile

INOR 323. Lanthanide extraction with a trialkylphosphine oxide capped ligand: Variation of extraction conditions to optimize lanthanide recovery. **M. Glander**, S.M. Biros, E.J. Werner

INOR 324. Variation of ligand caps and substituents of tripodal CMPO-based agents for f-element extraction. **A. Martinez**, W. Larrinaga, E.J. Werner

INOR 325. Time-correlated single-photon counting measurements of electron transfer between heterobinuclear units and bipyridine. **A. Stone**, D. Cobani, A. Hill

Section K

Orange County Convention Center
West Hall C

Undergraduate Research at the Frontiers of Inorganic Chemistry

General

C. Nataro, E. C. Sylvester, *Organizers*

5:30 - 7:30

INOR 326. Ask not what VIPEr can do for you – ask what you can do for VIPEr. **E.C. Sylvester**, **C. Nataro**, A.K. Bentley, H.J. Eppley, E.R. Jamieson, S. Lin, A.R. Johnson, J.R. Raker, B.A. Reisner, S.R. Smith, J.L. Stewart, L.A. Watson, N. Williams

INOR 327. Bonding with Nicolai and Henry in the D(earborn): A VIPEr content building workshop on molecular orbital theory and bonding. **S.C. Silver**, K.A. Grice, S.R. Smith

INOR 328. Coupling epoxides and dry ice under mild conditions: Development of an undergraduate laboratory experiment. **S. Poland**, **Z. Ni**, **J. McLemore**

INOR 329. Undergraduate laboratory development: Finding cost-effective catalysts for the coupling of epoxides and CO₂. **S. Poland**, **A. Braaksma**, **L. Fenimore**

INOR 330. Training undergraduate research students in cluster synthesis and crystallization techniques for single-crystal x-ray diffraction. **C. Thompson**, E.S. Eitheim



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

INOR 331. Lewis acid-mediated SuFEx reactions toward nitrogen-based sulfonylated compounds.. **C. Woroch**, N.D. Ball, C. Am Ende

INOR 332. Accessing phosphine boronates by C(sp²)-H and C(sp³)-H borylation using a cationic iridium complex. **K.C. Morris, S. Richardson-Solorzano**, S.E. Wright, T.N. Stewart, J. Wilson, C.D. Miller, **T.B. Clark**

Section K

Orange County Convention Center
West Hall C

Undergraduate Research at the Frontiers of Inorganic Chemistry

Organometallic Chemistry

C. Nataro, E. C. Sylvester, *Organizers*

5:30 - 7:30

INOR 333. Synthesis and characterization of chromium-centered radicals supported by tris(phosphinomethyl)phenylborate ligands. S. Senthil, J.T. Stephan, M. Swift, V.G. Young, Jr., **P.J. Fischer**

INOR 334. Ferrocene-linked binucleating ligands for holding two dissimilar metal ions. **Z. Gehman**, N.A. Piro

INOR 335. Influence of a second coordination sphere borane on rhodium(I) oxidative addition of chelating aldehydes. **M. Reese**, B.R. Nichols, N. Akhmedov, J.L. Petersen, B.V. Popp

INOR 336. Preparation of organometallic cobalt(III) complexes containing bidentate chiral amine ligands as potential transfer hydrogenation catalysts. **L. Do Carmo**, J.P. Lee

INOR 337. Mechanistic studies of the iridium-catalyzed *ortho* C-H borylation of benzylic amines. **N. Chuang**, A. Samoshin, C. Oliver, S.N. Hyland, H. Guan, **T.B. Clark**

INOR 338. Design and synthesis of amine bis(phenolate) ligands for applications in catalysis. **C.L. Griffith**

INOR 339. Iron tricarbonyl complexes of redox active ligands relevant to electrocatalytic reactions. **J. Brown**, **A. Josling**, M. Carroll

INOR 340. Substituent effects on solvatochromism of [CoCp₂][Mo(bpy)Cl₄]. **K. Lee**, W.T. Eckenhoff

INOR 341. Substituted sulfonamide alcohols as ligands for titanium and tantalum catalyzed asymmetric aminoallene hydroamination. **F. Sha**, **H.S. Slocumb**, **S. Towell**, **Y. Zhen**, A.R. Johnson

INOR 342. Synthesis of group 6 carbonyls with phosphine ligands for CO₂ reduction. N. Walker, **B.J. Bellott**

INOR 343. Synthesis and reactivity of molybdenum carbon dioxide complexes. **B.J. Jiannotti**, **M.T. MacDonald**, **S.C. Oldenburg**, M. Graziani, L. Briggs, G.R. Lorzing, X. Duan, P.M. Graham



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INOR 344. Suzuki-Miyaura coupling employing palladium catalysts with 1,1'-bis(ditert-butylphosphino)ferrocene in different coordination modes. C. Nataro, R. Bal

Section K

Orange County Convention Center
West Hall C

Undergraduate Research at the Frontiers of Inorganic Chemistry

Solid State, Materials and Nano Chemistry

C. Nataro, E. C. Sylvester, *Organizers*

5:30 - 7:30

INOR 345. Using a polymer stabilized aryl phosphine complex of iron in the purification of natural gas.. H. Nguyen, J.W. Gohdes

INOR 346. Incorporating fluorescent probes into the cavities of a metal-organic framework. E. Alvarez, G.J. McManus

INOR 347. Structural characterization of an azide containing coordination polymer. L. Lamos, G.J. McManus

INOR 348. Incorporation of rare earth chelates into a sol-gel matrix using post-annealing immersion. K.S. Brewer, M.Z. Woodward, O.M. Simone, E.M. Walicki

INOR 349. Synthesis and crystal structure of novel 3D porous metal-organic framework material for photocatalysis. C. Thrickmorton, B. Yan

INOR 350. Photophysical characterization, aggregation induced emission and particle size distribution of nanoggregates of diallyl- and 1-hydroxypropyl-substituted tetraphenyl siloles and germales. C. Lucy, J.L. Mullin, C.M. Prudente, H. Tracy

INOR 351. Analysis of protein-capped gold and silver nanoparticles by infrared spectroscopy. E.C. Rose, Z. Schonrock, A.K. Bentley

INOR 352. Noble metal nanoparticle interactions in aqueous solutions. S.S. Ibarra, S.A. Worku, A.K. Bentley

INOR 353. Synthesis and DFT calculations of $\text{Cu}_4(\text{I})_4(\text{SbR}_3)_4$ cuboids with near-IR thermoluminescence. S.A. Shubert-Zuleta, L. Taylor, M.J. Rose

INOR 354. Synthesis of copper(II) complexes with 3-hydroxyimidazole-1-oxide derivatives for development of single molecule magnets. C. Taylor, P. Baran, A. Kensinger, Y. Wojciechowski, R. Boca

INOR 355. Effect of electrolyte concentration on the cycle life of cryptomelane type manganese dioxide cathodes in aqueous zinc ion batteries. J. Laughlin, Z. Zec, A. Poyraz

INOR 356. Synthesis of diimide phosphonic acid derivatives. B.E. Galeas, J.S. Soriano, P.O. Adelani



TECHNICAL PROGRAM

- INOR 357.** Magnetic phenomena in cobalt-based ionic liquids. **J. Foster**, R.E. Del Sesto
- INOR 358.** Preparation of zinc metal-organic materials towards drug delivery vessels. **A. Bigness**, J.M. Montgomery, C.V. Gauthier
- INOR 359.** Selective hydrogenations with mono- and bimetallic Au catalysts. **C.S. Guzman**, E.R. Hand, N. Dwarica, J. Bruno, B. Chandler
- INOR 360.** Morphological control of zinc oxide nanoparticles imaged with scanning electron microscopy. **W. He**, J.C. Mann, J.M. Fritsch
- INOR 361.** Analysis of the origins of ferroelectricity in substituted perovskites using neutron and x-ray total scattering techniques. **K. Barker**, G. Laurita
- INOR 362.** Preparation methods for lead-free titanate perovskites. **A.R. Turtz**, G. Laurita
- INOR 363.** Synthesis and characterization of Ho-substituted bismuth pyrochlores. **J.D. Ross**, G. Laurita
- INOR 364.** Designing flexible aromatic ligands for the synthesis of metal-organic frameworks. **M. McCormack**, G.J. McManus
- INOR 365.** Developing novel tricarboxylic acid linkers as a design platform for flexible metal-organic frameworks. **N. Giorgi**, G.J. McManus
- INOR 366.** Elucidation of the living ring opening (co-)polymerization of L-lactide and ϵ -caprolactone by magnesium initiator complexes. **A.E. Stahl**, D.B. Green, J.M. Fritsch
- INOR 367.** Synthesis of *bis*-ligated zinc complexes and their use in ring opening (co-)polymerization of L-lactide and ϵ -caprolactone. **K. Brooks**, D.B. Green, J.M. Fritsch
- INOR 368.** Toward twisting hierarchically branched nanocrystals: Amino acid-mediated growth of metal dendrimers. **S. Severson**, J.D. Smith, S.E. Skrabalak

MONDAY MORNING

Section A

Orange County Convention Center
Valencia Ballroom A

ACS National Awards in Inorganic Chemistry: Plenary Session

S. A. Koch, N. S. Radu, *Organizers*
A. De Bettencourt Dias, *Presiding*

8:30 Introductory Remarks.



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

8:35 INOR 369. Award Address (ACS Award for Distinguished Service in the Advancement of Inorganic Chemistry sponsored by Strem Chemicals, Inc.). Fundamental coordination chemistry, speciation, biological activities and metals in medicine, especially using vanadium. **D.C. Crans**

9:05 INOR 370. Award Address (F. Albert Cotton Award in Synthetic Inorganic Chemistry sponsored by the F. Albert Cotton Endowment Fund). Cooperative adsorption and gas separations in metal-organic frameworks. T. McDonald, D.A. Reed, R. Siegelman, J. Oktawiec, H.Z. Jiang, E. Kim, D.E. Jaramillo, K. Colwell, R. Torres-Gavosto, D.J. Xiao, M. Gonzalez, J.E. Bachman, Z.R. Herm, M.K. Taylor, L.E. Darago, J. Mason, E.D. Bloch, B.M. Wiers, J. Zadrozny, D. Gygi, V.Y. Mao, B. Dinakar, L. Porter-Zasada, B. Keitz, C. McGuirk, P.J. Milner, J. Martell, A. Forse, T. Runcevski, A. Demessence, W.L. Queen, L.J. Murray, D.M. D'Alessandro, M. Dinca, **J.R. Long**

9:35 INOR 371. Award Address (Francis P. Garvan–John M. Olin Medal sponsored by the Francis P. Garvan–John M. Olin Medal Endowment). Mechanism based design of organometallic precursors for FEBID. **L. McElwee-White**

10:05 Intermission.

10:20 INOR 372. Award Address (ACS Award in Organometallic Chemistry sponsored by The Dow Chemical Company Foundation). Alkane dehydrogenation catalyzed by late-metal complexes, and related "tandem" systems. **A.S. Goldman**

10:50 INOR 373. Award Address (Harry Gray Award for Creative Work in Inorganic Chemistry by a Young Investigator sponsored by the Gray Award Endowment). Proton-coupled electron transfer pathways by which molecular catalysts mediate electrochemical fuel production. **J.L. Dempsey**, N. Elgrishi, T. Huang, D.A. Kurtz, B. McCarthy, E. Rountree

11:20 INOR 374. Award Address (ACS Award in Inorganic Chemistry sponsored by ACS). Molecular chemistry as a 'bottom-up' route to nanoscale magnetic materials. **G. Christou**

11:50 INOR 375. Award Address (Alfred Bader Award in Bioinorganic or Bioorganic Chemistry sponsored by the Alfred R. Bader Fund). Novel chemistry for biological iron-sulfur clusters: Radical initiation via organometallic chemistry. **J.B. Broderick**

Innovative Chemistry & Materials for Electrochemical Energy Storage

Solid & Polymer Electrolytes

Sponsored by ENFL, Cosponsored by CATL, INOR and PMSE

MONDAY AFTERNOON

Section A

Orange County Convention Center
Room W221A

Undergraduate Research at the Frontiers of Inorganic Chemistry

Organometallics and Catalysis



TECHNICAL PROGRAM

C. Nataro, E. C. Sylvester, *Organizers*
N. Crowder, *Presiding*

1:30 INOR 376. Evolving the use of metal carbonyl complexes for structure and kinetic studies: Applications in polymer chemistry. **T.M. Folsom**, D.J. Darensbourg

1:50 INOR 377. Effect of electron density on catalytic amine dehydrogenation using Ru(II)-ampy Complexes. **C.R. Ghareeb**, E.E. Joslin

2:10 INOR 378. Structure and reactivity of transition metal and main group proazaphosphatane complexes. **M. Johnson**

2:30 Intermission.

2:45 INOR 379. Catalytic intramolecular hydroamination of aminoallenes using titanium complexes of chiral, tridentate, dianionic imine-diol ligands. **B.S. Mitchell**, F. Sha, C. Ye, A.R. Johnson

3:05 INOR 380. Hydroamination reactions catalyzed by $[\text{Au}_2(\mu\text{-Cl})(\mu\text{-bis}(\text{phosphino})\text{ferrocene})][\text{BArF}_2\text{4}]$. **N. Wamser**, C. Nataro

3:25 INOR 381. Zwitterionic chromium(I)-centered radicals: Isolable cousins of thermally unstable d^6 tricarbonyl complexes. **P.J. Fischer**, S. Senthil, J.T. Stephan, M. Swift, V.G. Young, Jr.

3:45 Concluding Remarks.

Section B

Orange County Convention Center
Room W224B

F. Albert Cotton Award in Synthetic Inorganic Chemistry: Symposium in Honor of Jeffrey R. Long

J. K. McCusker, *Organizer*
M. Dinca, *Organizer, Presiding*

1:30 INOR 382. Characterization of the physical properties of complexes of the rare-earth metals in the +2 oxidation state. **W.J. Evans**

1:55 INOR 383. Designing molecule-based materials for bottom-up control of magnetic anisotropy. **J.D. Rinehart**, J. Hilgar, M.G. Bernbeck, A. Butts

2:20 INOR 384. Employing radical-ligands in lanthanide-based single-molecule magnet design. **S. Demir**, C.M. Legendre, F. Benner

2:45 INOR 385. Coordination chemistry of +3 actinides. **S.A. Kozimor**

3:10 Intermission.



TECHNICAL PROGRAM

3:25 INOR 386. Synthetic chemistry for quantum information science. M.J. Amdur, M. Fataftah, D. Laurenza, L. Sun, C. Yu, J. Zadrozny, **D.E. Freedman**

3:50 INOR 387. Magnetic properties of heterometallic organometallics. T.P. Latendresse, G. Risica, C.M. Dickie, C.P. Burns, B.O. Wilkins, **M. Nippe**

4:15 INOR 388. Engineering multimetallic compounds to activate small molecules. **L.J. Murray**

4:40 INOR 389. What can we learn from the nuclear inelastic scattering of γ -rays? G.J. Long, **F. Grandjean**

5:05 Concluding Remarks.

Section C

Orange County Convention Center
Room W224A

Harry Gray Award for Creative Work in Inorganic Chemistry by a Young Investigator: Symposium in Honor of Jillian L. Dempsey

E. M. Matson, A. J. Miller, *Organizers*
N. Elgrishi, *Presiding*

1:30 INOR 390. Direct P(V)-ate to P(III) electrocatalytic conversions. **D.G. Nocera**, J.S. Elias, C. Cyrille

1:55 INOR 391. Chemistry from 3D printed objects. **M.R. Hartings**

2:20 INOR 392. Metal organic frameworks for electrocatalytic water oxidation. S. Lin, B.J. Gibbons, **A.J. Morris**

2:45 INOR 393. Understanding the photoacid sensitization cycle and cause of photovoltaic action in light-driven ion pumps. J. Glancy, S. Luo, R.N. Bhide, L. Schulte, W. White, L. Renna, **S. Ardo**

3:10 Intermission.

3:25 INOR 394. Interfacial chemistry as an enabling tool in the development of colloidal electrocatalysts. **B.M. Cossairt**, D. Henckel, D. Ung, T. Robison

3:50 INOR 395. Unravelling the complex excited-state dynamics of semiconductor nanocrystals. C. Mi, M. Saniepay, L.M. Janes, **R. Beaulac**

4:15 INOR 396. Developing a deeper understanding of the role of precursors and solvent in the synthesis of multinary transition metal chalcogenide nanoparticles for applications in photovoltaics. J. Lee, R.C. Miller, L.J. Moloney, **A.L. Prieto**

4:40 INOR 397. Ph-dependent optical bandgaps in cdse quantum dots. **E.A. Weiss**

Section D



TECHNICAL PROGRAM

Orange County Convention Center
Room W224C

ACS Award in Organometallic Chemistry: Symposium in Honor of Alan S. Goldman

R. G. Bergman, M. Brookhart, K. I. Goldberg, *Organizers*
J. F. Hartwig, *Organizer, Presiding*
N. Williams, *Presiding*

1:30 INOR 398. Bond activation reactions by boryl pincer complexes. Y. Cao, W. Shih, **O. Ozerov**

1:50 INOR 399. Multistep synthesis of a tridentate pi-donating pyridone pincer designed to drive C-H oxidative addition. **N. Williams**, E.R. Jarvo, L.A. Watson

2:10 INOR 400. Selectivity in the C-H and X-H bond activation of alcohols, amines, ketones, and esters by [Tp⁺RhL]. **W.D. Jones**, J. Yuwen, A. Olivares

2:30 INOR 401. Iridium PCP complexes: The importance of steric effects. **D.M. Heinekey**, T. Lekich, L.M. Guard

2:50 Intermission.

3:05 INOR 402. New Ir^{III} complexes for aerobic alkane dehydrogenation. S.B. Rubashkin, K.E. Kim, **K.I. Goldberg**

3:25 INOR 403. Pincer complexes for electrochemical dinitrogen fixation. **A.J. Miller**, B.M. Lindley, Q.J. Bruch

3:45 INOR 404. Empirical microkinetic modeling of enantioselective hydroformylation. **C.R. Landis**, A. Brezny

4:05 INOR 405. Metallacarbatranes and related compounds derived from tris[(1-isopropylbenzimidazol-2-yl)dimethylsilyl]methane. M. Rauch, M.J. Hammond, S. Ruccolo, **G. Parkin**

4:25 INOR 406. Selective functionalization of C-H bonds. **J.F. Hartwig**

Section E

Orange County Convention Center
Room W221C

Structure-Property Correlations in Functional Inorganic Materials

Materials design of functional oxides

J. A. Aitken, E. E. Rodriguez, *Organizers, Presiding*

1:30 INOR 407. Investigation of local distortions and long range polarity in pyrochlore oxides through cation and anion substitution. **G. Laurita**

2:00 INOR 408. Materials by Design: From conception to execution. **T.T. Tran**, Y. Lin, S. Thon, T. McQueen



TECHNICAL PROGRAM

2:20 INOR 409. Medium range 2D order and structural frustration in doped VO₂ revealed by diffuse x-ray scattering. M.A. Davenport, L.M. Whitt, M. Krogstad, S. Rosenkranz, R. Osborn, **J.M. Allred**

2:50 INOR 410. Role of solid state chemistry in the design of advanced heat reflecting color pigments: YInMn blues and beyond. **M. Subramanian**

3:20 Intermission.

3:50 INOR 411. Faceted rare earth and alkaline earth oxide perovskite nanoparticles as catalyst supports. **K.R. Poepelmeier**, R.J. Paull, Z.R. Mansley, R. Kennedy, L. Marks

4:20 INOR 412. Designing oxide perovskites that break corner sharing toward realizing polar materials. **A.M. Fry**

4:50 INOR 413. Phase manipulation and luminescence studies of gadolinium silicate nanoparticles for application in neuromodulation. **A.A. Dickey**, E. Zhang, S.H. Foulger, J.W. Kolis

5:10 INOR 414. Structure–property relationships in complex transition metal oxides for high-rate energy storage applications. **K.J. Griffith**, I. Seymour, C. Kocer, A.J. Morris, C.P. Grey

Section F

Orange County Convention Center
Room W224D

Through the Lens of Inorganic Chemistry: Understanding Heterogeneous Processes in Energy Conversion & Storage

S. Marinescu, V. Thoi, J. Y. Yang, *Organizers*
E. Miller, *Presiding*

1:30 INOR 415. Adiabatic and non-adiabatic electron transfer at heterogeneous dye-sensitized titanium dioxide interfaces. **G.J. Meyer**, L. Troian-Gautier, K. Hu, E. Piechota, R. Sampaio, C.P. Berlinguette

2:00 INOR 416. Tuning the surface and phase of 2D transition metal dichalcogenides for hydrogen generation. **E. Miller**

2:30 INOR 417. Chemistry of nano-structured oxides. **A. Vojvodic**

3:00 Intermission.

3:15 INOR 418. Direct electrodeposition of composite electrode films for rechargeable batteries: A tool for systematically studying degradation. M.C. Schulze, L.A. Kraynak, **A.L. Prieto**

3:45 INOR 419. Molecule-like trap states in halide perovskites: From solar-cell absorbers to white-light emitters. M.D. Smith, A. Jaffe, A. Lindenberg, **H. Karunadasa**

4:15 INOR 420. Halide ion mobility in mixed halide perovskites and its influence on photovoltaic performance. **P.V. Kamat**, R. Scheidt

Section G



TECHNICAL PROGRAM

Orange County Convention Center
Room W221D

ACS Award for Distinguished Service in the Advancement of Inorganic Chemistry: Symposium in Honor of Debbie C. Crans

Bioinorganic, Metallodrug, and Oxometalates

B. Baruah, N. E. Levinger, M. Lim, *Organizers*
E. S. Honig, *Presiding*

1:30 Introduction.

1:35 **INOR 421.** Speciation of vanadium anti-diabetic and anti-cancer drugs in biological media controls activities. **P. Lay**, A. Levina, D.C. Crans

2:00 **INOR 422.** Small molecule and biometal adjuvants for oncolytic immunotherapy. **J. Diallo**

2:25 **INOR 423.** Transition metal coordination complexes for MRI. **J.R. Morrow**, E.M. Snyder, D. Asic, A. Patel, C.J. Bond

2:50 **INOR 424.** Thirty plus years working with Debbie Crans. **G.R. Willsky**

3:15 Intermission.

3:30 **INOR 425.** “Smart” biodegradable nanocarriers and antibodies as targeting delivery vehicles for gold-based metallodrugs. **M. Contel**

3:55 **INOR 426.** Bis(maltolato)oxovanadium(IV) effects on luteinizing hormone receptor signal transduction. D. Althumairy, D.C. Crans, J. Pace, G. Barisas, **D. Roess**

4:20 **INOR 427.** All-inorganic metal oxido- and hydroxido-clusters with inorganic protection groups. **Y. Hayashi**, S. ., K. Kawamoto

4:45 **INOR 428.** Interactions of polyoxometalates with proteins. **C.C. McLauchlan**, D.C. Crans

5:10 **INOR 429.** Designing novel monocoordinated transition metal compounds towards versatile biological properties. **N. Barba-Behrensa**, R. Castro-Ramírez, J.L. Brumaghim, P. Gamez

Section H

Orange County Convention Center
Room W221E

ACS Award in Inorganic Chemistry: Symposium in Honor of George Christou

A. S. Veige, *Organizer, Presiding*



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- 1:30 INOR 430. MOF design to applications: Impact of pore system control on gas separations. **M. Eddaoudi**
- 1:50 INOR 431. Trinuclear, basic metal pyrazolates: Redox activity and electronic structure. **R.G. Raptis**, J. López-Plá, I. Chakraborty, E.V. Govor
- 2:10 INOR 432. Low-coordinate and low-oxidation state vanadium and chromium complexes. C.I. Wagner, **P.P. Power**
- 2:30 INOR 433. Zerovalent and divalent carbon compounds as donor ligands in coordination chemistry. P. Quinlivan, D. Shlian, E. Amemiya, S. Gulati, **G. Parkin**
- 2:50 INOR 434. Synthesis and structural characterization of new divalent lanthanide complexes. **G.S. Girolami**, N.T. Anderson
- 3:10 Intermission.
- 3:30 INOR 435. Mechanism of ni-photocatalyzed aryl etherification. R. Sun, Y. Qin, S. Rucolo, C. Schnedermann, C. Cyrille, **D.G. Nocera**
- 3:50 INOR 436. Activated diradicals: from small molecule bioreagents to nanomedicine applications and nanocatalysis of CO₂. **J.M. Zaleski**
- 4:10 INOR 437. From anion-pi interactions to radicals: Supramolecular chemistry meets magnetism. **K.R. Dunbar**
- 4:30 INOR 438. Understanding molecular shape in uranium tris(imido) species. K. Gettys, N. Anderson, M. Zeller, **S.C. Bart**
- 4:50 INOR 439. Uranyl oxo reduction and functionalisation by elements from across the periodic table. **P.L. Arnold**, B. Cowie, N. Bell, M. Zegke, J. Purkis, M. Dutkiewicz, B. Shaw, N. Magnani, J.B. Love, R. Caciuffo, O. Walter, N. Kaltsoyannis, S. Parsons

Section I

Orange County Convention Center
Room W232A

Chemistry at the Interface of Solution-processed Inorganic Materials

B. M. Cossairt, *Organizer*
A. B. Greytak, *Organizer, Presiding*
D. C. Lee, *Presiding*

1:30 Introductory Remarks.

1:35 INOR 440. Surface science of semiconductor nanocrystals. **P. Kambhampati**

2:00 INOR 441. Colloidal ii-vi semiconductor nanorods: Growth and assembly controlled by surface ligands. **D.C. Lee**

2:25 INOR 442. Surface chemistry of colloidal nanocrystals, from 0D to 2D. **Z. Hens**



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

2:50 INOR 443. Colloidal quantum dots for visible-light photo-redox catalysis. K.P. McClelland, Z. Zhang, E.A. Weiss

3:15 Intermission.

3:30 INOR 444. Novel low-dimensional tin halide compounds: structures, properties and perspective applications. M. Kovalenko

3:55 INOR 445. Lewis acid-base chemistry of doped silicon nanocrystals. N.R. Neale, R. Limpens, G.F. Pach

4:20 INOR 446. New developments in alkahest chemistry: Exploring the mechanisms of bulk material dissolution. R.L. Brutchey

Section J

Orange County Convention Center
Room W232B

Chemistry of Materials - Materials for Energy & Catalytic Applications

C. G. Lugmair, *Organizer*
O. Gunaydin-Sen, W. Zhang, *Presiding*

1:30 INOR 447. Mapping hot carrier extraction efficiency in plasmonic metal/metal oxide heterostructures. C. Tan, B. Sadtler

1:50 INOR 448. Chemical redox kinetics of LiFePO₄ using UV vis spectroscopy. D. Gupta, G. Koenig

2:10 INOR 449. Investigation of pillaring ti₃C₂T_x (MXene) with Al₁₃ Keggin ions. A.S. Rosas, S.F. Kim, M. Garcia Cervantes, T.E. Mallouk

2:30 INOR 450. Properties of bulk ammonia borane – polyethylene oxide hydrogen storage composites via thermal and spectroscopic (IR, NMR) techniques. O. Gunaydin-Sen, K. Kharel, R. Fu

2:50 Intermission.

3:05 INOR 451. Versatile strategy based on polydopamine surface chemistry to fabricate 3D conductive lithium metal anodes. W. Zhang, L. Qi, L. Shang, X. Li, D.A. Weitz

3:25 INOR 452. Metal-tetrametaphosphate polyanions: Synthesis, characterization, and electrochemical evaluation for sodium ion battery application. N.S. Alhaqbani

3:45 INOR 453. Antiferroelectric transition in an organic acid-base salt. J. Lengyel, X. Wang, E. Choi, T. Besara, R.U. Schoenemann, S.K. Ramakrishna, J. Holleman, L. Balicas, S. McGill, N.S. Dalal, M. Shatruk

4:05 INOR 454. Insights on the thermal and chemical stability of V₂CT_x MXene under different environments. R.K. Thakur, C.A. Carrero



TECHNICAL PROGRAM

Innovative Chemistry & Materials for Electrochemical Energy Storage

Supercapacitors

Sponsored by ENFL, Cosponsored by CATL, INOR and PMSE

Elucidation of Mechanisms & Kinetics on Surfaces

Experimental Surface Science

Sponsored by CATL, Cosponsored by ENFL, ENVR, INOR and PHYS

Undergraduate Research Posters

Inorganic Chemistry

Sponsored by CHED, Cosponsored by INOR and SOCED

MONDAY EVENING

Section A

Orange County Convention Center
West Hall C

Sci-Mix

S. A. Koch, N. S. Radu, *Organizers*

8:00 - 10:00

74, 170, 171, 173, 174, 178, 185, 186, 188, 191, 197, 198, 199, 210, 211, 212, 213, 218, 219, 220, 270, 271, 272, 273, 277, 287, 293, 295, 300, 303, 321, 327, 332, 334, 335, 344, 345, 352, 368. See previous listings.

670, 671, 678, 679, 680, 681, 686, 688, 689, 690, 695, 710, 711, 716, 717, 718, 736, 737, 740, 741, 748, 749, 750, 761, 763, 765, 767, 783, 827, 829, 831, 832, 917, 1023, 1125. See subsequent listings.

TUESDAY MORNING

Section A



TECHNICAL PROGRAM

Orange County Convention Center
Room W221A

Mechanistic Studies of Inorganic Reactions: A memorial Symposium for Elena Rybak-Akimova

I. V. Korendovych, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 INOR 455. De novo design of functional metalloproteins. **I.V. Korendovych**, O. Makhlynets

9:15 INOR 456. Development of nickel mediated aziridination reactions. D. Liu, J. Bacsá, **C.E. MacBeth**

9:45 Intermission.

10:00 INOR 457. Mechanistic insights into PCET by copper-oxygen species relevant to enzyme intermediates. **W.B. Tolman**

10:40 INOR 458. M(II)/O₂-dependent aliphatic carbon-carbon bond cleavage reactions. **L.M. Berreau**

11:10 INOR 459. Energy conversion mechanisms involving metal-oxyl radicals. T.P. Keane, **D.G. Nocera**

Section B

Orange County Convention Center
Room W224B

Magnetism Across Length Scales

Magnetism in Extended-Structure Solids

G. Christou, S. Hill, G. F. Strouse, *Organizers*
M. Shatruk, *Organizer, Presiding*
J. Chan, *Presiding*

8:30 Introductory Remarks.

8:35 INOR 460. Crystal growth and characterization of co-doped Ce₂Fe₄Sb₅. **J. Chan**

9:00 INOR 461. Expanding the *R-T* landscape: Magnetic properties of rare earth-transition metal compounds. **C.M. Thompson**, G. Agbaworvi

9:25 INOR 462. Understanding itinerant magnetism of CuFe_{2-x}Co_xGe₂ through chemical bonding analysis. **Z. Tener**, V. Yannello, S. Stoian, M. Shatruk

9:45 INOR 463. New Zintl phases featuring a layered structure with ferromagnetic ordering and negative magnetoresistance. K.P. Devlin, **S. Kauzlarich**



TECHNICAL PROGRAM

10:10 Intermission.

10:25 **INOR 464.** Magnetism of transition metals in intermetallics: Effects of cluster size. **S.E. Latturner**

10:50 **INOR 465.** Tuning the effective dimensionality of triangular-based magnetic lattices by control of stoichiometry. **V.O. Garlea**

11:15 **INOR 466.** Revisiting bond breaking and making in EuCo_2P_2 : Where are the electrons? **V. Yannello**, F. Guillou, A. Yaroslavtsev, Z. Tener, F. Wilhelm, A. Yaresko, S. Molodtsov, A. Scherz, A. Rogalev, M. Shatruck

11:35 **INOR 467.** Low-dimensional metal halide-formates: Synthesis, crystal growth, structure, and magnetism. **K. Kovnir**

Section C

Orange County Convention Center
Room W224A

Small Molecule Activation for Oxidative & Reductive Catalysis

Models and Concepts in Small Molecule Activation

J. J. Concepcion, *Organizer*
J. D. Blakemore, *Organizer, Presiding*
J. Concepcion, *Presiding*

8:30 Introductory Remarks.

8:35 **INOR 468.** Developing scaling relationships to understand and improve molecular electrocatalysis. **J.M. Mayer**, D. Martin, M. Pegis, C. Wise, B. Koronkiewicz, A. Brezny

9:05 Discussion.

9:10 **INOR 469.** Small molecule reduction by molecular Al(III) complexes: Reactions of organohydrides. **L.A. Berben**, T.J. Sherbow, E.J. Thompson, A. Arnold

9:35 Discussion.

9:40 **INOR 470.** H_2 evolution catalysis with diverse $[\text{Cp}^*\text{Rh}]$ complexes: A thermochemical approach. **D. Lionetti**, Y. Peng, J.A. Hopkins, E. Boyd, W. Henke, V. Day, J.D. Blakemore

10:05 Discussion.

10:10 Intermission.

10:30 **INOR 471.** Mechanisms of molecular catalysis of CO_2 and O_2 electroreduction with metalloporphyrins. **C. Cyrille**

11:00 Discussion.



TECHNICAL PROGRAM

11:05 INOR 472. Small molecule activation with manganese(I) and (II) complexes. **D.C. Lacy**

11:30 Discussion.

11:35 INOR 473. *Operando* x-ray spectroscopy reveals the active form of an HER-active electrocatalyst. **B. Lassalle-Kaiser**, A. Zitolo, E. Fonda, M. Robert, E. Anxolabehere-Mallart

12:00 Discussion.

Section D

Orange County Convention Center
Room W224C

Alfred Bader Award in Bioinorganic or Bioorganic Chemistry: Symposium in Honor of Joan B. Broderick

J. Betz, *Organizer*
S. R. Smith, *Organizer, Presiding*

8:30 Introductory Remarks.

8:40 INOR 474. Zinc receptors in control of cell fate decisions. **T.V. OHalloran**

9:10 INOR 546. Anatomy of a radical SAM enzyme. **C.L. Drennan**

9:40 INOR 476. Insights regarding how *H. pylori* HypA protein acts as a nickel traffic cop. **M.J. Maroney**, H.Q. Hu, H. Huang, P. Basak

10:10 Intermission.

10:30 INOR 477. Mechanism of nitrogen fixation by nitrogenase. **B.M. Hoffman**

11:00 INOR 478. Electron flow through multicopper oxidases. **H.B. Gray**, J. Shin, J.R. Winkler

Section E

Orange County Convention Center
Room W221C

Francis P. Garvan_John M.Olin Medal-Olin Medal: Symposium in Honor of Lisa McElwee-White

L. J. Murray, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 INOR 479. Surface chemistry controlled synthesis and performance of metal and metal-like nanoparticles. **J. Millstone**



TECHNICAL PROGRAM

9:05 INOR 480. Looking for inspiration in colloidal solutions from the ages: Synthesis of plasmonic nanomaterials. **C.J. Murphy**

9:35 INOR 481. AACVD of metal oxides: from precursor synthesis to TCOs, photocatalysts and superhydrophobic materials. **C.J. Carmalt**

10:05 Intermission.

10:20 INOR 482. Transforming 2D films into 3D surfaces. **T.W. Odom**

10:50 INOR 483. N-Heterocyclic Carbenes as ligands for metal surfaces including flat(111) surfaces, nanoparticles and nanoclusters: Implications in SAM formation, Catalysis, atomic layer processing (deposition and etch) and sensing.. **C.M. Crudden**

11:20 INOR 484. Using surface chemistry to direct the morphology and deposition of thin films and nanoobjects of materials for electronics and energy applications. **A.V. Walker**

11:50 INOR 485. Germanium nanocages and nanoparticles from a microwave-assisted galvanic replacement reaction with Ag nanoparticles. X. Qi, **S. Kauzlarich**

Section F

Orange County Convention Center
Room W224D

Through the Lens of Inorganic Chemistry: Understanding Heterogeneous Processes in Energy Conversion & Storage

S. Marinescu, V. Thoi, *Organizers*
J. Y. Yang, *Organizer, Presiding*

8:30 INOR 486. Activity descriptors for molecular hydrogen evolution electrocatalysts. B. Ceballos, D.W. Cunningham, **J.Y. Yang**

9:00 INOR 487. Interplay between homogeneous coordination complexes and surface-adsorbed films in fuel-production catalysis. **J.L. Dempsey**, K.J. Lee, K. Lodaya

9:30 INOR 488. Modelling surface nitrides with macrocycle-supported cluster chemistry. **N.C. Tomson**

10:00 Intermission.

10:15 INOR 489. Surface-mounted cluster catalysts: dynamic ensemble nature, and dominance of rare metastable sites in defining catalytic activity, selectivity, and durability. **A. Alexandrova**

10:45 INOR 490. Homogeneous catalysis meets heterogeneous catalysis: Alkanes and alkenes transformations. Z. Syed, D.M. Kaphan, M. Ferrandon, C. Liu, A.J. Kropf, F. Perras, M. Pruski, **M. Delferro**

11:15 INOR 491. Managing reactivity of hydrides in CO₂ reduction to formate with [Fe₄N(CO)₁₂]. **L.A. Berben**, A. Taheri, D.B. Cluff, N.D. Loewen



TECHNICAL PROGRAM

Section G

Orange County Convention Center
Room W221D

ACS Award for Distinguished Service in the Advancement of Inorganic Chemistry: Symposium in Honor of Debbie C. Crans

Organometallics, Catalysis, and Photoactivity

B. Baruah, N. E. Levinger, M. Lim, *Organizers*
G. Eaton, *Presiding*

8:00 Introduction.

8:05 **INOR 492.** Catalytic studies of cobalt-containing complexes for hydrogen generation: Cheaper but challenging. **A. Holder**, M. Celestine, J.L. Bullock, B.W. Legere, N.K. Evaristo, J.K. Knarr, K.N. Burley, H.M. Maass

8:30 **INOR 493.** Synthesis of ureas by oxovanadium(v)-catalyzed carbon dioxide activation. **T. Moriuchi**

8:55 **INOR 494.** V-catalysed bromination of tetrapyrrolic rings. **V. Conte**, P. Galloni, G. Pomarico

9:20 Intermission.

9:35 **INOR 495.** Template based chromium doped manganese oxide nanostructures: Hydrothermal synthesis and catalytic studies for the mild oxidation of organic compounds. **A. Altaf**, **A. Badshah**

10:00 **INOR 496.** Application of N-heterocyclic carbene complexes in bio-inspired catalysis. **F.E. Kuehn**

10:25 **INOR 497.** Redox-promoted reactions of organometallic complexes, and Debbie Crans' many great contributions to the field of Inorganic Chemistry. **B.T. Donovan-Merkert**

10:50 **INOR 498.** Carbenes and phosphalkenes-reactivity and applications in photoactive materials. **J.D. Protasiewicz**

11:15 **INOR 499.** Debbie Crans, bio-inorganic chemistry, and an actinide connection. **J.L. Kiplinger**

11:40 **INOR 500.** Vanadium complexes in oxidation catalysis: Metal-ligand cooperation. **A. Pombeiro**

Section H

Orange County Convention Center
Room W221E

Chemistry of Materials - Metal Organic Frameworks

C. G. Lugmair, *Organizer*
J. A. Byers, Q. Zhang, *Presiding*



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- 8:30 INOR 501. Multivariate zirconium MOFs for tuneable redox activity. **G. Pour**, F.J. Uribe-Romo
- 8:50 INOR 502. Doping of metal-organic frameworks towards electronics. J. Calvo, A. Talin, V. Stavila, M. Allendorf, **M.C. So**
- 9:10 INOR 503. Hierarchically porous zirconium metal-organic framework: facile synthesis, characterization and applications. **Q. Zhang**
- 9:30 INOR 504. Spin-switchable Hofmann-type networks based on tetrakis(cyanoacetylides): Larger pores for larger guests. **D. Müller**, C. Knoll, J.M. Welch, G. Giester, M. Reissner, P. Weinberger
- 9:50 INOR 505. Stilbene-based metal-organic frameworks: synthesis, structure, photoluminescence and CO₂ adsorption properties. **S.T. Golafale**, C.W. Ingram
- 10:10 Intermission.
- 10:25 INOR 506. Metal-organic frameworks with single-component white-light-emission. **A. Peedikakkal**
- 10:45 INOR 507. Synthesis and characterization of materials for proton conduction studies. **P.O. Adelani**
- 11:05 INOR 508. Illuminating the growth of metal-organic nanotubes through isorecticular synthesis and liquid-cell transmission electron microscopy. **K.M. Vailonis**, K. Gnanasekaran, X.B. Powers, D.M. Jenkins, N.C. Gianneschi
- 11:25 INOR 509. Photocatalytic applications from visible-light responsive metal-organic framework systems. **K. Stylianou**
- 11:45 INOR 510. Using aperture opening events in UiO-66 to encapsulate organometallic catalysts for CO₂ conversion. **J.A. Byers**, C. Tsung, Z. Li, T.M. Rayder, E. Adillon

Section I

Orange County Convention Center
Room W232A

Chemistry at the Interface of Solution-processed Inorganic Materials

A. B. Greytak, *Organizer*
B. M. Cossairt, *Organizer, Presiding*
S. L. Brock, *Presiding*

8:30 Introductory Remarks.

- 8:35 INOR 511. In situ studies of nanocrystal nucleation and growth. M. Greenberg, M. Campos, B. Abecassis, S. Ghose, **J.S. Owen**
- 9:00 INOR 512. Colloidal chemistry in molten inorganic salts. V. Srivastava, V. Kamysbaev, N.B. Ludwig, M.H. Hudson, E. Dunietz, S. Vaikuntanathan, **D. Talapin**
- 9:25 INOR 513. Colloidal indium nitride nanocrystals as nanoscaled charge-storage units, and the origin of the quantum-confinement resilience effect. Z. Liu, L.M. Janes, M. Saniepay, **R. Beaulac**



TECHNICAL PROGRAM

9:50 Intermission.

10:05 INOR 514. X-type ligand displacement at CdSe quantum dot surfaces promoted by addition of charge carriers. **J.L. Dempsey**, C. Hartley

10:30 INOR 515. Between the sheets: Post-synthetic transformations in halide perovskites. M.D. Smith, I. Smith, A. Slavney, A. Saldivar Valdes, **H. Karunadasa**

10:55 INOR 516. Sol-gel assembly of quantum dots: Creating and modifying interfaces for redox stability and facilitated carrier transport. L. Mawella Vithanange, L. Silva, I. Hewavitharana, J. Davis, **S.L. Brock**

Section J

Orange County Convention Center
Room W232B

Nobel Laureate Signature Award for Graduate Education in Chemistry: Symposium in Honor of Bryan M. Hunter & Harry Gray

M. G. Hill, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 INOR 517. Solar hydrogen and a path from Gray to green. **R. Eisenberg**

9:05 INOR 518. Sustainable energy reactions as probed by electron paramagnetic resonance. **R.D. Britt**

9:35 INOR 519. Luminescent tungsten arylisocyanide complexes. **J.R. Winkler**, J. Fajardo

10:05 Intermission.

10:20 INOR 520. Protonated metallocenes as extremely reactive PCET reagents. **J.C. Peters**

10:50 INOR 521. Electrochemical reshaping of living tissues: Non-invasive surgical modalities for reshaping cartilage and cornea. **M.G. Hill**

11:20 INOR 522. **Award Address** (Nobel Laureate Signature Award for Graduate Education in Chemistry sponsored by Avantor™ Performance Materials, Inc.). Trapping an iron(VI) water-splitting intermediate in nonaqueous media. **B.M. Hunter**, H.B. Gray

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TECHNICAL PROGRAM

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TUESDAY AFTERNOON

Section A

Orange County Convention Center
Room W221A

Mechanistic Studies of Inorganic Reactions: A memorial Symposium for Elena Rybak-Akimova

I. V. Korendovych, *Organizer, Presiding*

1:30 INOR 523. Double dawson cluster on the ribosome. **D.C. Crans**, C.C. McLauchlan

2:10 INOR 524. Metal-oxido and hydroxido complexes: Intermediates in water oxidation and dioxygen activation. **A. Borovik**

2:50 INOR 525. Kinetic isotope effects in the non-heme Fe oxygenase factor inhibiting HIF (FIH). **M. Knapp**, V.D. Chaplin, J. Hangasky



TECHNICAL PROGRAM

3:20 Intermission.

3:35 **INOR 526.** Regioselective radical trifluoromethylation via photoinduced Co–CF₃ bond activation. **J.D. Soper**

4:05 **INOR 527.** Phosphinidene transfer reactions of anthracene-supported phosphinidene transfer reagents. W. Transue, M. Geeson, **C.C. Cummins**

Section B

Orange County Convention Center
Room W224B

Magnetism Across Length Scales

Magnetism in Nanomaterials

S. Hill, *Organizer*
M. Shatruk, G. F. Strouse, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 **INOR 528.** Chemical synthesis of magnetically hard rare-earth metal nanoparticles. **S. Sun**

2:05 **INOR 529.** Magnetic nanoparticles as recoverable catalysts and catalysts supports: Reduced iron nanoparticles as a versatile platform. **A.H. Moores**, J. Terra

2:35 **INOR 530.** Magnetic nanoclusters and nanoparticles. **G.C. Hadjipanayis**, F.M. Abel, O. Tosun, S. Pourmiri, D.J. Sellmyer, R. Skomski, B. Balasubramanian, V. Tzitzios

3:05 Intermission.

3:20 **INOR 531.** Advanced magnetic x-ray spectro-microscopy - a path towards studying novel spin textures at fundamental magnetic length and time scales. **P. Fischer**

3:50 **INOR 532.** Extracting structure-property correlations from colloiddally-prepared, magnetoresistive ferrites. **J.D. Rinehart**, B. Zhou

4:20 **INOR 533.** Effects of Zn doping and vacancy formation on the magnetic properties and magnetocaloric effect in MnCoGe. **Y. Wang**, V. Yannello, H. Zhang, Y. Long, M. Shatruk

4:40 **INOR 534.** Unconventional magnetic behavior of La_{0.4}Ce_{0.6}Co₂P₂. **J. Roth**, K. Kovnir, X. Tan, A. Yaroslavtsev, C.M. Thompson, O. Garlea, A. Menushenkov, A. Arico, M. Shatruk

Section C

Orange County Convention Center
Room W224A



TECHNICAL PROGRAM

Small Molecule Activation for Oxidative & Reductive Catalysis

Ligand Effects and Electron Transfer

J. J. Concepcion, *Organizer*
J. D. Blakemore, *Organizer, Presiding*
J. Concepcion, *Presiding*

1:30 Introductory Remarks.

1:35 INOR 535. Utilizing the secondary coordination sphere to enable small molecule catalysis. **J.Y. Yang**

2:00 Discussion.

2:05 INOR 536. Pyridinol-based CNC Pincer catalysts for carbon dioxide reduction: The big impact of one small remote group. **E.T. Papish**, S. Das, C.M. Boudreaux, D.B. Burks, R.R. Rodrigues, C.E. Webster, J.H. Delcamp

2:30 Discussion.

2:35 INOR 537. Electrophile reactivity with an intermediate ruthenium complex in catalytic CO₂ reduction. **M.D. Massey**, I.P. Mercer, C.K. Schauer

3:00 Discussion.

3:05 Intermission.

3:25 INOR 538. Unraveling intramolecular electron transfer kinetics in dyad ruthenium photocatalysts. **P. Farras**, S. Hennessey, A.D. Llobet

3:50 Discussion.

3:55 INOR 539. Redox hopping electron transport toward efficient electrocatalysis by metal-organic frameworks. P. Celis-Salazar, M. Cai, **A.J. Morris**

4:20 Discussion.

4:25 INOR 540. Mechanism of heterogeneous water oxidation catalysis by [Ru(bda)(L)₂]. **R. Sampaio**, Y. Xie, E. Fujita, J.J. Concepcion

4:50 Discussion.

4:55 INOR 541. Photo- and electro-catalytic transformations of small molecules using well-defined coordination complexes. **J. Lloret Fillol**

5:20 Discussion.

Section D



TECHNICAL PROGRAM

Orange County Convention Center
Room W224C

Alfred Bader Award in Bioinorganic or Bioorganic Chemistry: Symposium in Honor of Joan B. Broderick

J. Betz, S. R. Smith, *Organizers*
D. P. Ballou, *Presiding*

1:30 Introductory Remarks.

1:35 **INOR 542.** Moving beyond methionine synthase: New insights into cobalamin-dependent methyltransferase reactions. **S. Booker**

2:05 **INOR 543.** New role for an old cofactor. M. Pandelia, A. Arcinas, M.I. Radle, N. Lanz, **C. Krebs**, S.J. Booker, B. Zhang

2:35 **INOR 544.** Chemistry of diphthamide biosynthetic radical SAM enzymes. **H. Lin**

3:05 Intermission.

3:30 **INOR 545.** Electrochemical conversations with AdoMet radical enzymes. **S.J. Elliott**, L.M. Walker, S. Bonitatibus

4:00 **INOR 475.** Frontiers in ribonucleotide reductases: nucleotide-dependent control of quaternary structure and enzyme activity. **J. Stubbe**, C.L. Drennan, N. Ando, Y. Aye, Q. Lin, E. Brignole, G. Kang, F. Asturias

Section E

Orange County Convention Center
Room W221C

Francis P. Garvan_John M.Olin Medal-Olin Medal: Symposium in Honor of Lisa McElwee-White

L. J. Murray, *Organizer, Presiding*

1:30 **INOR 547.** Cooperative bond activation across metal-metal multiple bonds and catalytic applications of early/late heterobimetallic complexes. **C.M. Thomas**, K.M. Gramigna

2:00 **INOR 548.** Taming nitrene reactivity with silver: Construction (and destruction!) of *N*-heterocycles. **J.M. Schomaker**

2:30 **INOR 549.** Catalytic carbonyl-olefin metathesis and oxygen atom transfer. **C. Schindler**

3:00 Intermission.

3:15 **INOR 550.** Building cyclic peptides via a dehydroamino acid approach. **V.M. Dong**

3:45 **INOR 551.** Kinetic and mechanistic understanding of oxidative addition and reductive elimination of Pt(II) and Pt(IV) complexes. **J. Love**



TECHNICAL PROGRAM

4:15 INOR 552. Guide to supramolecular and transition metal coordination chemistry. **K. Bowman-James**

4:45 INOR 810. Expanding the surface of carbon bowls: Is it better for multiple metal binding? **M.A. Petrukhina**

Section F

Orange County Convention Center
Room W224D

Solid-State Inorganic Chemistry

V. Poltavets, *Organizer*
S. Bobev, F. Ramezanipour, *Presiding*

1:30 INOR 554. Metal flux synthesis and effects of Eu/Ca ratio on structure type and magnetism of Ca/Eu/Mg/Si Zintl phases. **J. Haddock**, S. Latturmer

1:50 INOR 555. Experimental study of the lithiation of Si- and Ge-based type-I clathrates. **S. Bobev**

2:10 INOR 556. Paths to stabilizing electronically aberrant compounds: A defect-stabilized polymorph and constrained atomic motion in PtGa₂. **H. Mitchell Warden**

2:30 INOR 557. Intermetallic carbides and borides grown from Pr/Ni flux. **T.O. Engstrand**

2:50 INOR 558. High pressure synthesis and characterization of the new $J_{\text{eff}}=1/2$ pyrochlores A₂Rh₂O₇ (A = Y, Lu). **C. Wiebe**, A. Hallas, A. Sharma, C. Mauws, H. Zhou, M. Tachibana, G. Luke

3:10 Intermission.

3:25 INOR 559. Controlling the negative thermal expansion and response to pressure in ReO₃-type fluorides by the deliberate introduction of excess fluoride: Mg_{2-x}Zr_xF_{4+2x}. **S.J. Baxter**, B. Hester, A.P. Wilkinson

3:45 INOR 560. Tuning the magnetic properties by manipulation of the oxygen-vacancies in oxygen-deficient perovskites. **F. Ramezanipour**, R.K. Hona, A. Huq

4:05 INOR 561. Temperature tunability in doped Sr_{1-x}Ca_xFeO₃ for rapid reversible oxygen uptake and release. **E.J. Popczun**, D. Tafen, Y. Zhou, S. Natesakhawat, D. Alfonso, J.W. Lekse

4:25 INOR 562. First principles investigation of metal-insulator transitions in rare earth nickelates induced by chemical doping. P. Yoo, S. Yao, **P. Liao**

4:45 INOR 563. Effect of vacancy order on the structure and charge-transport of oxygen deficient perovskites. **R.K. Hona**

5:05 INOR 564. Oxygen-release behaviors in B-site-layer-ordered/disordered perovskites Ca₂FeMnO₆ with unusually high valence Fe⁴⁺. **M. Goto**, T. Saito, Y. Shimakawa

Section G



TECHNICAL PROGRAM

Orange County Convention Center
Room W221D

ACS Award for Distinguished Service in the Advancement of Inorganic Chemistry: Symposium in Honor of Debbie C. Crans

Physical-inorganic, Nano-materials, Polyoxometalate and Photophysical studies

B. Baruah, N. E. Levinger, M. Lim, *Organizers*
M. D. Johnson, *Presiding*

1:30 Introduction.

1:35 **INOR 565.** Langmuir monolayers and Brewster angle microscopy for the analysis of the molecular conformations of insulin. **A. Sostarecz**

2:00 **INOR 566.** Measuring ionic strength in a nanodroplet one story of how debbie crans greatly expanded my horizon. **N.E. Levinger**, E. Gaudamauskas, D.C. Crans

2:25 **INOR 567.** Chemistry in confinement. **M.D. Johnson**

2:50 **INOR 568.** Electron spin relaxation of vanadium(IV) complexes. **S. Eaton**, T. Ngendahimana, G.R. Eaton, C. Lin, J. Zadrozny

3:15 Intermission.

3:30 **INOR 139.** Neutron scattering in the studies of molecular magnetism. **Z. Xue**, S. Stavretis, D.H. Moseley, Y. Cheng, L.L. Daemen, C.M. Brown, A.A. Podlesnyak, X. Wang, C. Hoffmann, A.J. Ramirez-Cuesta, T. Chang, Y. Chen, F. Fei, H. Cui, X. Chen, Z. Zhu, M. Guo, J. Tang

3:55 **INOR 570.** Luminescent oligothiophene-, naphthalimide- and carbazole-based lanthanide ion complexes. **A. De Bettencourt Dias**

4:20 **INOR 571.** Isomerization in Ru and Os polypyridine complexes containing chelating phosphine sulfoxide ligands. **J. Rack**

4:45 **INOR 572.** Does polyoxometalate speciation involve soft-oxometalates? **S. Roy**

5:10 **INOR 573.** Polyoxometalate capped gold nanoparticles: SERS application. **B. Baruah**

Section H

Orange County Convention Center
Room W221E

Structure-Property Correlations in Functional Inorganic Materials

J. A. Aitken, E. E. Rodriguez, *Organizers, Presiding*



TECHNICAL PROGRAM

1:30 INOR 574. Comparison of structure, properties, and electrocatalytic activity of phosphorus-rich metal phosphides. **E.G. Gillan**, A. Flores, M.D. Lovander

1:50 INOR 575. Pd solubility in transition metal carbides and their catalytic activity for the methanol oxidation reaction. **B.M. Leonard**, J.M. Thode

2:10 INOR 576. Dimensional control over the oxidation state of Mn ions in SrTiO₃. W. Harrigan, H. Mansoor, **K.R. Kittilstved**

2:30 INOR 577. Solid-solution semiconductors: Compositional tuning of metal oxides for the capture and conversion of solar energy. **P.A. Maggard**

2:50 INOR 578. Oxygen vacancy induced defect spin centers by design in single crystals of Ba₂CaWO₆. **M. Sinha**, T.J. Pearson, W. Phelan, T.T. Tran, T. Reeder, D.E. Freedman, T. McQueen

3:10 Intermission.

3:30 INOR 579. Chemistry of tetrel pnictides: Benefits and challenges of frameworks composed of elements of drastically different reactivities. **K. Kovnir**

3:50 INOR 580. Ultralow thermal conductivity and high thermoelectric performance in a new composite structure. **H. Kleinke**

4:10 INOR 581. Yb_{2-x}A_xCdSb₂ (A = Ca, Sr): Zintl phases with low thermal conductivity and high Seebeck coefficient. **K.P. Devlin**, S. Kauzlarich

4:30 INOR 582. Crystal growth and characterization of bismuth-doped topological LnSbTe (Ln = La, Ce, Pr). **A. Weiland**, D.G. Chaparro, J. Chan

4:50 INOR 583. How magnetism and structure couple in magnetocaloric materials. **J.D. Bocarsly**, S.D. Wilson, R. Seshadri

5:10 INOR 584. Cerium/copper flux synthesis of new cerium borocarbides. **M.B. Hertz**, S. Lattuner, R.E. Baumbach, Y. Lai

Section I

Orange County Convention Center
Room W232A

Chemistry at the Interface of Solution-processed Inorganic Materials

B. M. Cossairt, *Organizer*

A. B. Greytak, *Organizer, Presiding*

O. Chen, *Presiding*

1:30 Introductory Remarks.



TECHNICAL PROGRAM

1:35 INOR 585. Complex role of PVP in shape-controlled growth of Ag nanocubes: Structure directing agent, stabilizer, reducing agent and more. S. Jharimune, Z. Chen, R. Pfukwa, J. Chang, B. Klumperman, **R.M. Rioux**

2:00 INOR 586. Synthesis and self-assembly of anisotropic ‘patchy’ nanocrystals. **O. Chen**

2:25 INOR 587. Toward atomic precision in nanoscience. **R. Jin**

2:50 Intermission.

3:05 INOR 588. Towards functional assemblies of ligand-stabilized gold nanoclusters. **H. Hakkinen**

3:30 INOR 589. System-level control of structural hierarchy. **R. Macfarlane**

3:55 INOR 590. Symmetry breaking in seeded growth of metal nanocrystals. **S.E. Skrabalak**

Section J

Orange County Convention Center
Room W232B

Organometallic Chemistry: New Ligand Platforms

N. S. Radu, *Organizer*
D. Tapu, *Presiding*

1:30 INOR 591. New ferrocene-based N-heterocyclic carbenes: simple and versatile ligand platform. **A.V. Polezhaev**, I. Nikovskiy, A. Pavlov, V. Novikov, Y. Nelyubina

1:50 INOR 592. Computational insights into the manipulation of the ground and excited states of iridium(III) complexes via benzannulation. **L. Lystrom**, B. Liu, W. Sun, S. Kilina

2:10 INOR 593. Towards asymmetric catalytic aziridination by design of C_2 symmetric tetra-NHC complexes. **J. DeJesus**, S.B. Isbill, N.L. Dominique, R.W. Ozburn, S. Roy, D.M. Jenkins

2:30 INOR 594. New architectures in the chemistry of polyNHCs: Synthesis and coordination. **D. Tapu**

2:50 INOR 595. Synthesis and coordination chemistry of pyridine-phosphaalkene ligands: An entry point into new dearomatized Ru(II) complexes? **M.F. Cain**, M.L. Nakashige

3:10 INOR 596. Preparation and reactivity of cobalt-nitrenoid species supported by anionic PNP pincer ligands. **V. Krishnan**, I. Davis, A. Liu, Z.J. Tonzetich

3:30 INOR 597. Synthesis, structure, and reactivity of pincer complexes featuring an all phosphorous donor set ligand with a pyrrole-derived backbone. **M.N. Cosio**

3:50 INOR 598. Synthesis of metal-phosphine complexes containing redox-active “hydride relays” for efficient hydrogenation catalysis. **C. Zall**, N. Garcia, N. Devi, W. Fernandez



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

4:10 INOR 599. Structure-activity relationships of highly tuneable phosphonic diamide-phosphine ligands for Ni and Pd catalyzed functional polyethylene synthesis. **J. Brandt**, B.P. Carrow

4:30 INOR 600. Electrochromic ligand platforms involving the 6,6'-biazulenene core. **M.V. Barybin**

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Innovative Chemistry & Materials for Electrochemical Energy Storage

Beyond Li-Ion

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Light-Driven Chemistry: Photoelectrochemistry & Photocatalysis



TECHNICAL PROGRAM

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TUESDAY EVENING

Section K

Orange County Convention Center
West Hall C

Chemistry at the Interface of Solution-processed Inorganic Materials

Chemistry at the Interface of Solution-processed Inorganic Materials

B. M. Cossairt, A. B. Greytak, *Organizers*

5:30 - 7:30

INOR 601. Thermochemical characterization of synthetic strategies for the triangulated kagome lattice (TKL) material $\text{Cu}_9\text{X}_2(\text{cpa})_6$. **J.D. Taylor**, L.R. Reid, S.F. Skinner, J.H. Lovett, J.C. Lupton, J. Moses, B.M. Ortolano, R.A. Coro, S.D. Richardson, L.W. Ter Haar

INOR 602. Expanding the tool box for the preparation of complex transition metal phosphide (TMP) nanoparticles: Evaluating phosphidation rates in binary TMP phases. **T.P. Su'a**, M.N. Poli, S.L. Brock

INOR 603. Identification of chemical parameters that govern the kinetics of oxidative assembly: Establishing a chemical toolbox for programmed assembly of metal chalcogenide nanoparticles. **K.L. Silva**

INOR 604. Effect of oxidative gelation on the redox stability of metal chalcogenide gels: Modification of nanoparticle-nanoparticle dichalcogenide interfaces obtained from the oxidative gelation mechanism. **L. Mawella Vithanage**, S.L. Brock

Section K

Orange County Convention Center
West Hall C

Chemistry of Materials

C. G. Lugmair, *Organizer*

5:30 - 7:30

INOR 605. One step synthesis of N-C-SiO₂ composite aerogels and their adsorption property for cigarette smoke. **S. Chai**, G. Zan, Y. Ding, Q. Wu

INOR 606. Stabilization of mononuclear and dinuclear rhodium clusters on layered niobate and titanate supports. **R. Uppuluri**, A.S. Rosas, T.E. Mallouk



TECHNICAL PROGRAM

INOR 607. Investigation of structure-property relationship in a family of uranyl tetrahalides paired with substituted methylpyridinium cations. **N. Byrne**, R.G. Surbella, C.L. Cahill

INOR 608. Measurements of binary adsorption isotherm on MIL-53: A rigid and flexible material. **H. Nguyen**, L. Espinal, R. van Zee

INOR 609. Porous molecular crystals supported by interdigitated yet dispersive non-covalent bonds. **T. Kang**, H. Kim, S. Jeoung, Y. Park, D. Moon, H. Moon, D. Lee

INOR 610. Thermodynamics and up-conversion of Cr³⁺/Ho³⁺ co-doped 12CaO.7Al₂O₃ synthesized in argon. S. Liao, J. Cai, Y. Liu, **Y. Min**

INOR 611. Dramatically improved reversible oxygen binding in a bimetallic metal-organic framework. **R.M. Torres-Gavosto**, H.Z. Jiang, K. Chakarawet, L.E. Darago, D.A. Reed, J.R. Long

INOR 612. Synthesis of octa-cyanopropylsilsesquioxane cage structure and the electrorheological effects. **J.R. Omambala**

INOR 613. Rapid detection of the chemotherapeutic agents by a water stable luminescent metal-organic framework. **J. Ren**, C. Stackhouse, S. Ma

INOR 614. Designing mn-doped semiconductor nanocrystals generating hot electrons under visible light excitation. **D.G. Parobek**

INOR 615. Cyclodextrin-containing metal-organic frameworks (CD-MOFs) for highly efficient toxicant removal applications. **A. Yonchak**, D. Jones, M. Levine

INOR 616. Heat-up synthesis of colloidal pyrite CuSe₂ nanocubes and magnetic CuCr₂Se₄ nanorods. **F. Akbari Afkhami**, A. Gupta

INOR 617. Tunable electrical conductivity in metal-organic framework powders. **J. Calvo**, M.C. So

INOR 618. Earth-abundant and biocompatible alkali pnictogen dichalcogenide colloidal semiconductor nanocrystals. **B. Rosales**, M. White, J. Vela

INOR 619. Highly stable gold nanoparticles within a polymer particle template and their multi-catalytic properties. **P.N. Eyimegwu**, W. Jang, R. Taylor IV, H. Byun, J. Kim

INOR 620. Simple method for processing ph-responsive cotton fabric sensor. **T.O. Salami**

INOR 621. Detoxification of chemical warfare agents by using functionalized graphene-based composite. **S. Jang**, H. Jung, H. Jung, Y. Jin

INOR 622. Facile method to create hierarchically porous metal-organic frameworks. **Q. Wang**

INOR 623. Molecular beam epitaxy of transition metal dichalcogenides. **P.L. Garrett**, A. Roy, S. Banerjee

INOR 624. Surface alteration of aluminum alloy: Graphene protection and corrosion test. **B. Baruah**



TECHNICAL PROGRAM

- INOR 625.** Insights into the flexibility of ZIF-7 and its impact on adsorption. **B. Wooler**, Y. Du, M. Nines, K. Mao, P. Kortunov, C. Paur, J. Zengel, S. Weston, P. Ravikovitch
- INOR 626.** Pyridinethiolate heterobimetallic precursors to 10-14 binary intermetallics. **C. Daniels**, J. Vela
- INOR 627.** Fabrication of metal-organic graphene analogue materials using langmuir-blodgett method. S. Yoon, D.Y. Sasaki, **M.C. So**
- INOR 628.** Synthesis and characterization of an improved nanocomposite cathode materials for Li-ion batteries. **C. Otero Velez**, S. Nieto Ramos
- INOR 629.** Wettable PVDF nanofiber composite for separator technology. **D.B. Dwyer**, E. Mera, W. Bernier, W.E. Jones
- INOR 630.** Fluoride detection with redox-active metal–organic frameworks. **H. Wentz**, M.G. Campbell
- INOR 631.** Post synthetically modified covalent organic frameworks as an effective heterogenous catalyst for modified Mannich type reactions.. **H. Vardhan**
- INOR 632.** Highly conjugated amino and phenyl-ethynyl linkers for photocatalytic titanium-based metal organic frameworks. **A. Almonte**, D.A. Vazquez-Molina, D. Fairchild, F.J. Uribe-Romo
- INOR 633.** Efficient MOF-sensitized solar cells made of [100]-oriented pillared porphyrin framework films. **M.A. Gordillo Varela**, D. Panda, S. Saha
- INOR 634.** Energy transfer in a novel light-harvesting luminescent metal-organic framework. **A. Khatun**
- INOR 635.** Preparation of functional nanocomposites from layered zirconium phosphates. **E. Snyder**, B.M. Mosby
- INOR 636.** Evaluation of diazonium gold(III) salts in forensic chemistry: Latent fingerprint development on metal surfaces. A. Ahmad, A. Alawadhi, J. Park, **H. Abdou**, A. Mohamed
- INOR 637.** Investigation of interlayer and surface interactions in layered zirconium phosphate. **E. Cruz**, B. Mosby
- INOR 638.** Optimization of a classic organic light emitting diode device. **C. Burson**, **K. Bodenstedt**, **S. Li**, M.A. Omary
- INOR 639.** Diplatinum macrocycles as anion and temperature sensors. B. Cockrell, M. Fonseca, T. Nguyen, L. Tran, V. Tran, **S.O. Elsiddeq**
- INOR 640.** Design and characterization of PANI@UiO-66 composites as a highly tunable photoelectrode material. **J.J. Shanahan**, E.C. Sullivan, J.J. Keleher, D. Kissel
- INOR 641.** Functional frameworks of the f-elements. **R.G. Surbella**

Section K

Orange County Convention Center
West Hall C

Coordination Chemistry: Synthesis & Characterization



TECHNICAL PROGRAM

A. Larsen, *Organizer*

5:30 - 7:30

INOR 642. Correlation of hydrolysis conditions for rutile white pigment production via short sulfate process. **C. Tian**

INOR 643. Mononuclear and dinuclear ruthenium complexes of *cis*- and *trans*-thioindigo: Geometrical and electronic structure analyses. **M. Chatterjee**, G.K. Lahiri

INOR 644. Ternary pentagonal-bipyramidal oxovanadium(V) complexes containing five- and six-membered chelate rings: Syntheses, structures and properties. **A.K. Srivastava**, S. Ghosh

INOR 645. Ligandless copper(I) carboxylates. **J. Ducilon**, A.T. Noll, J.T. Sockman, H.M. Kidd, S.L. Sandri, A.M. Ishver, A.T. Royappa

INOR 646. Coordination chemistry and redox activity of heteroleptic azodioxide complexes. **K.A. Emhoff**, L. Balaraman, A.M. Salem, W. Boyd

INOR 647. Synthesis and reactivity of Pt(II)-Me pyrazolate complexes. **B. Zahora**, K.I. Goldberg

INOR 648. Simple building blocks into complex frameworks: The relationship between gold and triphos (PPh(CH₂CH₂PPh₂)₂). **D.T. Walters**, R. Babadi Aghakhanpour, X.B. Powers, K. Ghiassi, M.M. Olmstead, A.L. Balch

INOR 649. Synthesis and characterization of dinitrosyl iron complexes using pyrazole-derived ligands. **M. Le**, L. Li

INOR 650. Mono- and bis-cross-bridged tetraazamacrocycles with thiol pendant arms for biomolecule conjugation. J. Nimsey, A.J. Manning, M. Gorbet, A. Ranjan, **T.J. Hubin**

INOR 651. Primary amine pendant arms useful for conjugation of cross-bridged tetraazamacrocycles to other bioactive groups. E.M. Allbritton, M.R. Koper, F. Okorochoa, **T.J. Hubin**

INOR 652. Synthesis and characterization of palladium mononuclear complexes with electron donor *N,O* species. **C. Jimenez**, R. Guzmán-Mejía, J. González-Campos, R. Herrera, J. Aviña-Verduzco

INOR 653. Synthesis and characterisation of zinc (II) and nickel (II) complexes with 3-hydroxy-4-(2-hydroxy phenyl amino)cyclobut-3-ene-1,2-dione. **K.M. Udoisang**, A. Johnson, **N.E. Efiang**

INOR 654. Luminescent homoleptic 4'-arylterpyridyl complexes of group 13 cations. **B.M. Lovaasen**

INOR 655. Seven coordinate molybdenum and tungsten complexes containing Tpm and Tpm derivatives and the impact of ligand substitution on NMR chemical shifts. S.A. O'Reilly, **C. Seager**, C. Carley

INOR 656. Syntheses and crystal structures of heavy transition and main group metals with thiosulfate. **W.R. Blomberg**, E.M. Villa

INOR 657. Substitution effects of redox-active arylazothioformamide ligands: synthesis, spectral properties, and binding association determination with copper(I) salts. **K.L. Gutman**, Y. Kan, Z.M. Heiden, M.F. Roll, J.G. Moberly, K.V. Waynant



TECHNICAL PROGRAM

INOR 658. Synthesis of multimetallic clusters of lithium and 1st row transition metals with 2,6-bis(*tert*-butyldimethylsilylamino)pyridine ligands. **M. Smith**, G. Guillet

INOR 659. Synthesis of multimetallic clusters with 2,6-bis(triethylsilylamino)pyridine as supporting ligand. **D. Elwell**, G. Guillet

INOR 660. Metal-Metal bonded complexes supported by artificial sweeteners: Tetra and bis saccharinate and acesulfamate complexes of dirhodium(II,II). **S.C. Haefner**

INOR 661. Synthesis and characterization of new macrocyclic complexes with nitrogen and sulfur donor atoms. **O.A. Clark**, M.W. Jones

INOR 662. “Green” solventless versus solvent mediated synthesis of copper(i) and silver(i) complexes encompassing phenathroline and azolate ligands. **A. Kolek**, R. Kidwell, R. Jawaid, V. Nesterov, M. Omary

INOR 663. Comparison of Cu-ligand complexes for A β -42 therapeutic chelating agents. **A. Tabaka**, **E. Sanchez**, M.A. Havens, J.J. Keleher, D. Kissel

INOR 664. New bis(amidine) ligands for highly luminescent Cu₄ arrays and polynuclear Group 11 complexes. O. Ugarte Trejo, **A. Calderón Díaz**, **N.Z. Maya**, C. O’Dea, **J. Arras**, E. Miller, N. Bhuvanesh, C. McMillen, **M. Stollenz**

Section K

Orange County Convention Center
West Hall C

Electrochemistry

N. S. Radu, *Organizer*

5:30 - 7:30

INOR 665. Using optoelectrochemical sensing to determine ion concentrations in surface marine environments. **M. Leiskau**, J.M. DeCosta, C.A. Sweet, A.R. McCabe, C. Murphy

INOR 666. Reversible lithium capacity of iron-doped titania nanoparticles. **J. Clapham**, V. Barone, **B.D. Fahlman**

INOR 667. Fundamental studies and sensing applications of selenium redox chemistry. **E. Christensen**, **M.P. Diagne**, **G.R. Nemeth**, **E. Wiita**, M.C. Buzzeo

INOR 668. Electrochemical properties of hydroxyl-substituted terpyridine complexes as a function of pH. **C. Teahan**, **C.L. Montgomery**, S.L. Shepherd, M. Bezpalko, W.S. Kassel, D.P. Harrison, T. Dudley, J.J. Paul

INOR 669. Theoretical Pourbaix diagrams of hydroxy-substituted polypyridyl ruthenium complexes. H. Praveen, **T. Dudley**, C.L. Montgomery, C. Teahan, **J.J. Paul**

Section K



TECHNICAL PROGRAM

Orange County Convention Center
West Hall C

Environmental & Energy-Related Inorganic Chemistry

S. A. Koch, *Organizer*

5:30 - 7:30

INOR 670. Sulfonamide and thioamide chelators as mercury extractants and sensors for potential application to high-level waste processing at the savannah river site. **A.O. Fasiku**, I. Chakraborty, T.M. Jonah, G.A. Flores, R.G. Raptis, K. Kavallieratos

INOR 671. Light induced selective separation of metals with a redox active ligand. **S. Salpage**, R.C. Lanzetta, Y. Zhou, J.C. Wang, T.E. Albrecht-Schmitt, K. Hanson

INOR 672. Thiosalen nickel complexes as light driven proton reduction catalysts. **M. Hodl**, P. Hutchison, C. Tinker, J. Dewar, W.T. Eckenhoff

INOR 673. Predicting the reductive mechanism of a hydrogen evolving catalyst. **P. Hutchison**, W.T. Eckenhoff

INOR 674. Organic modifications to improve electrical conductivity in carbon nanotube thin films. **Y. Zhu**, M.E. Hagerman

INOR 675. Cobalt complex with dithiothiophene ligand for the light driven production of H₂. **L. Rhodes**, M. Hodl, W.T. Eckenhoff

INOR 676. In-situ mixing of polymer heterojunctions with inkjet printing for solar applications. **A.J. Rapaport**, **M.E. Hagerman**

INOR 677. Water dispersible cadmium selenide nanoparticles for solar films. **S.D. Ambos**, J.D. Kehlbeck, **M.E. Hagerman**

INOR 678. Ligand effects of Re(4,4'-R-2,2'-bipyridine) on carbon dioxide reduction ability. **R. Kiss**, L.D. Schmitt, A.J. Lees

INOR 679. Redox mediators for dye sensitized solar cells: Metal complexes of chelating nitrogen donor ligands. **S. Knorr**, R.R. Rodrigues, J.H. Delcamp, E.T. Papish

INOR 680. Withdrawn

Section K

Orange County Convention Center
West Hall C

Inorganic Catalysts

S. A. Koch, *Organizer*



TECHNICAL PROGRAM

5:30 - 7:30

INOR 681. Investigation of a series of nickel phosphine catalysts for “green” suzuki-miyaura coupling reactions. **L. Perez Carapia, L. Bruce, J.P. Lanorio**

INOR 682. Synthesis of mesoporous titanium dioxide from industrial titanyl sulfate solution. **C. Tian, Y. Zhang**

INOR 683. Synthesis of doped porous titania from industrial TiOSO₄ solution and its application on SCR degradation of NO. **C. Tian**

INOR 684. Metallo-antibiotics as participant in oxidative stress mechanisms. **I. Perez Cabrera, E. Zheng, S. Islam, L. Ming**

INOR 685. Synthesis and characterization of [Ru(tpyOH)(bpy)(H₂O)][OTf]₂(tpyOH = 4'-hydroxy-2,2':6',2''-terpyridine, bpy = 2,2'-bipyridine) for water oxidation catalysis. **D. Isaacs, M. Bezpalko, W.S. Kassel, J.J. Paul**

INOR 686. Transition metal catalyzed oxidation of alcohols and ethers. **A. Rahman, W. Wang, H. Zhong**

INOR 687. Green catalysis via palladium-NHC complexes tethered to imidazole-based ionic liquid ligands. **R.T. Johnson, N. Cyr, D. Paull**

INOR 688. CeO_x and CeO_x-ZnO porous nanorods decorated with Au nanoparticles for the water-gas shift reaction (WGS). **C.S. de Oliveira, D. Zanchet, E. Teixeira Neto, F. Sigoli, M. Rangel, I.O. Mazali**

INOR 689. Withdrawn

INOR 690. Intramolecular C–H functionalization followed by a [2_σ+2_π]-addition via an intermediate nickel-nitridyl complex. **Z. Sun, W. Lee, T.R. Cundari**

INOR 691. Dinuclear copper(II) complexes based on bis(pyrazolyl)methane ligands and their catecholase activities. **N.P. Jayaweera, R.F. Semeniuc**

INOR 692. Ceria properties influenced by incorporation of CTAB during hydrothermal treatment of ceria synthesis. **S. Eaimsumang, A. Luengnaruemitchai**

INOR 693. Solid oxide fuel cell (SOFC) cathode catalyst by aerosol processing. **C.D. Ligon, J. Edwards, F. Chen, K. Senevirathne**

INOR 694. Controlled ring-opening polymerization of *rac*-lactide by titanium complexes. **K. Upitak, P. Hormnirun**

INOR 695. Single-Site Aluminium complexes in catalysis of *rac*-lactide polymerization. **S. Kamavichanurat, P. Hormnirun**

INOR 696. Effects of zirconium heterometal substituted polyoxometalate on the reactivity of tungsten peroxo species for CWA decontamination. **S.L. Giles, J. Lundin, G.C. Daniels, B.T. Rasley, J.H. Wynne**

INOR 697. Electrocatalytic reduction of CO₂ to HCOOH using dirhodium(II,II) catalysts. **H.D. Manamperi, C. Turro**

INOR 698. Mechanistic probing of a dinuclear nickel electrocatalyst. **J. Belnap, K. Chabal, D. Ramirez, M.T. Kieber-Emmons**



TECHNICAL PROGRAM

INOR 699. Zinc complexes of tetradentate mono-anionic ligands as catalysts for ROP of *rac*-lactide. **I. Kremer Shitrit**, M. Kol

INOR 700. Cooperative polymerization of racemic lactide by catalyst enantiomers. **R. Hador**, M. Kol

INOR 701. Iridium(III) polypyridyl based new catalysts for highly chemoselective hydrogenation of aldehydes. **M. Pandrala**, A. Resendez, **S.V. Malhotra**

INOR 702. Withdrawn

INOR 703. Mechanistic study for the electrocatalytic CO₂ reduction by M[(bpy-R)(CO)₄] (M = Mo, W) complexes. **X. Li**, J. Panetier

INOR 704. Electrocatalytic hydrogen production via aromatically bridged butterfly [2Fe-2S] clusters. **M.O. Hamilton**, H.W. Pitts, R.S. Glass, D.L. Lichtenberger

INOR 705. Withdrawn

INOR 706. Towards rectified ruthenium polypyridyl complexes for the photochemical reduction of carbon dioxide. **C. Sparks**, D.J. Boston

Section K

Orange County Convention Center
West Hall C

Lanthanide & Actinide Chemistry

A. De Bettencourt Dias, *Organizer*

5:30 - 7:30

INOR 707. Solvent dependent sensitization of ytterbium and neodymium via an intramolecular excimer. **M. Deng**, G. Ung

INOR 708. Search for intervalence charge transfer in mixed-valent plutonium complexes. **B. Long**, C.J. Windorff, T.E. Albrecht-Schmitt

INOR 709. Stark effect in various lanthanide and actinide complexes. **J. Campbell**

INOR 710. Novel d-f bimetallic complexes containing macrocyclic ligand. **P.K. Yuen**, C. Lau, A. Yuen

INOR 711. Sandwich structure of mononuclear lanthanide complexes. **P.K. Yuen**, C. Lau, A. Yuen

INOR 712. Hybrid and expanded porphyrins: coordination chemistry of the actinide elements. **J.T. Brewster**, H. Zafar, J.L. Sessler

INOR 713. Influence of phosphorus substituents on homoleptic lanthanide and actinide phosphinodiboranate structures. **R. Harrison**, S.R. Daly



TECHNICAL PROGRAM

INOR 714. Radiation induced redox chemistry of californium-249. **D. Meeker**, G. Horne, T.S. Grimes, P.R. Zalupski, J.F. Wishart, S.P. Mezyk, T.E. Albrecht-Schmitt

INOR 715. Lanthanum dialkyl and monoalkyl phosphates as precursors for lanthanum phosphates. **M. Albqmi**, A.W. Apblett

INOR 716. Controlling the coordination environment of uranium to enable spectroscopic identification for microscopy analysis. D.J. Moulding, H.V. Stafford, D.L. Jones, M. Williams, **A.W. Woodward**, L.S. Natrajan

INOR 717. Halogen atom effect on the near-infrared emission of porphyrinate ytterbium (III) complexes. **D. Meyer**, H. He

INOR 718. Synthesis and spectroscopic studies of porphyrinate ytterbium (III) complexes. **E. Micheli**, H. He

INOR 719. Novel Modifications of UCl_6 and UBr_5 . **H.L. Deubner**, S.I. Ivlev, D. Kraus

INOR 720. Synthesis and characterization of lanthanide-silica based core/shell nanoparticles for scintillator applications. **F. Guerrero**

INOR 721. Reduction chemistry of $Ln[N(SiHMe_2)_2]_3$ complexes. **E.M. Hanada**, J.W. Ziller, W.J. Evans

INOR 722. Withdrawn

INOR 723. Stabilizing lanthanide periodates: Preventing hydrothermal reduction with a sacrificial oxidant. **C.N. Reedy**, E.M. Villa

INOR 724. Structural divergence of heavy metal complexes with isomeric thiophenecarboxylates. **A.G. Lang**, E.M. Villa

INOR 725. Neodymium, erbium, ytterbium, oh my! A new family of salicylhydrazone complexes with three near IR lanthanoid emitters: Synthesis and characterization. **K. Ayers**, G. Ung

INOR 726. Synthesis and characterization of novel lanthanide ethylenediamine tetra(methylene phosphonic acid) complexes for targeted radiotherapy. **C.D. McKinley**, F.D. White, T.E. Albrecht-Schmitt

INOR 727. Lanthanide and actinide bis-triazinyl pyridine complexes. **D. Dan**

Section K

Orange County Convention Center
West Hall C

Main Group Chemistry

T. Hudnall, *Organizer*

5:30 - 7:30

INOR 728. Mixing various reduced forms of corannulene bowls. **A. Zabula**, S.N. Spisak, A.S. Filatov, M.A. Petrukhnina, A.Y. Rogachev



TECHNICAL PROGRAM

INOR 729. Cyanoxime derivatives of main group V elements. **K. Pinks**, N. Gerasimchuk

INOR 730. Towards Alkali and Alkaline-Earth metal complexes of 2,5-bis(3,5-dimethylpyrazolylmethyl)pyrrole. D. Haugh, **A.Y. O'Brien**, M. Gillett-Kunnath, K. Ruhlandt-Senge

INOR 731. Berylliumcarboxylates, their formation and structural diversity. **M. Müller**, M.R. Buchner

INOR 732. Synthesis of ligand systems bearing icosahedral dodecaborate substituents. **K.M. Lehman**, J.A. Dopke, R.J. Staples

INOR 733. N,N,N-pincer ligand system for potential alkali and alkaline-earth metal complexes. **J. Burke**, R. Giufré, A.Y. O'Brien, M. Gillett-Kunnath, K. Ruhlandt-Senge

INOR 734. Palladium-catalyzed coupling reactions of icosahedral dodecaborates. **C.R. Jones**, J.A. Dopke, R.J. Staples

INOR 735. Synthesis of conjugated imines bearing icosahedral dodecaborate moieties. **A.C. Bach**, J.A. Dopke, R.J. Staples

Section K

Orange County Convention Center
West Hall C

Mechanistic Studies of Inorganic Reactions: A memorial Symposium for Elena Rybak-Akimova

I. V. Korendovych, *Organizer*

5:30 - 7:30

INOR 736. NMR-guided directed evolution of Kemp eliminases. **S. Bhattacharya**, A. D'Souza, A. Volkov, J. Yoon, C. Costeas, O. Makhlynets, I. Korendovych

INOR 737. Solution calorimetric studies of N_xO_y binding to transition metal complexes. **L. Farias Serafim**, J.V. Davis, M. Menaka Gamage, B. Captain, C.D. Hoff

INOR 738. Cages for capturing phytate and more complex anions. **S. Pramanik**, M. Reinmuth, S. Kaur, V. Day, K. Bowman-James

INOR 739. Multi-tasking supramolecular host-guest chemistry. **S. Kaur**, V. Day, K. Bowman-James

INOR 740. Photooxidation of Pt(II) aminothiolato complexes to sulfenato and sufinato complexes. **I. Bychinskaya**, T. Pham, M. Selke

INOR 741. Design of peptides to block association of HIV virus with human cells. **A. Kulesha**, M. Jayachandran, P. Gosavi, J. Rempillo, I. Korendovych

Section K



TECHNICAL PROGRAM

Orange County Convention Center
West Hall C

Organometallic Chemistry: New Ligand Platforms

N. S. Radu, *Organizer*

5:30 - 7:30

INOR 742. Synthesis, characterization, and reactivity of N-phosphino-2-(phosphino)pyrrole ligands and their nickel complexes: applications for C–C and C–N cross-coupling reactions. **H. Fokwa**

INOR 743. Functional groups effect on the electronics of macrocyclic pyridinophane. **M. Mekhail**, K.N. Green, A. Yepremyan

INOR 744. Toward the synthesis and characterization of a new anionic NHC and its corresponding transition metal complexes. **M. Grimes**, **I. Sellars**, D. Tapu

INOR 745. Synthesis and complexation of a new Cerberus NHC: Synthesis and coordination. **B. Clinebell**, **R. Gaynor**, R. Hooper, A. Mason, M. Montgomery, **D. Tapu**

INOR 746. Synthesis and complexation of a new anionic chelating N-heterocyclic carbene. **A. Duenas**, **E. Swales**, **S. Young**, R. Gaynor, B. Clinebell, D. Tapu

INOR 747. Reactivity of imidazole substituted biaryl mono-phosphine complexes. **H. Henriksen**, B.E. Silva, D. Grotjahn

INOR 748. Synthesis, characterization and reactivity of bifunctional transition-metal complexes containing hydride-relay functionality. **N. Devi**, **C.M. Zall**

INOR 749. Synthesis of biphenyl-based tetradentate pyridyl N-heterocyclic carbene (NHC) ligands and their application for electrocatalytic CO₂ reduction. **S. Sinha Roy**, H. Dulaney, W. Yang, J.W. Jurss

INOR 750. Synthesis of multidentate ligands with a pyrrole-derived backbone and the reactivity of resultant organometallic complexes. **M.N. Cosio**

INOR 751. Synthesis of redox-active phosphine ligands containing organic hydride donors within a flexible, modular design. **D. Eason**, S. Longe, J.L. Chaloupka, N. Devi, C. Zall

Section K

Orange County Convention Center
West Hall C

Organometallic Chemistry: Synthesis & Characterization

N. S. Radu, *Organizer*

5:30 - 7:30



TECHNICAL PROGRAM

INOR 752. Photophysics of platinum(II) complexes with abnormal *N*-heterocyclic ligands: Insights from theory and experiment. J. Soellner, **P. Pinter**, T. Strassner

INOR 753. Synthesis of a sterically hindered three-coordinate Pd(II) complex for C–F reductive elimination. **S.F. Kim**, L. Wang, L. Chen, B.P. Carrow

INOR 754. Cyclopentadienyl pyridazines and oxazines and their applications in energy and advanced electronics. **N.C. Tice**, C. Olmstead, S. Wild, J.L. Jenkins, C.A. Synder

INOR 755. Homometallic and heterometallic 1D wires: Preparation, structures, magnetic and spectroscopic properties. **C. Turner**, N. Gerasimchuk

INOR 756. Chemistry of binary copper(I) pyrazolates with carbon monoxide. **R. Dias**, D. Parasar, N. Jayaratna

INOR 757. Volatilization of mixed metal group 13 amides and the stability of their metal ratios. **A.P. Purdy**

INOR 758. Diastereoselective cycloiridation and transmetallation of metal-based sandwich complexes. **R.A. Arthurs**, C.J. Richards

INOR 759. Synthetic methodologies of metallocene-fused polyacenes. **B. Curole**, J. Bergeron, U. Pokharel, J.P. Selegue

INOR 760. Developing one-pot, one-step routes to transition metal imino-pyridine complexes. **T.E. Shaw**, T. Jurca

Section K

Orange County Convention Center
West Hall C

Small Molecule Activation for Oxidative & Reductive Catalysis

New Frontiers in Model Chemistry and Catalysis

J. D. Blakemore, J. J. Concepcion, *Organizers*

5:30 - 7:30

INOR 761. Ultrafast photoinduced CO release from manganese tricarbonyl complexes. **W. Henke**, C.J. Otolski, W. Moore, C.G. Elles, J.D. Blakemore

INOR 762. Functionalization of Mn bipyridine catalysts for electrocatalytic CO₂ reduction: A study of electron-donating effects in the second coordination sphere. **V. Blaszczak**, M.E. McKinnon, D.C. Grills, M.Z. Ertem, J.J. Rochford

INOR 763. Chemical and electrochemical properties of [Cp*Rh] complexes supported by a hybrid phosphine-quinoline ligand. **J.A. Hopkins**, V. Day, J.D. Blakemore, D. Lionetti

INOR 764. Chromophores and anchoring strategies for light-driven water splitting. **L. Wang**, Y. Xie, R. Sampaio, J.J. Concepcion



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- INOR 765.** Tuning the redox properties of [Cp*Rh] catalysts with monosubstituted 2,2'-bipyridyl ligands. **W. Moore**, W. Henke, D. Lionetti, J.D. Blakemore
- INOR 766.** CO₂-expanded electrolytes: a new medium for the enhancing CO₂ reduction catalysis. **D. Sconyers**, C. Shaughnessy, B. Subramaniam, K.C. Leonard, J.D. Blakemore
- INOR 767.** Formation and reactivity of substituted η⁴-cyclopentadiene (Cp*H) complexes of rhodium. **Y. Peng**, D. Lionetti, J. Douglas, V. Day, J.D. Blakemore
- INOR 768.** Thermodynamic hydricities and acidities of transition metal hydrides containing mixed triphosphine and monophosphine ligands. **W. Fernandez**, C.M. Zall, D.L. Williams
- INOR 769.** Synthesis and characterization of nitrosamine: A redox switchable hno/no donor. **A. Green**, T.H. Warren, A.P. Cardenas
- INOR 770.** Palladium and platinum diphosphine complexes for CO and CO₂ hydrogenation. S.H. Schreiner, **E. Kober**
- INOR 771.** Quantification of lewis acid effects in heterobimetallic complexes. **A. Kumar**, D. Lionetti, V. Day, J.D. Blakemore
- INOR 772.** Electrochemical properties of heterobimetallic complexes of Zinc. **S. Kelsey**, A. Kumar, D. Lionetti, J.D. Blakemore
- INOR 773.** Noncovalent immobilization of molecular f-element complexes on electrode surfaces. **J.D. Blakemore**, K. Johnson, D. Lionetti, V. Day

Section K

Orange County Convention Center
West Hall C

Solid-State Inorganic Chemistry

V. Poltavets, *Organizer*

5:30 - 7:30

- INOR 774.** Identifying anthropogenic biases in exploratory syntheses; evaluating the effects of experiment design on machine learning models. **Y. Huang**, A.J. Norquist, J. Schrier
- INOR 775.** Development of a solid state undergraduate teaching laboratory. **K.L. Tracey**, **B.J. Bellott**
- INOR 776.** Synthesis of AAl₂SnQ₄X. **K. Murphy**, **B.J. Bellott**
- INOR 777.** Robot-ready, high throughput synthesis of lead halide perovskites. E.E. Brown, X. Jia, P. Cruz Parrilla, M. Nellikkal, I.M. Pendleton, J. Schrier, **A.J. Norquist**
- INOR 778.** Incommensurate crystal structures of doped rhenium silicides: Promising thermoelectric properties. **V. Decocq**, F. Wang



TECHNICAL PROGRAM

INOR 779. Tetragonal tungsten bronzes revisited. **M.T. Yeung**, K.R. Poeppelmeier

INOR 780. Structural and photoluminescence characterization of RE³⁺- substituted Ba₂SrGaO₄F *via* microwave synthesis. R. Green, **V. Pierre**

INOR 781. Structural and photoluminescence characterization of the RE³⁺- substituted hexagonal anti-perovskite Na₂CaVO₄F. R. Green, **T. Kelly**

INOR 782. Electronic and structural *ab initio* calculations of ReSiAl models. **A. Neeson**, F. Wang

Section K

Orange County Convention Center
West Hall C

Through the Lens of Inorganic Chemistry: Understanding Heterogeneous Processes in Energy Conversion & Storage

S. Marinescu, V. Thoi, J. Y. Yang, *Organizers*

5:30 - 7:30

INOR 783. Complementary insights from ex situ, in situ, and operando spectroscopy and diffraction studies of insertion and conversion based inorganic materials for electrochemical energy storage. **A.C. Marschlok**, K.J. Takeuchi, E.S. Takeuchi

WEDNESDAY MORNING

Section A

Orange County Convention Center
Room W221A

Inorganic Catalysts

S. A. Koch, *Organizer*
A. Bengali, J. W. Jurss, *Presiding*

8:30 INOR 784. Base metal-catalyzed, additive-free C–O bond cleavage of β-O-4 lignin model compounds. **O. Brown**

8:50 INOR 785. Bifunctional catalysis using nickel SNS amido and thiolate complexes. **Y.M. Albkuri**, C. Guo, C. Bucher, B. Gabidullin, R. Baker

9:10 INOR 786. Hydrosilation of organic substrates using earth abundant transition metal catalysts. **A. Bengali**, S. T. Madrahimov, W. Fan, V. Yempally



TECHNICAL PROGRAM

9:30 INOR 787. Mechanistic study for the reduction of CO₂ to CO using M[bpyMe(ImMe)](CO)₃Cl⁺ complexes: Probing the role of the imidazolium moiety in the secondary coordination sphere. **X. Li**, S. Sung, M. Nippe, J. Panetier

9:50 INOR 788. Why pincer metal catalysts for green chemistry? **A. Poater**

10:10 Intermission.

10:30 INOR 789. Design of earth-abundant nitridyl catalysts for C-H functionalization. **Z. Sun**, t.R. Cundari

10:50 INOR 790. DNA hybrid catalysts for asymmetric transformations. **J. Cope**, W. Harrison, D. Russel, A. Bartlett, B. Donnadieu, M.P. Hendrich, J. Emerson

11:10 INOR 791. Electro- and photocatalytic CO₂ reduction with nickel complexes bearing tunable bipyridyl-*N*-heterocyclic carbenes. **J.W. Jurss**, X. Su, H. Shirley, H. Sanjanwala, J.H. Delcamp

Section B

Orange County Convention Center
Room W224B

Magnetism Across Length Scales

Magnetism in Molecules and Molecule-Based Materials

S. Hill, M. Shatruk, G. F. Strouse, *Organizers*
G. Christou, *Organizer, Presiding*
V. Zapf, *Presiding*

8:30 Introductory Remarks.

8:35 INOR 792. Highlights for the quantum materials initiative at ORNL. **C. dela Cruz**

9:00 INOR 793. Control of the magnetism at an interface: The long/short and hot/cold of the topic. **M.W. Meisel**

9:25 INOR 794. Functionalized trispyrazolylborate spin crossover complexes: towards single molecule spin state detection. **C. Besson**, C. Ma, H. Flötotto, C. Meyer

9:50 INOR 795. Vanadium tetracyanoethylene for coherent magnonics. **E. Johnston-Halperin**

10:15 Intermission.

10:30 INOR 796. Manipulating spin in molecules and materials. T. Pearson, S. Coste, J.P. Walsh, **D.E. Freedman**

10:55 INOR 797. Magnetic resonance investigations of systems featuring metal-metal bonds: Insights into the design of single-molecule magnets. **S. Greer**, K.M. Gramigna, J. Nehr Korn, B. Malbrecht, C.M. Thomas, S. Stoian, T. Betley, S. Hill

11:15 INOR 798. Giant molecules: Exploring synthetic parameters on the path to new Mn/O torus-like clusters. **A.R. Hale**, K.A. Abboud, G. Christou



TECHNICAL PROGRAM

Section C

Orange County Convention Center
Room W224A

Small Molecule Activation for Oxidative & Reductive Catalysis

New Frontiers in Fundamentals and Applications

J. J. Concepcion, *Organizer*
J. D. Blakemore, *Organizer, Presiding*
J. Concepcion, *Presiding*

8:30 Introductory Remarks.

8:35 INOR 799. Platform system for kg-scale carbon dioxide conversion and solar fuels production. **S.W. Sheehan**

9:00 Discussion.

9:05 INOR 800. Homogenous hydrogenation of carbon dioxide to formate in water and organic solvent by Rh-bisdiphosphine molecular catalysts. **J. Laureanti**, A.P. Walsh, J.C. Linehan, M. O'Hagan, W. Shaw

9:30 Discussion.

9:35 INOR 801. Multifaceted mechanisms of CO₂ reduction to CO by iridium(III) phenyl-pyridine photo- and electro-catalysts. **G. Manbeck**, E. Fujita, D.E. Polyansky, M.Z. Ertem

10:00 Discussion.

10:05 Intermission.

10:25 INOR 802. Earth-abundant catalysts with tunable redox-active ligands for CO₂ reduction in acetonitrile and aqueous solutions. **J.W. Jurss**, X. Su, K.M. McCardle, L. Chen, J. Panetier

10:50 Discussion.

10:55 INOR 803. Mechanistic investigation of oxygen atom transfer pathway for Ru based water oxidation catalysts. **M.Z. Ertem**, J.J. Concepcion

11:20 Discussion.

11:25 INOR 804. Structure-function studies of carbene-supported electrocatalysts for CO₂ reduction. **S. Gonell**, C.K. Schauer, J.T. Muckerman, A.J. Miller

11:50 Discussion.

Section D



TECHNICAL PROGRAM

Orange County Convention Center
Room W224C

Alfred Bader Award in Bioinorganic or Bioorganic Chemistry: Symposium in Honor of Joan B. Broderick

S. R. Smith, *Organizer*
J. Betz, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 **INOR 805.** Shining light on photosynthetic reaction center biohybrids for hydrogen production. **L.M. Utschig-Johnson**, K.L. Mulfort, O. Poluektov, D.M. Tiede

9:05 **INOR 806.** Spectroscopic studies of hydrogen reduction by [FeFe]-hydrogenase HydA1 from *Chlamydomonas reinhardtii*. **Y. Guo**

9:35 **INOR 807.** From peyrone's salt to genomics: Tracking platinum compounds through cells. **V. DeRose**

10:05 Intermission.

10:25 **INOR 808.** Formation of a reactive, alkyl thiolate-ligated Fe^{III}-superoxo intermediate derived from dioxygen. **J. Kovacs**, M.N. Blakely, M.A. Dedushko, P. Poon, A. Downing, G. Villar-Acevedo, D. Rogers

10:55 **INOR 809.** Fe-S clusters as cellular iron sensors: Roles for Fe-S binding glutaredoxins in iron regulation. **C.E. Outten**

11:25 Concluding Remarks.

Section E

Orange County Convention Center
Room W221C

Francis P. Garvan_John M.Olin Medal-Olin Medal: Symposium in Honor of Lisa McElwee-White

L. J. Murray, *Organizer, Presiding*

8:30 **INOR 553.** From anti-diabetic to anti-cancer compounds: Conducting research while working with undergraduates. **D.C. Crans**, J.T. Koehn, H. Murakami, S.M. Petry, E. Gaudamauskas, P. Chatterjee, B. Baruah, J.J. Smee

9:00 **INOR 811.** New applications for hafnium pyridylamido catalysts. **A.M. LaPointe**, J.M. Eagan, R. Di Girolomo, T. Lin, G.W. Coates

9:30 **INOR 812.** Heterobimetallic d-4f catalysts for alkyne semi-hydrogenation. **C.C. Lu**, B.L. Ramirez

10:00 Intermission.



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

10:15 INOR 813. Structure and behavior of imine soft donor ligands for f-element coordination. **A.E. Gorden**

10:45 INOR 814. Aromatic and anti-aromatic metallacycles: An actinide story. **J.L. Kiplinger**

11:15 INOR 815. Many-electron reductive activation of small molecules with dinuclear 4f- and 5f- organometallics. **P.L. Arnold**, M. Seymour, F. Lam, K. Wang, T. Ochiai, R. Kelly, A. Price

11:45 INOR 816. N,O-chelated complexes of early transition metals for the catalytic synthesis of materials. **L. Schafer**

12:15 Concluding Remarks.

Section F

Orange County Convention Center
Room W224D

Coordination Chemistry: Characterization & Applications

A. Larsen, *Organizer*
J. J. Wilson, *Presiding*

8:30 INOR 817. Preventing cell death with ruthenium coordination complexes. **J.J. Wilson**, J.J. Woods, J. Spivey

8:50 INOR 818. Super-electron-donor dimetal complexes acting as frustrated Lewis pairs: Electrocatalytic production of hydrogen from weak acids. **M.O. Hamilton**, M. Humphries, D.L. Lichtenberger

9:10 INOR 819. Large and in charge: Development of expanded macrocycles for the chelation of large metal ions of therapeutic and industrial relevance. **N.A. Thiele**, J.J. Wilson

9:30 INOR 820. Ce/Mn clusters from reductive aggregation: Unusual long-range Mn---Mn exchange-coupling through Ce^{IV}. **S. Das Gupta**, K.A. Abboud, G. Christou

9:50 INOR 821. Ligand-induced tuning of the ground state spin of Ce₃Mn₈ clusters, a molecular mimic of the perovskite repeating unit. **T. Cao**, K.A. Abboud, G. Christou

10:10 INOR 822. Paramagnetic Co(II) complexes with appended fluorophores as bimodal imaging agents. **A. Patel**, J.R. Morrow, S. Mohammed, P. Cullen

10:30 Intermission.

10:40 INOR 823. Coordination chemistry of the rhodizonate anion with divalent toxic metals: Binary and ternary rhodizonate complexes for spectrophotometric M(II) detection. **J.A. Silverman**, S.J. Saluga, K. Kavallieratos

11:00 INOR 824. Scorpionate-supported cobalt(II) borohydride complexes. **A.M. Aboelenen**, **J.L. Petersen**, **M.P. Jensen**

11:20 INOR 825. Colorimetric sensing using the 3d metal based coordination complexes and further modifications. **I. Bhowmick**, C.R. Collins, S. Regalado-Love, D.J. Boston



TECHNICAL PROGRAM

11:40 INOR 826. Capture of low concentration perfluorooctanesulfonate from aqueous solutions using metal-organic frameworks. **D. Barpaga**, J.A. Soltis, V. Shutthanandan, S. Basuray, S. Chatterjee, R. Motkuri

Section G

Orange County Convention Center
Room W221D

Chemistry of Materials - Metal Organic Frameworks

C. G. Lugmair, *Organizer*
P. J. Milner, T. Wang, *Presiding*

8:30 INOR 827. Probing the connection between low-frequency vibrational modes and macroscopic structural behavior of metal organic frameworks. **N.D. Kline**, B. Goetz, A. Tripathi, C. Ellis, J.L. Mendoza-Cortes, C. Serre

8:50 INOR 828. Design and construction of multivariate hierarchical metal-organic frameworks for heterogeneous catalysis. **L. Feng**, H. Zhou

9:10 INOR 829. Cooperative capture of carbon dioxide in diamine-appended metal-organic frameworks. **P.J. Milner**, R. Siegelman, J. Martell, A. Forse, J. Lee, M. Gonzalez, S. Weston, J. Neaton, J.A. Reimer, J.R. Long

9:30 INOR 830. Structure tuning in a series of holmium-based MOFs: Building a radiotherapeutic system. **J.P. Vizuet**, G. McCandless, K.J. Balkus

9:50 INOR 831. Core-shell structured cyclodextrin metal-organic frameworks: Construction & multifunctional development. **Y. Chen**, J. Gong

10:10 Intermission.

10:25 INOR 832. Investigation of singlet oxygen photosensitization by porphyrinic metal-organic frameworks. **B.M. Liu**, A.E. Arredondo, T.F. Bennett, K.J. Nelms, Y. Liu, M. Selke

10:45 INOR 833. Stable Indium-organic framework exhibiting *soc* topology as a versatile bifunctional catalyst for highly efficient one-pot strecker synthesis of α -aminonitriles. **G. Verma**, S. Kumar, B.A. Carr, Z. Niu, H. Vardhan, L. Wojtas, S. Ma

11:05 INOR 834. Defect studies of nanoporous aluminum metal-organic frameworks. **C. Lin**

11:25 INOR 835. Vanadium docked covalent-organic frameworks: an effective heterogenous catalyst for modified mannich-type reaction, prins reaction and sulphide oxidation. **H. Vardhan**

11:45 INOR 836. Increasing the optical transmittance via decreasing crystallite dimensions—insights on MOF luminescence sensing applications. **T. Wang**, A.I. Benin, F. Doty, V. Stavila, M. Allendorf

Section H

Orange County Convention Center
Room W221E



TECHNICAL PROGRAM

Organometallic Chemistry: Applications to Materials & Polymer Science

N. S. Radu, *Organizer*
C. M. Kozak, *Presiding*

8:30 INOR 837. Influence of second sphere h-bonding interactions on photoluminescent heteroleptic-iridium complexes. **B. Balonova**, B. Blight

8:50 INOR 838. Blue OLED emitters. **T. Strassner**

9:10 INOR 839. Access to a doubly boron-doped dihelicene or an oxadiborepin from the same precursor. **J. Radtke**, M. Wagner

9:30 INOR 840. Photochemical decomposition of Pt precursors for photoassisted chemical vapor deposition. **H. Liu**, S.R. Wheeler, B. Salazar, A.V. Walker, L. McElwee-White

9:50 INOR 841. Defining the role of organometallic species in atom transfer radical polymerization. **F. Lorandi**, M. Fantin, T. Ribelli, G. Szczepaniak, R. Poli, K. Matyjaszewski

10:10 INOR 842. Mechanistic spectroscopic analysis of carbonate synthesis from CO₂ and epoxides using amino-bis(phenolate) complexes. **C.M. Kozak**, K. Ni, K. Devaine-Pressing

10:30 INOR 843. Photochemistry of (η^3 -allyl)Ru(CO)₃X precursors for photoassisted chemical vapor deposition. **C.R. Brewer**, O.M. Hawkins, N.C. Sheehan, B. Salazar, A.V. Walker, L. McElwee-White

10:50 INOR 844. Mechanism-based precursor design for focused electron beam-induced deposition of Pt nanostructures. **H. Lu**, J.A. Spencer, F. Ferreira da Silva, O. Ingólfsson, H. Fairbrother, L. McElwee-White

11:10 INOR 845. Ligand effects in Au(I) precursors for focused electron beam induced deposition. **W.G. Carden**, R.M. Thorman, I. Unlu, T.M. Kim, H. Fairbrother, L. McElwee-White

Section I

Orange County Convention Center
Room W232A

Chemistry at the Interface of Solution-processed Inorganic Materials

A. B. Greytak, *Organizer*
B. M. Cossairt, *Organizer, Presiding*
E. Miller, *Presiding*

8:30 Introductory Remarks.

8:35 INOR 846. Controlling the phase and stability of metallic MoS₂ nanosheets for hydrogen generation. **E. Miller**

9:00 INOR 847. Single atomic vacancy catalysis. **M. Chhowalla**



TECHNICAL PROGRAM

9:25 INOR 848. At the interphase of molecular and bulk: Chemical functionalization of phosphorene nanosheets. **A. Velian**, C. Chang, Y. Sakazaki

9:50 Intermission.

10:05 INOR 849. Properties and applications of solution-processed inorganic two-dimensional materials. **M. Hersam**

10:30 INOR 850. Synthetic control of the interfacial chemistry of carbon. S. Chu, A. Murray, C.J. Kaminsky, M. Jackson, **Y. Surendranath**

10:55 INOR 851. Tailoring the properties of 2D materials via surface chemistry. **J.E. Goldberger**

Section J

Orange County Convention Center
Room W232B

Mechanistic Studies of Inorganic Reactions: A memorial Symposium for Elena Rybak-Akimova

I. V. Korendovych, *Organizer, Presiding*

8:30 INOR 852. Tuning the reactivity and relative stability of manganese dioxygen intermediates via systematic ligand modification. **J. Kovacs**, P. Poon, M.A. Dedushko, G. Yang, A. Johansen, S.A. Toledo, X. Sun, E.V. Rybak-Akimova

9:10 INOR 853. Bond electron densities in macrocyclic complexes: what is visible in a routine X-ray diffraction experiment. **A.Y. Nazarenko**

9:40 INOR 854. Mechanistic studies for the nickel promoted nitrile-self and nitrile-amide condensations for the production of imidoamidines (N-NacNacs).. **C. Guifarro**, E.V. Rybak-Akimova

10:10 Intermission.

10:20 INOR 855. Surprising analogy between singlet oxygen and orbital magnetism in two-coordinate cobalt(II) compounds. **L. Davis**, G.S. Girolami

10:50 INOR 856. Alkali metal substitution in supramolecular metal-rich sandwiches. **M.A. Petrukhina**

11:20 INOR 857. Adventures in exploring the high-valent nonheme iron-oxo landscape. **L. Que**

Innovative Chemistry & Materials for Electrochemical Energy Storage

Beyond Li-Ion

Sponsored by ENFL, Cosponsored by CATL, INOR and PMSE



TECHNICAL PROGRAM

Activation of Light (C1-C4) Hydrocarbons: Theory & Experiments

Sponsored by CATL, Cosponsored by ENFL, ENVR, INOR and PHYS

Light-Driven Chemistry: Photoelectrochemistry & Photocatalysis

Sponsored by CATL, Cosponsored by COLL, ENFL, I&EC, INOR and PHYS

Chemical Catalysis for Bioenergy Consortium: Addressing Deactivation during Biomass Conversion

Sponsored by CATL, Cosponsored by ENFL, ENVR and INOR

WEDNESDAY AFTERNOON

Section A

Orange County Convention Center
Room W221A

Mechanistic Studies of Inorganic Reactions: A memorial Symposium for Elena Rybak-Akimova

I. V. Korendovych, *Organizer, Presiding*

1:30 INOR 858. Insight into possible mechanisms for for oxidation of N_2 or N_2O to nitrate. **C.D. Hoff**

2:10 INOR 859. Mechanistic role of anion- π and halogen-bonded complexes in electron-transfer reactions involving halide anions. **S.V. Rosokha**

2:40 INOR 860. Instrument repair to data collection to colleague. **R.J. Staples**, E.V. Rybak-Akimova

3:10 Intermission.

3:20 INOR 861. Exploring synthetic iron model oxidation pathways by kinetic and mechanistic techniques: Insights and challenges. **J.P. Caradonna**

4:00 INOR 862. Novel ligands of pincer- and tripod-design: Their application to surface-supported catalysis and metal-ion sensing. **R.P. Planalp**, L. Fulton, B. Barron, T. Bullick, D. DiRocco

4:30 INOR 863. Pyridine pincer versatility: A tribute to the memory of Elena V. Rybak-Akimova. **K. Bowman-James**

5:10 Concluding Remarks.

Section B



TECHNICAL PROGRAM

Orange County Convention Center
Room W224B

Magnetism Across Length Scales

Magnetism in Molecules and Molecule-Based Materials

M. Shatruk, G. F. Strouse, *Organizers*
S. Hill, *Organizer, Presiding*
K. Preuss, *Presiding*

1:30 INOR 864. [TCNE]-based (TCNE = tetracyanoethylene) ferromagnets, ferrimagnets, synthetic/artificial antiferromagnets, and weak ferromagnets. **J.S. Miller**

1:55 INOR 865. Novel high field phases in molecule-based multiferroics. **J. Musfeldt**, A.J. Clune, K. Hughey, J. Singleton, J. Lee, W. Tian, J. Fernandez-Baca, N.S. Dalal, Z. Liu, M. Ozerov

2:20 INOR 866. High-magnetic-field explorations of molecular architecture and fundamental physics in organic quantum magnets. **J. Singleton**, P. Goddard, J. Musfeldt, A.J. Clune, K. Hughey, J. Manson, J. Brambleby

2:45 INOR 867. Dithiazolyl radicals: Molecular magnets, coordination chemistry and radical-radical cocrystals. D. Leckie, M. Harb, N. Stephaniuk, **J.M. Rawson**

3:10 Intermission.

3:25 INOR 868. Correlation of electronic structure to function: reactivity and magnetism. **T. Betley**

3:50 INOR 869. Exploring tunable nanoscale metal complexes through ligand design. **J. Brusso**

4:15 INOR 870. Prospects for molecular magnetism in quantum information science. **M.R. Pederson**

4:40 INOR 871. Effects of environmental engineering on electronic spin qubits. **J. Zadrozny**, C. Lin, T. Ngendahimana, C. Jackson, S. Johnson, S. Eaton, G. Eaton

Section C

Orange County Convention Center
Room W224A

Chemistry of Materials - Synthesis & Properties

C. G. Lugmair, *Organizer*
D. A. Loy, T. E. Stevens, *Presiding*

1:30 INOR 872. Studying the growth of Ce/O nanoclusters. **B.K. Russell-Webster**, K.A. Abboud, G. Christou

1:50 INOR 873. 1-Dimensional Fe(II) spin crossover polymers – An in-fight between rigidity, solvate and anion. **C. Knoll**, D. Müller, J.M. Welch, G. Giester, M. Reissner, R. Miletich, P. Weinberger



TECHNICAL PROGRAM

2:10 INOR 874. Influence of organic bridging groups on the mechanical properties of organosilica materials. **D.A. Loy**, K.M. Frederick

2:30 INOR 875. Luminescent bismuth(III)- and lanthanide-doped bismuth(III)-organic materials: Synthesis, structural characterization, and photophysical behavior. **A.K. Adcock**, K.E. Knope

2:50 Intermission.

3:05 INOR 876. Synthesis and magnetic properties of iron nitrides. **T.E. Stevens**, R.E. Lewis, C.J. Pearce, M.A. Rodriguez, S. Dickens, B.B. McKenzie, S. Atcitty, T.C. Monson

3:25 INOR 877. Preparation of functional zirconium phosphates by stepwise interlayer and surface modification. E. Cruz, **B.M. Mosby**

3:45 INOR 878. Fluorocarbon R134a adsorption in pore-engineered metal-organic framework materials for sorbent-based chiller applications. **D. Barpaga**, J. Zheng, B. Trump, P. Bhattacharya, R. Motkuri

4:05 INOR 879. Structural and spectroscopic features of novel linear Cu_4 arrays. **M. Stollenz**, A. Calderón Díaz, N.Z. Maya, C. O'Dea, J. Arras, N. Bhuvanesh, C. McMillen

Section D

Orange County Convention Center
Room W224C

Chemistry of Materials - Metal Organic Frameworks

C. G. Lugmair, *Organizer*
R. Motkuri, *Presiding*

1:30 INOR 880. How do enzymes orient when trapped on metal-organic framework (MOF) surfaces? **Z. Yang**

1:50 INOR 881. Metal-organic frameworks-based porous frustrated lewis pairs as the new heterogeneous hydrogenation catalyst. **Z. Niu**, S. Ma

2:10 INOR 882. New lanthanide containing metal-organic frameworks from linear aromatic dicarboxylate ligands: Syntheses, structures and luminescence sensing capabilities. **C. Hossack**, Z. Min, M. Singh-Wilmot

2:30 INOR 883. Customized hierarchical porous metal organic frameworks engenders stable enzymatic nanoreactors. **N.M. Khashab**

2:50 INOR 884. Stimuli-responsive electronic and photonic metal-organic frameworks. **S. Saha**, M. Gordillo, A. Khatun, D. Panda

3:10 Intermission.

3:25 INOR 885. Studies of chemical bonding and “breathing” in MOFs and their complexes with small molecules by new method: Solid-state synchronous fluorescence spectroscopy. C. Grinnell, **A. Samokhvalov**



TECHNICAL PROGRAM

3:45 INOR 886. Genetically engineered peptides used in MOF synthesis. **S. Lympelopoulou**, I. Efimov, Z. Westcott, C. Perry, D. Bradshaw

4:05 INOR 887. Tubular shape metal-organic framework for controlled drug release. **Q. Wang**

4:25 INOR 888. Understanding the free energy landscape in the early stages of MOF nucleation. **L. Kollias**, D.C. Cantu, V. Glezakou, R. Rousseau, M. Salvalaglio

4:45 INOR 889. Metal-organic frameworks for efficient adsorption cooling applications. **R. Motkuri**, D. Barpaga, J. Zheng, J. Jenks

Section E

Orange County Convention Center
Room W221C

Environmental & Energy-Related Inorganic Chemistry

S. A. Koch, *Organizer*

A. W. Apblett, I. Chakraborty, *Presiding*

1:50 INOR 890. Mercury (II) complexes derived from N, N- and N, S-donor ligands. **I. Chakraborty**, I. Lehman-Andino, S. Kandel, R. Raptis, K. Kavallieratos

2:10 INOR 891. Sorption of uranium from ground water and sea water. **A.W. Apblett**, C.K. Perkins, H. Albusaidi

2:30 INOR 892. Alternative basic additives for copper bipyridyl complex mediated DSSCs. **Y. Wang**, T. Hamann

2:50 Intermission.

3:10 INOR 893. Enhanced charge transport by fluorine-modified organic cation for additive-free 2D perovskite solar cells with a PCE >13%. **F. Zhang**, K. Zhu

3:30 INOR 894. Low-spin Co(II) redox shuttles for dye sensitized solar cells. **A.L. Raithe**, T. Kim, T. Hamann

3:50 INOR 895. Thermochemical energy storage materials for combination with solar thermal collector systems. **D. Müller**, C. Knoll, J.M. Welch, A. Werner, M. Harasek, C. Schnabl, P. Weinberger

4:10 INOR 896. Reduction of CO₂ to oxalate by a copper(I) complex: Effects of redox mediators. **F. Khamespanah**, D.B. Crochet, U.R. Pokharel, F.R. Fronczek, A.W. Maverick

Section F

Orange County Convention Center
Room W224D

Chemistry of Materials - Synthesis & Properties



TECHNICAL PROGRAM

C. G. Lugmair, *Organizer*
A. B. Martinson, *Presiding*

1:30 INOR 897. Bulky aminocyanophosphine glasses: A new class of inorganic polymers. **B.L. Chaloux**, T.J. Dabrow, A. Epshteyn

1:50 INOR 898. Rationally designed route to the one-pot synthesis of right bipyramidal nanocrystals of copper. **Z. Lyu**, M. Xie, K. Gilroy, Z. Hood, M. Zhao, S. Zhou, J. Liu, Y. Xia

2:10 INOR 899. Design and synthesis of defect-ordered perovskites: Controlling the electrical properties through modification of defect-arrangement for fuel-cell applications. **F. Ramezanipour**, R.K. Hona, A. Huq

2:30 INOR 900. Additive manufacturing of transparent silica glass from solutions. **I. Cooperstein**, S. Magdassi

2:50 Intermission.

3:05 INOR 901. 3D printed organic-ceramic complex hybrid structures with high silica content. **E.Z. Shukrun Farrell**, I. Cooperstein, S. Magdassi

3:25 INOR 902. Sequential infiltration synthesis of conductive oxides. R. Waldman, O. Heinonen, S.B. Darling, **A.B. Martinson**

3:45 INOR 903. Formation of the faujasite zeolite followed by in situ spectroscopies. **S. Prodingner**, M.A. Derewinski, J.A. Lercher

4:05 INOR 904. Molecular materials derived from boron difluoride (BF₂) formazanate complexes. **R.R. Maar**, S. Barbon, J.B. Gilroy

Section G

Orange County Convention Center
Room W221D

Organometallic Chemistry: Catalysis

N. S. Radu, *Organizer*
O. Ozerov, *Presiding*

1:30 INOR 905. Ru pincer complexes for acceptorless dehydrogenative conversion of alcohols: mechanistic investigations. D. Nguyen, **R. Gauvin**

1:50 INOR 906. Supported pincer-iridium(III) complexes on metal oxides for electrophilic C–H functionalization. **Z.H. Syed**, D.M. Kaphan, F. Perras, M. Pruski, M. Ferrandon, E.C. Wegener, C. Yang, A.J. Kropf, C. Liu, F. Dogan, K.I. Goldberg, M. Delferro

2:10 INOR 907. Withdrawn



TECHNICAL PROGRAM

2:30 INOR 908. Studies of mechanism of dehydrogenative borylation of terminal alkynes by (PNP)Ir complexes. **O. Ozerov**, B.J. Foley, J. Zhou

2:50 INOR 909. Photocatalytic CO₂ reduction with novel supramolecular Mn(I) complexes. **D.C. Fabry**, H. Koizumi, D. Ghosh, Y. Yamazaki, H. Takeda, Y. Tamaki, O. Ishitani

3:10 INOR 910. Examining intermediates, speed bumps, bifurcations, and more with quasiclassical organometallic reaction dynamics. **D.H. Ess**

3:30 INOR 911. Mechanistic analysis of cu(i)-catalyzed boracarboxylation of vinyl arenes. **N.N. Baughman**, N. Akhmedov, B.V. Popp

3:50 INOR 912. Cobalt-catalyzed C-H methylation for late stage functionalization. **S.D. Friis**, L. Ackermann, M.J. Johansson

4:10 INOR 913. Withdrawn

4:30 INOR 914. Acidification of C-H bonds by transition metals: Thermodynamic and kinetic aspects from experiment and DFT. **E.B. Hulley**, W. Christman, R. Tenney

Section H

Orange County Convention Center
Room W221E

Coordination Chemistry: Characterization & Applications

A. Larsen, *Organizer*
A. Hossain, *Presiding*

1:30 INOR 915. Molecular recognition of biologically relevant anions with transition metal complexes. **A. Hossain**, M. Rhaman, M.H. Hasan

1:50 INOR 916. New derivative of zinc(II) salphen complex: Biogenic amines optical sensor. **M. Sahudin**, N. Abd Karim, M. Suait, L. Tan

2:10 INOR 917. Chirality as key for determining the spin-state in Fe(II) spin crossover complexes. **D. Müller**, C. Knoll, J.M. Welch, M. Reissner, G. Giester, M. Wildner, P. Weinberger

2:30 INOR 918. Some novel metal complexes of mixed carboxylates-nitrogen containing lewis bases. **J.A. Obaleye**, A.A. Ajibola

2:50 INOR 919. Measuring the influence of metal ion on hydrogen atom reactivity in a series of group 10 complexes with a proton and redox non-innocent ligand. **B.J. Charette**, A.F. Heyduk

3:10 Intermission.

3:20 INOR 920. Synthesis and X-ray structures of family of dinuclear silver (I) pyrazolates. Assessment of their antibacterial efficacy. **S. Kandel**, I. Chakraborty, J. Stenger, R. Raptis



TECHNICAL PROGRAM

3:40 INOR 921. Second-generation zirconium photosensitizers: oxidative photoredox reactions with an air- and moisture-stable photocatalyst. **Y. Zhang**, C. Milsmann

4:00 INOR 922. Dinitrogen reduction and functionalization by multimetallic uranium complexes. **M. Mazzanti**

4:20 INOR 923. Supramolecular aggregates of single-molecule magnets. **T. Ghosh**, D. Takahashi, W. Wernsdorfer, K.A. Abboud, G. Christou

4:40 INOR 924. Solid-state structural rearrangement of a trinuclear copper complex due to ethylene adsorption. **D. Parasar**, N. Jayaratna, M.G. Cowan, R. Dias

Section I

Orange County Convention Center
Room W232A

Bioinorganic Chemistry: DNA, RNA & Inorganic Drugs

S. A. Koch, *Organizer*

R. E. Bachman, E. L. Que, *Presiding*

1:30 INOR 925. Determining structure-activity relationships of ruthenium complexes for Alzheimer's disease therapy. **M. Webb**, S. Huffman, S. Fisher, B. Wall, M. Will

1:50 INOR 926. Cancer cell death induced by rhenium anticancer agents. **J.J. Wilson**, S.C. Marker, A.P. King, C.C. Konkankit

2:10 INOR 927. Synthesis, characterization, and reactivity of novel platinum indazole complexes with potential anti-cancer activity. **R.E. Bachman**, K. Wills, K. Barwick, A. Bachman, O. Zalesak, K.A. Wheeler, G. Ferrence

2:30 INOR 928. Bio-inspired ruthenium(II) arene complexes: Synthesis, characterization and evaluation of their anticancer properties. **T.A. Khan**, K. Bhar, A.K. Sharma

2:50 INOR 929. Hydrogen peroxide as a hydride donor and reductant under biologically relevant conditions. **A.G. Tennyson**

3:10 INOR 930. Withdrawn

3:30 Intermission.

3:40 INOR 931. Transition metal platforms for ¹⁹F magnetic resonance imaging: sensors for biomarkers and chemical environments. **E.L. Que**

4:00 INOR 932. Oligotetrapyrrole complexes as efficient photochemotherapeutic agents with remarkably high phototoxicity indices. **J. Rosenthal**, A. Potocny, M. Martin

4:20 INOR 933. Enhancing photoinduced ligand dissociation in polypyridyl Ru(II) complexes via electronic control. **L.M. Loftus**, K.L. Fillman, T.N. Rohrabough, C. Turro



TECHNICAL PROGRAM

4:40 INOR 934. Exploring rhodium (II) paddlewheel complexes with tethered axial coordination as potential chemotherapeutic agents. **D. Moore**, A. Darko

5:00 INOR 935. Paramagnetic probes based on low-spin Fe(III) macrocyclic complexes. **P.B. Tsitovich**, J.R. Morrow

5:20 INOR 936. Singlet oxygen formation vs. photodissociation for protic ruthenium anticancer compounds. **E.T. Papish**, F. Qu, J.L. Gray, J. Park, Y. Kim

Activation of Light (C1-C4) Hydrocarbons: Theory & Experiments

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Innovative Chemistry & Materials for Electrochemical Energy Storage

Advanced Materials & Synthesis

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Light-Driven Chemistry: Photoelectrochemistry & Photocatalysis

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Chemical Catalysis for Bioenergy Consortium: Addressing Deactivation during Biomass Conversion

Sponsored by CATL, Cosponsored by ENFL, ENVR and INOR

THURSDAY MORNING

Section A

Orange County Convention Center
West Hall F2

Chemistry of Materials - Nanomaterials

C. G. Lugmair, *Organizer*
A. R. Tao, *Presiding*

8:30 INOR 937. PbS quantum dot surface chemistry investigated via purification with gel permeation chromatography. **A. Roberge**, M. Kelley, A.B. Greytak



TECHNICAL PROGRAM

9:10 INOR 938. Understanding the thermal conversion of Prussian blue analogues. **E.T. Nguyen**, D.A. Hardy, G.F. Strouse

9:30 INOR 939. Tailoring the covalent functionalization of boron nitride nanomaterials using the Billups-Birch reaction. **C. de los Reyes**, A.D. Smith McWilliams, K. Hernández, K. Walz Mitra, S. Yazdi, E. Ringe, M. Pasquali, A.A. Marti

9:50 INOR 940. Charge and energy transfer in donor-acceptor fluorescence pairs. **M. Yang**, M. Zamkov

10:10 Intermission.

10:25 INOR 941. Understanding growth behavior of boehmite and alumina nanoparticles for inks. **B.A. Hernandez-Sanchez**, N.S. Bell, T.J. Boyle, L.J. Treadwell, M. Casillas, F.A. Fasulo

10:45 INOR 942. Subcellular compartment targeting manipulated by porous coordination cages for cancer nanotherapy. **Y. Fang**

11:05 INOR 943. New nanocrystalline materials via room temperature cation exchange. C. Lin, H.D. Hall, A.T. Akinmola, A. Fall, N. Huszainey, C.R. Teeple, M.S. Elkommos, J.M. Miller, **P.G. Van Patten**

11:25 INOR 944. Copper sulfide nanocrystals for plasmon-enhanced multiphoton optical absorption. **A.R. Tao**

11:45 INOR 945. Alloyed upconverting nanoparticles for multiphoton imaging and lasing at ultralow powers. **B.E. Cohen**, B. Tian, A. Fernandez-Bravo, E. Chan, P. Schuck

Section B

Orange County Convention Center
Room W224B

Magnetism Across Length Scales

Magnetism in Molecules and Molecule-Based Materials

S. Hill, M. Shatruk, G. F. Strouse, *Organizers*
G. Christou, S. Demir, *Presiding*

8:30 INOR 946. Magnetic quantum tunneling in Fe-doped Li_3N : stable but manipulable states. **E. del Barco**, M. Fix, J. Atkinson, P. Canfield, A. Jesche

8:55 INOR 947. Ligand-induced tuning of the ground state spin of Ce_3Mn_8 clusters, a molecular mimic of the perovskite repeating unit. **T. Cao**, K.A. Abboud, G. Christou

9:15 INOR 948. Multireference ab-initio studies of magnetic properties of TbPc2-type single-molecule magnets. **K. Park**

9:40 INOR 949. Magnetic blocking and coercivity in lanthanide single-molecule magnets. **S. Demir**, F. Benner, C.M. Legendre

10:05 Intermission.



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- 10:20 INOR 950.** Controlled growth of Mn₁₂ single-molecule magnet polymers and oligomers. **C. Lampropoulos**
- 10:45 INOR 951.** Exploring the coordination chemistry of mpmH as a new ligand in 3d-cluster chemistry. P. Abbasi, D.I. Alexandropoulos, G. Delle Monache, T.C. Stamatatos, **M. Pilkington**
- 11:10 INOR 952.** Supramolecular aggregates of single-molecule magnets. **T. Ghosh**, K.A. Abboud, G. Christou
- 11:25 INOR 953.** Halogenated and unsubstituted lanthanoid (III) diphthalocyanines as potential qubits. **M. Dailey**, N. Byrne, K. McKenzie, C. Besson
- 11:40 INOR 954.** Roles of *f*-electrons in [Mn_m]Ce_n magnetic particles. **H. Cheng**, D. Chen, J. Gu, T. Ghosh, X. Zhang, G. Christou

Section C

Orange County Convention Center
Room W224A

Coordination Chemistry: Synthesis & Characterization

A. Larsen, *Organizer*
E. R. Trivedi, *Presiding*

8:30 INOR 955. Near-infrared emission of heterobimetallic Zn²⁺/Ln³⁺ schiff base complexes. J. Farnsworth, S. Eliseeva, M. Zeller, S. Petoud, **E.R. Trivedi**

8:50 INOR 956. Withdrawn

9:10 INOR 957. Unusual coordination chemistry and bond activation involving light alkaline earth metal carbene complexes. J.E. Walley, O. Wong, L. Freeman, G. Wang, D. Agakidou, G. Briener, D. Dickie, **R.J. Gilliard**

9:30 INOR 958. Synthesis of manganese-based precursors and nanoparticles for printing purposes. **T. Nguyen**, T.J. Boyle, L.J. Treadwell

9:50 INOR 959. Synthesis and characterization of metal alkoixdes modified by Mannich condensation generated multi-dentate alcohols for tailored materials production. **T.J. Boyle**, J.R. Farrell

10:10 Intermission.

10:20 INOR 960. Novel synthetic strategies towards the isolation of main group metal hydrides. **L. Freeman**, G. Wang, D. Dickie, R.J. Gilliard

10:40 INOR 961. Developing methods to cross-bridge pentaazamacrocycles. **T.J. Hubin**, A.G. Oliver, J.A. Krause, T.J. Prior

11:00 INOR 962. Self-sorting behavior in two dynamic covalent chemistry systems generated from pnictogen-assisted iodine oxidation. **N. Phan**, L.N. Zakharov, D.W. Johnson



TECHNICAL PROGRAM

11:20 INOR 963. Synthesis and characterisation of transition metal complexes with a two-photon absorbing photochromic ligand. **A.W. Woodward**, L. Jones, L.S. Natrajan

Section D

Orange County Convention Center
Room W224C

Electrochemistry

N. S. Radu, *Organizer*
A. Paolella, *Presiding*

8:30 INOR 964. Withdrawn

8:50 INOR 965. Carbide-derived novel mesoporous carbons for energy storage. **A.T. Brown**, V.S. Agrawal, M.C. Thomas, J. Lin, J.P. Ferraris, Y.J. Chabal, K.J. Balkus

9:10 INOR 966. Structure-function relationships in cobalt water oxidation electrocatalysts and their application for zinc electrorefining. C. Chen, S. Moncho Escriva, E.N. Brothers, **S.W. Sheehan**

9:30 INOR 967. Synthesis new hydrophobic cross-linked fluorinated polymers for corrosion protection on steel substrate. **W. Yaseen**

9:50 INOR 968. Reaction between metal disulfides interlayer and polysulfides in lithium-sulfur batteries. **A. Paolella**, K. Zaghbi

Section E

Orange County Convention Center
West Hall F4

Inorganic Catalysts

S. A. Koch, *Organizer*
M. Z. Ertem, R. F. Semeniuc, *Presiding*

8:30 INOR 969. Photochemical and thermal analysis of phosphine modified hydrogenase model compounds. **C.F. Works**

8:50 INOR 970. Rapid alcoholysis of cyclic esters using aluminium alkoxide. **S. Yimthachote**, K. Phomphrai

9:10 INOR 971. Withdrawn

9:30 INOR 972. Quantum chemical characterization of photocatalytic CO₂ reduction by transition metal complexes: Mechanistic insights from ¹³C kinetic isotope effects. **M.Z. Ertem**, A.M. Angeles Boza, T.W. Schneider

9:50 Intermission.



TECHNICAL PROGRAM

10:10 INOR 973. Probing the O-H and C-H activation for the neutral and charged species of ruthenium mono-oxide species. Ground and excited states calculations. **N.M. Almeida**, I.R. Ariyaratna, E. Miliordos

10:30 INOR 974. Magnetic and recyclable nickel nanoparticles for selective semi-hydrogenation of alkynes to (Z)-alkenes. **A.M. López Vinasco**, L.M. Martínez-Prieto, J.M. Asensio, J. Campora, B. Chaudret, P.W. van Leeuwen

10:50 INOR 975. Constructing exposed equatorial positions of metal centers in MOFs and developing their catalytic properties. S. Yuan, **P. Zhang**, H. Zhou

11:10 INOR 976. Encapsulation of metal nanocluster in amino acid functionalized metal-organic framework for heterogeneous catalysis. **T. Goh**

11:30 INOR 977. Dinuclear copper(II) bioinspired complexes: Investigations of their catecholase activity. **R.F. Semeniuc**, N.P. Jayaweera, A. Hall, K.A. Wheeler, M. Konkle

Section F

Orange County Convention Center
Room W224D

Inorganic Spectroscopy

C. V. Popescu, *Organizer*
J. A. Telser, *Presiding*

8:30 Introductory Remarks.

8:35 INOR 978. Withdrawn

8:55 INOR 979. Advanced paramagnetic resonance studies on high-oxidation state iron corroles. **J.A. Telser**, A. Schnegg, K. Holldack, J. Krzystek, S. Stoian, Z.J. Tonzetich, K.E. Thomas, A. Ghosh

9:15 INOR 980. Exploring the spectroscopic intricacies of heterometallic chain compounds. **J. Chipman**, J.F. Berry, D. Brogden

9:35 INOR 981. Development of a cobalt(III) polypyridyl spectrochemical series for application in understanding the ligand field electronic structure in iron(II)-based chromophores. **J.T. Yarranton**, J.K. McCusker

9:55 Intermission.

10:00 INOR 982. Investigating the photophysics and photochemistry of [(diimine)Re(CO)₄]⁺ using fast time-resolved IR spectroscopy. **M. George**

10:20 INOR 983. Novel spectroscopic technique for determination of energy levels and charge transfer in water-insoluble inorganic compounds: Solid-state synchronous luminescence spectroscopy. A. Alzahrani, S. Taylor, **A. Samokhvalov**

10:40 INOR 984. In-silico inorganic spectroscopy using the local spectroscopy data initiative (LSDI). **S. Dwaraknath**, S.E. Hayes, S. Ong, K. Persson



TECHNICAL PROGRAM

11:00 INOR 985. Steric control of MLCT deactivation in low spin Fe(II) polypyridyls. **B. Paulus**, S. Adelman, J.K. McCusker

Section G

Orange County Convention Center
West Hall B4 - Theater 10

Chemistry of Materials - Nanomaterials

C. G. Lugmair, *Organizer*
M. A. Mahmoud, V. Mochalin, *Presiding*

8:30 INOR 986. New tellurium precursor for nanocrystal synthesis: Tris(dimethylamino)phosphine telluride. **H. Sun**, F. Wang, W.E. Buhro

8:50 INOR 987. Enhancing the optical properties of semiconducting 2D materials by plasmonic nanoparticle 2D arrays. **M.A. Mahmoud**

9:10 INOR 988. Ethanoic acid-capped ruthenium nanoparticles: a promising HER catalyst? R. Gonzalez-Gomez, I. De Rosal, K. Philippot, **R. Poteau**

9:30 INOR 989. New insights into the role of water in chemical transformations of $Ti_{n+1}C_n$ MXenes. **S. Huang**, V. Mochalin

9:50 INOR 990. Composition tunable colloidal $Cs_{1-x}FA_xPbI_3$ perovskite nanocrystals for high V_{OC} solar cells. **A. Hazarika**, Q. Zhao, A. Gaulding, J. Christians, B. Dou, A. Marshall, T. Moot, J. Berry, J.C. Johnson, J. Luther

10:10 Intermission.

10:25 INOR 991. Preparation of Mn (II) doped CdSe nanowires via diffusion doping. **P. Kittikhunnatham**, A.B. Greytak

10:45 INOR 992. DNA-gold bioconjugate with outstanding resistance to nuclease degradation. S. Panickar, **A. Mohamed**

11:05 INOR 993. Environment sensitive photoresponse of spontaneously partially oxidized 2D transition metal carbides (MXenes). **V. Mochalin**, S. Chertopalov

11:25 INOR 994. Radiation stability of additive manufactured boron carbide-containing epoxy and silicone. **L.J. Treadwell**, K.M. Hattar, A. Monterosa, K. Manning, A.W. Cook

11:45 INOR 995. Comparing the effects of chemical doping and contact doping in 2D monolayers. **S.S. Esdaille**

Section H

Orange County Convention Center
West Hall B4 - Theater 11

Chemistry of Materials - Materials for Energy & Catalytic Applications



TECHNICAL PROGRAM

C. G. Lugmair, *Organizer*
E. G. Gillan, *Presiding*

8:30 INOR 996. Synthesis of ultrathin Au nanowires based on a novel, facile and rapid synthetic strategy. **X. Jiang**, Y. Tang, J. Zhou

8:50 INOR 997. Encapsulation of Ni₃Fe nanoparticles in n-doped carbon nanotube-grafted carbon nanofibers as high-efficiency hydrogen evolution electrocatalysts. **T. Li**, Y. Tang, Y. Zhang

9:10 INOR 998. Transition metal doped mesoporous CoP and FeP nanomaterials for the hydrogen evolution reaction. **M.R. Shakil**, H. Tasnim, A. Shirazi Amin, A. Meguerdichian, J.P. Dubrosky, P. Kerns, S.L. Suib

9:30 INOR 999. One-pot hydrothermal synthesis of vanadium doped cesium tungsten bronze: Enhanced HER performance upon vanadium incorporation. **H. Tasnim**, M.R. Shakil, A. Meguerdichian, L. Tabassum, J. Macharia, S.L. Suib

9:50 INOR 1000. AlFe₂B₂ as water oxidation electrocatalyst. **D.K. Mann**, J. Xu, N.E. Mordvinova, V. Yannello, J. Sousa, O.I. Lebedev, Y.V. Kolen'ko, M. Shatruk

10:10 Intermission.

10:25 INOR 1001. Deliberate synthetic control of one-dimensional α-MnO₂ type materials: Impact on resultant electrochemistry. **K.J. Takeuchi**, A.C. Marschilok, E.S. Takeuchi

10:45 INOR 1002. Comparison of structure, properties, and photocatalytic activity of polymeric carbon nitrides synthesized from a reactive trichloromelamine precursor. **E.G. Gillan**, A.T. Montoya

11:05 INOR 1003. Probing the material corrosion chemistry at the semiconductor/electrolyte interface for sustainable solar fuel generation. **W. Yu**, N.S. Lewis

11:25 INOR 1004. Linking molybdenum-sulfur clusters for electrocatalytic hydrogen evolution. **Z. Ji**, C. Trickett, X. Pei, O.M. Yaghi

Section I

Orange County Convention Center
Room W232A

Environmental & Energy-Related Inorganic Chemistry

S. A. Koch, *Organizer*
M. B. Chambers, J. Schrier, *Presiding*

8:30 INOR 1005. Light-initiated C–H activations by high valent molybdenum dioxo complexes. **M.B. Chambers**, S. Fosshat

8:50 INOR 1006. Single molecule dirhodium photocatalyst for production of dihydrogen using red to near-infrared light. **C. Xue**, T.J. Whittemore, J. Huang, C. Turro



TECHNICAL PROGRAM

9:10 INOR 1007. Toward a novel treatment for the removal of deposited uranium in case of human contamination. **A. Younes**, A. Duda, J. Ali, M. Cao, C.M. Drain, S. Alexandratos

9:30 INOR 1008. Polymer-assisted solution strategy: from thin films to patterns. **G. Zou**

9:50 INOR 1009. Electrocatalytic CO₂ reduction by imidazolium-functionalized molecular catalysts at mild potentials. **S. Sung**, X. Li, J. Meeder, J. Panetier, M. Nippe

10:10 Intermission.

10:30 INOR 1010. "Robot-ready" halide perovskite synthesis. **J. Schrier**

10:50 INOR 1011. Catalytic CO₂ reduction by mononuclear and dinuclear Re(I) complexes linked to anthracene. **S. Sinha Roy**, W. Yang, N. Liyanage, S. Davis, E. Amaty, J.H. Delcamp, J.W. Jurss

11:10 INOR 1012. Withdrawn

11:30 INOR 1013. Rhenium complexes with second coordination sphere functionality for electrocatalytic CO₂ reduction. **K. Talukdar**, J. Vaughan, S. Sahil, J.W. Jurss

Section J

Orange County Convention Center
Room W232B

Organometallic Chemistry: Applications to Organic Transformations

N. S. Radu, *Organizer*
K. Ding, *Presiding*

8:30 INOR 1014. Novel homogeneous cobalt catalyst for dceptorless dehydrogenations and dehydrogenative couplings of alcohols *via* "Borrowing Hydrogen". **K. Ding**, S. Xu

8:50 INOR 1015. Iron-catalyzed transfer hydromagnesiation of vinyl arenes: Mechanistic insights and indications of competing alkene insertion pathways. **J.A. Rogers**, B.V. Popp

9:10 INOR 1016. Novel dirhodium paddlewheel catalysts: Synthesis and application towards diazo-mediated cyclopropanation reactions. **C. Zavala**, A. Darko, D. Cressy, W. Sheffield

9:30 INOR 1017. Iron catalyzed hydrosilylation of esters. **S.R. Tamang**, A.F. Cozzolino, M. Findlater

9:50 INOR 1018. Theoretical structure-activity study of a new bifunctional reaction mode between four coordinate d⁴-metal-nitride complexes and carboxylic acids. M. Ataya, B.M. Lindley, A.J. Miller, **F. Hasanayn**

10:10 INOR 1019. Withdrawn

10:30 INOR 1020. Study of molybdenum catalysts for deoxydehydration (DODH) of vicinal diols. **T.C. Siu**, M.J. Lunn, A. John



TECHNICAL PROGRAM

10:50 INOR 1021. Hydrogenation knölkler derivative catalysts: On the way to functionalize CO₂. **A. Poater**

11:10 INOR 1022. Utilization of LUMO lowering boronic acids as organocatalysts within the PKR. **J.D. Ricker**, L. Geary

Section K

Orange County Convention Center
West Hall B4 - Theater 20

Lanthanide & Actinide Chemistry

A. De Bettencourt Dias, *Organizer*
T. Forbes, H. La Pierre, *Presiding*

8:30 INOR 1023. Understanding chemical bonds in actinide complexes through the interacting quantum atom energy decomposition analysis. **C.A. Celis-Barros**, T.E. Albrecht-Schmitt

8:50 INOR 1024. Zinc schiff base complexes as antennae for sensitization of near-infrared lanthanide luminescence. **J. Farnsworth**, S. Eliseeva, M. Zeller, S. Petoud, E.R. Trivedi

9:10 INOR 1025. Activation of the actinyl asymmetric stretching band in Raman spectroscopy: How, when, and why. **T. Forbes**

9:30 INOR 1026. Spatial control over Bi³⁺-doped YVO₄:Eu³⁺ core-shell nanoparticles and the effects of weak electric field on the photoluminescence behavior. **K. R Bajgiran**, A.T. Melvin, J. Dorman

9:50 Intermission.

10:00 INOR 1027. Perturbing the balance between ionic and covalent bonding in early actinide complexes. **H.S. La Pierre**, J. Su, N.T. Rice, T. Gomba, D. Russo, L.M. Aguirre-Quintana, J. Bacsa, E.R. Batista, P. Yang

10:20 INOR 1028. Structural and Spectroscopic Investigation of Aged Plutonium Oxalate Specie. **A. De Bettencourt Dias**, J.F. Corbey

10:40 INOR 1029. Improving the luminescence of Ln^{III} (Ln = Eu, Tb, Eu_xTb_y or Tm)-doped ZnAl₂O₄ nanospinels with a pyridine-2,6-bis(ethyl ester)-functionalized polymer. **R.A. Tigaa**, D.A. Hardy, A. De Bettencourt Dias, G.F. Strouse

11:00 INOR 1030. Insights into PuO₂ Microstructure Evolution as a Function of Processing Conditions. **A. De Bettencourt Dias**, L.E. Sweet

Innovative Chemistry & Materials for Electrochemical Energy Storage

General

Sponsored by ENFL, Cosponsored by CATL, INOR and PMSE



Chemical Catalysis for Bioenergy Consortium: Addressing Deactivation during Biomass Conversion

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Elucidation of Mechanisms & Kinetics on Surfaces

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THURSDAY AFTERNOON

Section A

Orange County Convention Center
West Hall F3

Coordination Chemistry: Synthesis & Characterization

A. Larsen, *Organizer*

E. M. Fatila, E. M. Villa, *Presiding*

1:30 INOR 1031. Oxygen-exchange kinetics of the anderson-type polyoxometalate Ion $\text{TeMo}_6\text{O}_{24}^{6-}$ in aqueous solution. **E.M. Villa**, G.M. Kuhl

1:50 INOR 1032. New ligand condensed from two identical thioamides into a S^NS thione-thiolate chelate: Pt(II) complexes and electrochemistry. **L. Zuckerman**, A.S. Hyre, J.K. Elinburg, R.N. Loy, A.L. Rheingold, L.H. Doerrer

2:10 INOR 1033. Studies on bis(cyclohexyl isocyanide) gold(I) complexes: From examining the mechanism of vapor-induced single-crystal-to-single-crystal phase transitions to varying non-coordinating anions. **P.M. Luong**, V. Moshayedi, M.M. Olmstead, A.L. Balch

2:30 INOR 1034. Reactivity of NHC-gold(I) complexes with tris(pyrazolyl)borate ligands: Preparation of heterobimetallic species and highly protected gold(I) cations. **D. Mendoza-Espinosa**, V. Salazar-Pereda, A. Priante-Flores

2:50 INOR 1035. Resolution of the chiral octanuclear iron-oxo-pyrazolate to its *P* and *M* enantiomers. **K. Lazarou**, K. Gonzalez, R.G. Raptis

3:10 Intermission.

3:20 INOR 1036. Investigating mechanochemical approaches for the synthesis of lanthanide complexes. **E.M. Fatila**, R.E. Cooper, B.J. Cooper, A.A. Brown, N.N. Daanen, S.E. Skrabalak, K. Preuss

3:40 INOR 1037. Exploring electronic communication between metal centers facilitated by non-innocent ligands. **C. Bell**, K. Clark, C. Moore



TECHNICAL PROGRAM

4:00 INOR 1038. Synthesis, isolation, and comparative studies on the transition metal diselenodiphenylphosphinate complexes, $M(\text{Se}_2\text{PPh}_2)_3$ ($M = \text{V}, \text{Cr}$). **J.L. Brown**

4:20 INOR 1039. Synthesis and characterization of pyrazolate supported $\text{Cr}^{\text{III}}_3(\mu_3\text{-O})$ cores. **J.M. Lopez**, R. Raptis

4:40 INOR 1040. Synthesis and characterisation of 4-aminopyridine copper(II) complexes. **O.O. Onawumi**, A.O. Ibrahim, O.A. Odunola

Section B

Orange County Convention Center
Room W224B

Magnetism Across Length Scales

Magnetism in Molecules and Molecule-Based Materials

G. Christou, S. Hill, G. F. Strouse, *Organizers*
M. Shatruk, *Organizer, Presiding*

1:30 INOR 1041. Magnetoelectric coupling at spin state transitions in Mn-based molecular compounds. **V. Zapf**, S. Chikara, V. Jakobsen, S. Lin, C. Batista, E. Krenkel, J. Eckert, B. Scott, N.C. Smythe, E. Dobbelaar, I. Kühne, G. Morgan

1:30 INOR 1042. Control of the speed of a light-induced spin transition through mesoscale core-shell architecture. **D.R. Talham**

1:30 INOR 1043. Conducting Fe(II) spin crossover complexes with organic TCNQ radicals. **O. Ungor**, H. Phan, M. Shatruk

1:30 INOR 1044. Design, synthesis, and investigation of new ligand combinations for light-responsive Fe(complexes). **G. Donalson**, Ö. Üngör, M. Jo, M. Shatruk

1:30 INOR 1045. Ultrafast transmission electron microscopy for the study of light-induced phase transitions in strongly cooperative spin-crossover materials. **R. van der Veen**

1:30 Intermission.

1:30 INOR 1046. Probing spin-phonon coupling in metal complexes. **Z. Xue**, D.H. Moseley, S. Stavretis, Z. Lu, M. Ozerov, J. Ludwig, D. Smirnov, R. Richardson, G. Knight, K. Thirunavukkuarasu, Y. Cheng, L.L. Daemen, A.J. Ramirez-Cuesta, Z. Zhu, M. Guo, J. Tang, F. Fei, H. Cui, X. Chen

1:30 INOR 1047. Assessing the magnetic properties of low-coordinate iron(II) complexes supported by β -diketiminato ligands and phosphorus-based co-ligands. **S. Stoian**

1:30 INOR 1048. Slow magnetic relaxation in axial lanthanide single molecule magnets. **A.B. Canaj**, M.K. Singh, C. Wilson, G. Rajaraman, M. Murrie

1:30 INOR 1049. Ce/Mn clusters from reductive aggregation: Unusual long-range Mn---Mn exchange-coupling through Ce^{IV} . **S. Das Gupta**, K.A. Abboud, G. Christou



TECHNICAL PROGRAM

1:30 Concluding Remarks.

Section C

Orange County Convention Center
Room W224A

Chemistry of Materials - Nanomaterials

C. G. Lugmair, *Organizer*
S. M. Kuebler, H. Lu, *Presiding*

1:30 INOR 1050. Copper indium selenide nanocrystal defects and surface chemistry. **D.W. Houck**, B.A. Korgel

1:50 INOR 1051. Surface modification of layered structured nanomaterials for drug delivery. **J.L. Colon**, J. González-Villegas, L. Ramírez-Pagán, M. Martínez

2:10 INOR 1052. Controlling the nanoscale morphology of silver deposited by electroless metallization. **S.M. Kuebler**, C.N. Grabill

2:30 INOR 1053. Structural design of lanthanide-doped upconversion nanocrystals for enhancing the multiphoton upconversion. B. Zhou, B. Tang, **Y. Ma**, T. Zhai

2:50 INOR 1054. Synthesis of pure and bare III-V Nanocrystals from bulk metals in a low temperature plasma. **N.B. Uner**, E. Thimsen

3:10 Intermission.

3:25 INOR 1055. Tunable luminescence in rare earth doped core-shell nanophosphors via adaptive absorption of the transition metal ions. **P. Darapaneni**, J. Dorman

3:45 INOR 1056. Characterization of quantum dots using dynamic nuclear polarization (DNP) surface enhanced NMR spectroscopy (SENS) to achieve high sensitivity. **Y. Chen**, M.P. Hanrahan, R. Blome-Fernández, J. Vela, A.J. Rossini

4:05 INOR 1057. Role of holes and non-planar distortions in borophenes, an *ab-initio* study. **N. Karmodak**, E.D. Jemmis

4:25 INOR 1058. Singlet fission of pentacene molecule on perovskite nanocrystals through dexter singlet energy transfer. **H. Lu**, X. Chen, J.C. Johnson, M.C. Beard

4:45 INOR 1059. Synthesis of multi-component nanostructures through controlled structural symmetry breaking of silver-halide intermediates. **B. Stephens**, T.J. Kempa

Section D

Orange County Convention Center
Room W224C

Coordination Chemistry: Synthesis & Characterization



TECHNICAL PROGRAM

A. Larsen, *Organizer*
M. Stollenz, *Presiding*

1:30 INOR 1060. Group 11 metal chloride bis(amidine) complexes upon insertion into NH...N' hydrogen bonds: Synthesis, structures, and molecular dynamics in solution. **M. Stollenz**, O. Ugarte Trejo, C. O'Dea, A. Ehnbohm, N. Bhuvanesh, C. McMillen

1:50 INOR 1061. Decoding the nuclear coordinate for ground-state recovery in iron(II) polypyridyls. **S. Adelman**, J.K. McCusker

2:10 INOR 1062. Magneto-structural characterization of two novel ytterbium frustrated magnets. **N. Jiang**, X. Bai, J. Bacsa, M. Mourigal, H.S. La Pierre

2:30 INOR 1063. Targeting the sub-zeptomolar Cu(I) affinity regime with preorganized phosphine sulfide-stabilized phosphine ligands. **F. Saeedifard**, T.M. Morgan, C.J. Fahrni

2:50 INOR 1064. Monovalent coinage metals and dithiophosphonate based ligands for functional materials. **L. Harris**, M.A. Omary

3:10 Intermission.

3:20 INOR 1065. Folding, self-assembly and characterization of giant metallo-supramolecules with atomic resolution. **Y. Li**, Z. Zhang, B. Song, Y. Zhang, S.W. Hla, X. Li

3:40 INOR 1066. Template-free synthesis of multinuclear complexes that contain macrocyclic bis(pyridine-diimine) and bis(pyridine-dienamido) ligands. **E. Reinhart**, R.F. Jordan

4:00 INOR 1067. Beryllium metal in liquid ammonia, an approach to the synthesis of beryllium amides. **M. Müller**, M.R. Buchner

4:20 INOR 1068. Synthesis, structure and magnetic studies of novel open-cage hexanuclear copper pyrazolato complexes. **D.I. Kreiger**, L. Mathivathanan, R. Herchel, R. Raptis

4:40 INOR 1069. Synthesis and characterization of a nickel(II) diphosphinimino NCN-pincer complex that may contain an agostic interaction. **K. Sheriff**, S. Pitts, D. Rucker, G. Guillet

Section E

Orange County Convention Center
West Hall F4

Main Group Chemistry

T. Hudnall, *Organizer*
K. Chansaenpak, *Presiding*

1:30 INOR 1070. Group 13 and 14 complexes supported by multidentate $N_2O_2^{3-}$ formazanate ligands. **R.R. Maar**, S. Barbon, J.B. Gilroy



TECHNICAL PROGRAM

- 1:50 INOR 1071. Supramolecular chemistry and chirality of tris(pyridyl) aluminate ligands. **R. Garcia-Rodriguez**
- 2:10 INOR 1072. Withdrawn
- 2:30 INOR 1073. Nanoencapsulation of near infrared boron-based dye: the strategy to enhance water solubility and biocompatibility. **K. Chansaenpak**, S. Tanjindaprateep, A. Kamkaew
- 2:50 Intermission.
- 3:00 INOR 1074. Interesting excited-state behavior in borafuorene derivatives. **J. Cassidy**
- 3:20 INOR 1075. Elucidation of the regiochemistry of acid-catalyzed hydroxylation of dodecaborates and iodododecaborates. **J.A. Dopke**, Z. Lincoln, J.W. Mazzuca, R.J. Staples
- 3:40 INOR 1076. “Simple” cationic zinc- and gallium-based Lewis acids. **R. Wehmschulte**, D.R. Powell
- 4:00 INOR 1077. Effects of photochromic moieties on pendant groups that participate in secondary bonding interactions. **M.C. Andrews**, A.F. Cozzolino
- 4:20 INOR 1078. Importance of secondary interactions such as $M \cdots \pi$ and $M \cdots F$ in alkaline earth metal complexes. **M.M. Gillett-Kunnath**, K. Ruhlandt-Senge

Section F

Orange County Convention Center
Room W224D

Nanoscience

B. G. Trewyn, *Organizer*
M. A. Walters, *Presiding*

- 1:30 INOR 1079. Attoliter polymer reactors as combinatorial tools for understanding alloy nanocrystal structure–function relationship. **J.S. Du**, V.P. Dravid, C.A. Mirkin
- 1:30 INOR 1080. David versus goliath: Effects of sterics and electronics on ligand binding at nanocrystal surfaces. **N.C. Anderson**, J.S. Owen, P. Chen, A. Buckley, J. De Roo
- 1:30 INOR 1081. Rational phase control in the synthesis of $CuInSe_2$ nanocrystals. **B.A. Tappan**, G. Barim, J. Kwok, R.L. Brutchey
- 1:30 INOR 1082. High-throughput, continuous flow synthesis of nanoparticle catalysts as a safe and sustainable nanomanufacturing method. **E. Roberts**, R.L. Brutchey
- 1:30 INOR 1083. Growth of CNT-weaved 2D hybrid films for flexible electronics. **H. Li**, L. Li, J. Shi, E. Shi, Y. Fang, A. Cao
- 1:30 INOR 1084. Self-assembly of macrocyclic supramolecule with multiple types of metal ions and characterization by STM. L. Wang, **B. Song**, Y. Li, X. Li, Y. Zhang, S. Hla



TECHNICAL PROGRAM

1:30 Intermission.

1:30 INOR 1085. Multimodal polysilsesquioxane nanoparticles for the combined treatment of triple-negative breast cancer using chemo, photodynamic and gene therapies. **J.L. Vivero-Escoto**

1:30 INOR 1086. Measuring the temperature of a nanoaperture optical trap with a single quantum dot. **C. Zhang**, R. Gelfand, J. Li

1:30 INOR 1087. Mucin1-specific redox-responsive mesoporous silica nanoparticles for combinatorial therapy of pancreatic ductal adenocarcinoma. **J.L. Vivero-Escoto**, M. Tarannum, P. Mukherjee

1:30 INOR 1088. Amide-carboxylate oligomeric nanoparticles for metal ion binding. **M.A. Walters**, T. Sang, T. Rubio, F. Maistrovicz, J. Kim

1:30 INOR 1089. Polyarylated boranes exhibit electrochromism and redox-controlled fluorescence switching. **M.W. Lee**

Section G

Orange County Convention Center
West Hall B4 - Theater 10

Bioinorganic Chemistry: Proteins & Enzymes & Model Systems

S. A. Koch, *Organizer*

P. Basu, K. N. Green, *Presiding*

1:30 INOR 1090. Hydrogen bonding vs acidity: Ligand tuning alters Cu/NO reductive coupling product in a Cu-chelate model of NOR. **M. Bhadra**, K.D. Karlin

1:50 INOR 1091. Substrate selectivity in asymmetric oxo-Mo(IV) dithiolene complexes with a MoOS₄core. **P. Basu**, S.A. Dille, B. Mogesa

2:10 INOR 1092. Evaluation of oxygen-transfer properties of dinuclear copper pyrazolato complexes. **L. Mathivathanan**, S. Herrera, R. Raptis

2:30 INOR 1093. Rational design of artificial hydrogenases. **S. Chakraborty**, D. Selvan, P. Prasad

2:50 INOR 1094. Catalytic aerobic oxidation of alcohols by copper complexes bearing redox-active ligands with tunable H-bonding groups. **K. Rajabimoghadam**

3:10 INOR 1095. Ultrafast vibrational spectroscopy reveals non-additive effects of mutation on binding site structure. **S.C. Edington**, C.R. Baiz, D.B. Halling, T.R. Middendorf, R.W. Aldrich, S. Bennett

3:30 Intermission.

3:50 INOR 1096. Withdrawn

4:10 INOR 1097. Withdrawn



TECHNICAL PROGRAM

4:30 INOR 1098. Withdrawn

4:50 INOR 1099. Manganese and iron tetraazamacrocyclic monomers, dimers, and trimers (oh my!). **K.N. Green**, T.J. Hubin, H.M. Johnston, S.M. Brewer

5:10 INOR 1100. Insights into the design of synthetic analogues of metalloenzymes. T.J. Paul, G. Sharma, V. Jayasinghe-Arachchige, Q. Hu, **R. Prabhakar**

Section H

Orange County Convention Center
West Hall B4 - Theater 11

Organometallic Chemistry: Catalysis

N. S. Radu, *Organizer*
M. G. Campbell, *Presiding*

1:30 INOR 1101. Oxygen atom transfer from nitrogen oxides for applications in organic synthesis. **L. Geary**

1:50 INOR 1102. Study of Rh catalysts for the single-step oxidative alkenylation of benzene. **W. Zhu**, J. Chen, Z. Luo, T.B. Gunnoe

2:10 INOR 1103. Exploring redox catalysis with well-defined dinuclear silver complexes. **M.G. Campbell**

2:30 INOR 1104. Tuning the catalytic activity/selectivity of water-soluble bimetallic RuPt nanoparticles by modifying their surface metal distribution. **D. Bouzouita**, S. Tricard, L. Martinez-Prieto, L. Guy, B. Chaudret

2:50 INOR 1105. Reactivity and catalytic properties of substituted η^4 -cyclopentadiene complexes of rhodium. **Y. Peng**, D. Lionetti, J. Douglas, V. Day, J.D. Blakemore

3:10 INOR 1106. CO₂ hydrogenation to formate via a Co(-1/1) cycle featuring two stable cobalt dihydrogen complexes. **M.V. Vollmer**, J. Ye, C.C. Lu, J.C. Linehan, L. Gagliardi

3:30 INOR 1107. Molecular iron complexes as catalysts for CO₂/epoxide coupling and copolymerization: Epoxide deoxygenation competes with carbonate formation. **C.M. Kozak**, F.M. Kerton, K.A. Andrea, E.D. Butler, T.S. Anderson

3:50 INOR 1108. Hydrogenation catalysis with [Co, Rh] and [Co, Ir] heterobimetallic complexes. **A. Kumar**, V. Day, J.D. Blakemore

4:10 INOR 1109. Mapping out the mechanism of Mn(I)-catalysed C–H bond functionalisation. **L. Hammarback**, I. Clark, I. Sazanovich, M. Towrie, A. Robinson, I.J. Fairlamb, J. Lynam

4:30 INOR 1110. Rare earth metal catalyzed intermolecular hydroamination of alkenes. **K. Hultzs**, J.B. Soltys, L. Schickhofer

Section I



TECHNICAL PROGRAM

Orange County Convention Center
Room W232A

Organometallic Chemistry: Synthesis & Characterization

N. S. Radu, *Organizer*
K. M. Clark, E. B. Hulley, *Presiding*

1:30 INOR 1111. Chemistry and photophysics of cyclometalated carbene platinum complexes: from theory to efficient phosphorescent emitters for OLED applications. **P. Piermaria**, T. Strassner

1:50 INOR 1112. Use of ligand steric properties to control the thermodynamics and kinetics of oxidative addition and reductive elimination with pincer-ligated Rh complexes. **S. Gu**, K.H. Taylor, G. Fortman, R.J. Nielsen, D. Dickie, W.A. Goddard, T.B. Gunnoe

2:10 INOR 1113. Design and reactivity of copper and zinc based frustrated Lewis pairs. **K.M. Clark**, Y. Gao, J. Byrd, T.J. Morris, S. Hall, C. Moore

2:30 INOR 1114. Synthesis, characterisation and catalytic activity of gold, rhodium and palladium complexes featuring fluorinated *N*-heterocyclic carbene ligands. **M. Jamil**, A.K. Brisdon

2:50 INOR 1115. Synthesis of Fe(IV)-Imids with a 16-membered, macrocyclic tetra NHC ligand. **M.R. Anneser**, G. Elpitiya, X.B. Powers, E.J. Johnson, J. Townsend, K.D. Vogiatzis, T. Betley, D.M. Jenkins

3:10 INOR 1116. Visible light photocleavage of metal-carbon bonds in organopalladium complexes. **P.M. Waddell**, B.P. Carrow

3:30 INOR 1117. Rhodium alkylidene formation from redox cascade activation of haloalkanes: Mechanism, scope, and [Rh=CR₂] reactivity. **E.B. Hulley**, T. Morrow, J. Gipper

3:50 INOR 1118. Donor-acceptor stabilized P₂ and As₂ complexes from oxidative coupling of terminal rhenium pnictides. **J. Abbenseth**, A. Hinz, C. Würtele, J.M. Goicoechea, M. Lein, S. Schneider

4:10 INOR 1119. Synthesis and characterization of a series of late transition metal carbene complexes. **M. Hoffbauer**

4:30 INOR 1120. Metal-ligand cooperative synthesis of benzonitrile via electrochemical reduction and photolytic splitting of dinitrogen. **F. Schendzielorz**, S. Schneider

Section J

Orange County Convention Center
Room W232B

Chemistry of Materials - Metal Organic Frameworks

C. G. Lugmair, *Organizer*
E. D. Bloch, Y. Fang, *Presiding*



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

1:30 INOR 1121. SION-105: A selective, fast-response, regenerable metal–organic framework for sampling excess fluoride levels in drinking water. **F.M. Ebrahim**, T.N. Nguyen, K. Stylianou

1:50 INOR 1122. Small-molecule storage with porous coordination cage-based materials. **E.D. Bloch**

2:10 INOR 1123. Rapid removal of metals from complex water mixtures with MOF/Polymer composites. D. Sun, L. Peng, S. Yang, N. Gasilova, W.S. Reeder, E. Oveisi, **W.L. Queen**

2:30 INOR 1124. Synthesis and characterization of a novel mixed-ligand MOF: from a 1D coordination polymer to a hydrogen-bonded 3D framework. **J.P. Vizuet**, G. McCandless, K.J. Balkus

2:50 INOR 1125. Separations of arenes via interactions with two metal sites in metal-organic frameworks. **P.J. Milner**, M. Gonzalez, M. Kapelewski, J. Lee, J. Neaton, J.R. Long

3:10 Intermission.

3:25 INOR 1126. CO₂ capture with MOFs containing nucleophilic metal hydroxide groups. **C. Bien**, C. Wade

3:45 INOR 1127. Incorporation of highly polarizable iodine moieties in metal-organic frameworks to study their selectivity for xenon over krypton. **D. Fairchild**, T.G. Glover, F.J. Uribe-Romo

4:05 INOR 1128. Withdrawn

4:25 INOR 1129. Incorporating heavy alkane into mesoporous metal-organic frameworks for enhancing methane uptake. **Y. Fang**

Section K

Orange County Convention Center
West Hall B4 - Theater 20

Lanthanide & Actinide Chemistry

A. De Bettencourt Dias, *Organizer*
K. Johnson, P. Miro, *Presiding*

1:30 INOR 1130. *meso*-Position functionalized porphyrinate lanthanide complexes for near-infrared emission. **H. He**, D. Meyer, E. Micheli

1:50 INOR 1131. Gadolinium(III) relaxivity modulation via oligonucleotide coordination. **M. Halim**, E. Kadeer, M. Heidarian, C. Hofstetter

2:10 INOR 1132. New ligands that sensitize luminescence and singlet oxygen in water-soluble lanthanide complexes. **K. Johnson**, C.V. Rodrigues, A. De Bettencourt Dias

2:30 INOR 1133. Homoleptic homobimetallic *f*-block complexes. **T. Gomba**, N.T. Rice, B. Yik, J. Bacsá, H.S. La Pierre

2:50 INOR 1134. Structures and energetics of polymethylated DOTA complexed with lanthanides. **Y.S. Lee**, Z. Mou, A.C. Opina, R.E. Swenson, O. Vasalatiy



TECHNICAL PROGRAM

3:10 Intermission.

3:20 **INOR 1135.** Speciation of uranyl-peroxide species: from molecules to nanocapsules. **P. Miro**, S. Rabbani, E. Hare

3:40 **INOR 1136.** Properties of conjugated imine and mixed-donor ligands and their uranyl complexes. **J. Niklas**, K. Hunter, A.E. Gordon

4:00 **INOR 1137.** 5,5'-Azobistetrazolate in lanthanide coordination chemistry - The impact of CO₂ and traces of ²⁴¹Am. **C. Knoll**, D. Müller, J.M. Welch, G. Giester, B. Lendl, P. Weinberger, G. Steinhauser

4:20 **INOR 1138.** Chelate stabilization of low-valent uranium complexes of unsaturated hydrocarbon ligands: Synthesis of a U(II) amide complex. **J.M. Boncella**, A.M. Tondreau, B. Billow, A.L. Odom

4:40 **INOR 1139.** Importance of counteranions in isolating new crystalline examples of complexes of f-elements in low oxidation states. **D.N. Huh**, J.W. Ziller, W.J. Evans

Activation of Light (C1-C4) Hydrocarbons: Theory & Experiments

Sponsored by CATL, Cosponsored by ENFL, ENVR, INOR and PHYS

Elucidation of Mechanisms & Kinetics on Surfaces

Sponsored by CATL, Cosponsored by ENFL, ENVR, INOR and PHYS

MEDI

Division of Medicinal Chemistry

J. Schwarz, *Program Chair*

SUNDAY MORNING

Section A

Orange County Convention Center
Room W414AB

Small Molecule Immunomodulators in Cancer

E. F. DiMauro, S. A. Mitchell, *Organizers, Presiding*



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

8:30 Introductory Remarks.

8:35 **MEDI 1.** Discovery of potent and structurally diverse IDO1 selective heme-displacing inhibitors from optimization of hits from a mass spectrometry based affinity (ALIS) screen. **Y. Han**, A. Achab, **C. Andrews**, J. Ballard, **I. Bharathan**, X. Chai, P. Chen, M. Cheng, D. Clausen, Y. Deng, A. Doty, H. Ferguson, X. Fradera, C. Gibeau, W. Glaab, L. Guo, S. He, B.A. Hopkins, X. Huang, W. Kang, J.A. Kozlowski, C. Lesburg, G. Li, J. Lim, K. Liu, M. Lu, T. Martinot, M.A. McGowan, J.R. Miller, E. Nickbarg, J. O'Neil, K. Otte, Q. Pu, S. Sanyal, N. Sciammetta, N. Smotrov, D. Sloman, N. Solban, X. Song, P. Spacciapoli, A. Bass, S. Vincent, C. White, D. Xiao, W. Yu, H. Zhou, H. Zhang, **D. Li**, A. Pasternak, D.J. Bennett

9:05 **MEDI 2.** Small molecule ectonucleotidase inhibitors for the immunotherapy of cancer. **C.E. Muller**

9:35 **MEDI 3.** Identification of BAY-218: A potent and selective small molecule AHR inhibitor, as a new modality to counteract tumor immunosuppression. **N. Schmees**, I. Gutcher, U. Roehn, H. Irlbacher, B. Bader, C. Kober, L. Roesse, R. Carretero, I. Oezen, L. Zorn, M. Platten, I. Hartung, B. Kreft, D. Stoeckigt, H. Weinmann

10:05 **MEDI 4.** Discovery of novel cyclic dinucleotide STING agonists for cancer treatment. **W. Chang**, M.D. Altman, B.M. Andresen, S. Cemerski, M. Childers, A. Haidle, T.J. Henderson, J.P. Jewell, R. Liang, J. Lim, H. Liu, M. Lu, A. Northrup, R. Otte, S.A. Perera, J. Presland, T. Siu, Q. Truong, S. Walsh, K. Zhao, J. Cumming, W. Trotter

10:35 Intermission.

10:50 **MEDI 5.** Discovery of JNJ-787: An Hpk1 inhibitor that enhances the anti-tumor immunity of anti-PD1 in mice. **L. Mevellec**, S. Descamps, C. Adelinet, B. Wroblowski, V. Vreys, A. Valckx, I. Boeckx, N. Van Slycken, C. Paulussen, L. Leclercq, T. Verhulst, B. Van der Leede, P. Angibaud, L. Meerpoel, J.P. Edwards, S. Laquerre, M. Lorenzi, J. Vialard

11:20 **MEDI 6.** Antiviral innate immunity through small molecules for protection against RNA viruses. **M. Gale**

11:50 **MEDI 7.** GS-4361: A novel IDO1 Inhibitor. **R.V. Kalla**, K. Elbel, M. Bartlett, J. Cosman, T.D. Perry, E. Elzein, X. Li, D.O. Koltun, E.Q. Parkhill, J.A. Zablocki, M. Clark, H. Maecker, S. Jawahar, D. Hendricks, A. Shornikov, D. Koditek, B. Stafford, D. Soohoo, J. Voigt, E. Lansdon, R. Mackman, B. Corkey

12:20 Concluding Remarks.

Section B

Orange County Convention Center
Room W331A

General Orals

J. B. Schwarz, *Organizer*
M. Lu, *Presiding*

8:30 **MEDI 8.** Discovery and optimization of inhibitors of the autophagy E1 enzyme, ATG7. **S. Huang**, S.J. Harrison, A.E. Gould

8:50 **MEDI 9.** Development of water soluble, brain permeable EP2 receptor antagonist: Lead-optimization and *in vitro* proof-of-concept studies. **R. Amaradhi**, A. Banik, S. Mohammed, V. Patro, A. Rojas, W. Wang, R. Dingedine, T. Ganesh



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

9:10 MEDI 10. SAR studies in the sulfonyl carboxamide class of core protein modulators of the hepatitis B virus. **S.D. Kuduk**

9:30 MEDI 11. Discovery and development of PI4KIII β inhibitors as immunosuppressive agents for the prolongation of allogeneic organ engraftment. **J. Reuberson**

9:50 MEDI 12. Target identification studies of a utrophin modulator for treatment of Duchenne muscular dystrophy. **I. Wilkinson**, A. Vuorinen, J. Reynolds, K. Perkins, H. Dugdale, S. Squire, A. Casagrande, M. Geese, F. Wilson, G. Wynne, S. Mohammed, K. Huber, K. Davies, A. Russell

10:10 MEDI 13. Synthesis and biological evaluation of a new class of aryl isonitriles as antimicrobial agents. **K. Kyei-Baffour**, H. Mohammad, M.N. Seleem, M. Dai

10:30 MEDI 14. Hit-to-lead evolution of small-molecule PPAR α agonists: Working towards non-invasive options for retinal diseases. **A.S. Duerfeldt**

10:50 MEDI 15. Discovery of [^{11}C]MK-6884: A positron emission tomography (PET) imaging agent for M4 PAM. **L. Tong**, W. Li, **X. Gao**, M. Lo, J.M. Wai, M.T. Rudd, D.M. Tellers, Z. Zeng, P. Miller, C. Salinas, K.A. Riffel, H. Haley, M. Purcell, M. Holahan, T. Bueters, J. Uslaner, J. Morrow, R. Mazzola

11:10 MEDI 16. Discovery and optimization of potent, selective, and bioavailable USP7 inhibitors to target tumor growth. **P. Leger**, D.X. Hu, B. Abraham, L. Adsusmilli, B. Biannic, D. Bradford, G. Cutler, X. Han, S. Jacobson, A. Jorapur, P. Kassner, D. Kaveri, J. Ketcham, A. Kim, J. Maung, J. McKinnell, Y. Ohol, A. Okano, L. Peiser, D. Pookot, P. Rana, N. Shah, G. Shibuya, M. Sun, S. Suthram, O. Talay, K. Young, J.B. Schwarz, D.J. Wustrow

11:30 MEDI 17. New ruthenium Formate catalyst MCAT-53TM for C-H activation useful for the synthesis of medically relevant molecules. **A. Mehta**, B. Saha, A. Koohang, M. Chorghade

11:50 MEDI 18. Discovery of a novel $\alpha 7$ nAChR positive allosteric modulator for the treatment of cognitive disorders. **B.M. Crowley**, J. Balsells-Padros, J. Bao, B.T. Campbell, C.J. Daley, D. Guiadeen, B.C. Huff, J. Della Rocca, E.M. Joshi, K.J. Leavitt, D. Paul, J.M. Sanders, S. Tye, X. Wang, S.M. O'Connor, A.J. Harvey, J. Uslaner, J.L. Duffy, I.M. Bell

Drug Discovery: Informatics Approaches

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TECHNICAL PROGRAM

SUNDAY AFTERNOON

Section A

Orange County Convention Center
Room W414AB

General Orals

J. B. Schwarz, *Organizer, Presiding*

1:30 MEDI 19. Design of clinical candidate eFT226, a first-in-class inhibitor of the RNA helicase eIF4A. **C. Nilewski**, J.T. Ernst, P.A. Thompson, A.X. Xiang, C.V. Tran, G.K. Packard, T.D. Michels, P.A. Sprengeler, B. Eam, N.P. Young, S. Fish, J. Chen, M. Barrera, H. Howard, A. Parra, E. Sung, J. Staunton, I.N. Hung, G.S. Parker, G.G. Chiang, C.J. Wegerski, A. Nevarez, J. Clarine, S. Sperry, K.R. Webster, S.H. Reich

1:55 MEDI 20. Design and synthesis of a dual kinase-bromodomain inhibitor targeting ALK and BRD4. **E. Watts**, D. Heidenreich, E. Tucker, B. Bellenie, S. Knapp, L. Chesler, S. Hoelder

2:20 MEDI 21. Design, synthesis, and optimization of 2'2'-cyclic dinucleotides as STING agonists. **M. Lu**, M.D. Altman, A. Beard, F. Bennett, T. Cernak, W. Chang, M. Childers, S. Dreher, C. Lesburg, C. Li, R. Liang, J. Lim, H. Liu, L. Nogle, T. Siu, D. Steinhuebel, B. Taoka, Q. Truong, S. Walsh, J. Presland, S. Perera, S. Cemerski, J. Cumming, W. Trotter

2:45 MEDI 22. Geopharmaceuticals: New drug scaffolds from Baltic amber. **E.A. Ambrose**, C. McDermott

3:10 MEDI 23. Discovery of a novel series of small molecule modulators of TNF alpha binding and signalling through a novel mechanism of action. **T. Norman**, F. Lecomte, J. Kennedy, B. Carrington, J. Porter, J. O'Connell, A. Lawson, R. Davis, S. Rapecki, B. Kroeplien, A. Burgin, T. Arakaki

3:35 MEDI 24. Structure-based drug design towards small molecule interleukin-6 inhibitors. **D. Schultz**, L. Mao, G. Shi, W. Zhou, R. Huigens, C. Li

4:00 MEDI 25. Design and synthesis of novel central nervous system penetrant metabotropic glutamate receptor subtype 2 (mGlu₂) negative allosteric modulators (NAMs) via scaffold hopping. **E.S. Childress**, J.M. Wieting, A.S. Felts, M.M. Breiner, M.F. Long, V.B. Luscombe, A.L. Rodriguez, H.P. Cho, A.L. Blobaum, C.M. Niswender, P.J. Conn, C.W. Lindsley

4:25 MEDI 26. Beyond the "Rule of 5" (bRo5): The evolution of efficient drug discovery. **C.A. Lipinski**

Section B

Orange County Convention Center
Room W331A

Targeted Protein Degradation: A Small Molecule Game-Changer for Medicine Discovery

A. B. Benowitz, M. P. Bourbeau, *Organizers, Presiding*



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

1:30 MEDI 27. Use of heterobifunctional molecules that direct targeted protein degradation to explore signaling pathways. **C. Loh**, J. Kelleher, M. Weiss, V. Campbell, K. Yuan, C. Klaus, N. Mainolfi

2:00 MEDI 28. Design, characterization, and function of PROTACs targeting B-cell lymphoma 6 (BCL6). **W. McCoull**

2:30 MEDI 29. Co-opting and degrading IAPs. **S.T. Staben**

3:00 MEDI 30. Harnessing bioPROTACs to achieve rapid and robust protein knockdown. **S. Lim**, J. Chang, A. Partridge

3:30 MEDI 31. Targeting the undruggable: PROTAC approach to target transcriptional factors. **S. Wang**

4:00 MEDI 32. Lead optimisation of a series of RIPK2 PROTACs: Ripping up the rule book. **J.D. Harling**

Drug Discovery: Informatics Approaches

Sponsored by CINF, Cosponsored by MEDI

Hudson Award

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Isabell Award

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Collaborations & Data Sharing in Rare & Orphan Disease Drug Discovery

Sponsored by CINF, Cosponsored by MEDI

Gin New Investigator Award

Sponsored by CARB, Cosponsored by CELL, MEDI, ORGN and PROF

SUNDAY EVENING

Section A



TECHNICAL PROGRAM

Orange County Convention Center
West Hall C

General Posters

J. B. Schwarz, *Organizer*

7:00 - 9:00

MEDI 33. Tip48/Tip49 inhibitors: Antipyrene derivatives with diamide linker as potential anticancer agents. **T. Hamada**, M. Ebisawa, T. Suzuki, T. Murata, T. Tsukada, R. Motoki, Y. Kagoshima, M. Hirasawa, K. Hagihara, Y. Fujii, R. Murakami, T. Takata, K. Iwanaga, N. Haginoya, K. Uoto

MEDI 34. Using small molecule adjuvants to combat antibiotic resistant bacteria in cystic fibrosis. **V.B. Hubble**, C. Melander

MEDI 35. Pt-Mal-LHRH attenuates breast cancer tumor growth and metastasis by targeting overexpression of the LHRH receptor. **M. Ndinguri**, C. Black, J. Rollins, L. Calderon

MEDI 36. Quinazoline derivatives as potential tubulin polymerization inhibitors. **F. Herrera-Vázquez**, R. Aguayo-Ortiz, L. Dominguez, F. Hernández-Luis

MEDI 37. Discovery of DS-6930: A potent selective PPAR γ modulator. **K. Fujii**, T. Shinozuka, T. Tsukada, E. Tokumaru, K. Shimada, Y. Onishi, Y. Matsui, S. Wakimoto, M. Kuroha, T. Ogata, K. Araki, J. Ohsumi, R. Sawamura, N. Watanabe, H. Yamamoto, K. Fujimoto, Y. Tani, M. Mori, J. Tanaka

MEDI 38. Identification of novel PPAR α/γ dual agonist by *in silico* screening and molecular dynamics simulations. **V. Nath**, V. Kumar

MEDI 39. Dual CDK4/ARK5 inhibition by ON 123300 for targeting metastatic colorectal cancer. **M. Reddy**, S. Cosenza, S. Divakar, B. Akula, M.R. Mallireddigari, P. Reddy

MEDI 40. Activity landscape modeling and molecular dynamics of dual inhibitors of DNMT1 and G9a. **E. Lopez**, F. Prieto-Martínez, J. Medina-Franco

MEDI 41. 4-Hydroxybenzthiazole inhibitors of catechol-O-methyltransferase. **P.J. De Leon**, J. Barrow

MEDI 42. MOEsaic: Application of matched molecular pairs to interactive SAR exploration. **A. Ajamian**

MEDI 43. Exploiting solvent effects in drug design and optimization. **A. Ajamian**

MEDI 44. Scaffold replacement and 3D ligand optimization applied to the discovery of tyrosine kinase inhibitors. **A. Ajamian**

MEDI 45. Protocol for validating small molecule structure assignment using calculated ¹³C NMR chemical shifts with quantum mechanics and MOE. **A. Ajamian**



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- MEDI 46.** First investigation of the antibacterial activity of the combination of 2-hexadecynoic acid and ciprofloxacin against multi-drug resistant *Staphylococcus aureus*. **S. Medina, T. Pereles-De-Leon, C. Ocasio-Malave, D. Diaz, N.M. Carballeira, D.J. Sanabria Rios**
- MEDI 47.** α -Glucosidase inhibition natural products from *Chromolaena odorata*. **C.T. Onyema, V.I. Ajiwe, A. Ata**
- MEDI 48.** Polyhydroxyalkanoate-celecoxib nanoparticles for systemic lupus erythematosus therapy with enhanced efficacy and reduced side effects. **J. Hu**
- MEDI 49.** Facial sebum levels and its relationship with the severity of acne vulgaris in African adolescents. **O.N. Ilesanmi**
- MEDI 50.** Benzoflavone derivatives as potent antihyperuricemic agents. **H. Singh, J. Singh, A. Singh, P. Bedi**
- MEDI 51.** La-DOTA-melanocortin 1 receptor targeting ligand clearance route is controlled by linker polarity. **H. Kil, N. Tafreshi, D. Pandya, M. Doligalski, C. Tichacek, M. Budzevich, E. Moros, T. Wadas, D. Morse, M. McLaughlin**
- MEDI 52.** Purifying complex reaction mixtures via high-performance flash chromatography. **J.R. Bickler**
- MEDI 53.** Binding affinity of flavins to riboflavin binding protein using fluorescence spectrometry and isothermal titration calorimetry; and estimated binding energies using computational approaches. **A. Jenkins, M. McMillan, J.B. Ealy**
- MEDI 54.** Discovery of (3S,4S)-3-methyl-3-(4-fluorophenyl)-4-(4-(1,1,1,3,3,3-hexafluoro-2-hydroxyprop-2-yl)phenyl)pyrrolidines as novel ROR γ t inverse agonists. **B. Jiang, J. Duan, C.A. Weigelt, S.M. Stachura, A. Karmakar, H. Hemagiri, D.K. Raut, A.K. Gupta, J. Khan, J.S. Sack, D. Wu, M. Yarde, D. Shen, M.A. Galella, Q. Zhao, L.M. Salter-Cid, P.H. Carter, T. Dhar**
- MEDI 55.** X-ray crystal structure determination of leukotriene A₄ hydrolase in complex with 4-methoxy-ARM1 and characterization of the aminopeptidase enzyme mechanism. **K. Lee, G. Petrucio, Y. Shim, S. Noble, M. Paige**
- MEDI 56.** Substrate-dependent hydrolysis by the leukotriene A₄ hydrolase in the presence of 4MDM. **K. Lee, Y. Shim, S. Noble, M. Paige**
- MEDI 57.** Novel 5-cyanopyrimidine derivatives induces inhibition EGFR signaling pathways in cancer cell lines. **D. Khochenkov, Y. Khochenkova, A.S. Bunev**
- MEDI 58.** Tip48/Tip49 inhibitors: Antipyrene derivatives with an oxadiazole ring as potential anticancer agents. **T. Tsukada, M. Ebisawa, Y. Sugimoto, T. Taniguchi, S. Hirano, F. Muro, T. Suzuki, T. Hamada, T. Murata, S. Takechi, R. Motoki, Y. Kagoshima, M. Hirasawa, K. Hagihara, Y. Fujii, K. Hashimoto, T. Takata, R. Murakami, K. Iwanaga, N. Haginoya, K. Uoto**
- MEDI 59.** Discovery and characterization of a novel allosteric binding site of HSP70 by fragment based screening. **S. O'Connor, Y. Le Bihan, R. van Montfort, I. Collins**
- MEDI 60.** 5-Cyanopyrimidine-based compounds inhibits migration in A549 lung cancer cells. **V. Dudanova, D. Khochenkov, Y. Khochenkova, A.S. Bunev**
- MEDI 61.** Methylphenidate (Ritalin®) and synthetic cathinones (bath salts): Are they similar? **B.J. Yadav, J. Eltit, R.A. Glennon**



TECHNICAL PROGRAM

- MEDI 62.** Pharmacological analysis of 1,2,3-triazoles as amide bioisosteres in potentiators of the cystic fibrosis transmembrane conductance regulator protein. **J. Doiron**, G.W. Breton, L. Tang, W. Wang, S.M. Rowe, S.G. Aller, M.L. Turlington
- MEDI 63.** Development of potent GPR35 agonists with activity at human and rodent receptors. **L.L. Wendt**, D. Thimm, C.E. Muller
- MEDI 64.** Library of covalent, bifunctional small-molecule probes for the targeting of cysteine residues. **E. Altmann**, S. Numao, P. Ertl, L. McGregor, S. Renner
- MEDI 65.** FRAGNET: A European consortium to advance fragment-based drug discovery and educate its future advocates. **M. Wijnmans**, J. van Muijlwijk-Koezen, I. de Esch
- MEDI 66.** Aurora-A inhibitor alisertib potentiates VEGFR inhibitors in glioblastoma cell lines. **K. Smith**, C. Mifsud, C. Zumber, N. Lehman
- MEDI 67.** Nanokinib: A cyclic library of hinge binder and chemocentric approach for the discovery of selective kinases inhibitor. **N. George**, P. Benderitter, P. Blom, M. Fouchet, A. Denis, J. Hoflack
- MEDI 68.** Structural evolution of novel opioid peptidomimetics with reduced abuse liabilities. **S. Henry**, N. Griggs, J.P. Anand, B. Sears, J.R. Traynor, E. Jutkiewicz, K. Sobczyk-Kojiro, H.I. Mosberg
- MEDI 69.** Regioselective alkylation, arylation, and heteroarylation of 3-substituted pyrazoles. **A. Bao**, A. Huang
- MEDI 70.** Novel imidazobenzodiazepine GABA_A receptor $\alpha 2/\alpha 3$ selective PAM for the treatment of refractory/resistance epilepsy. **L.K. Golani**, J.M. Witkin, J.M. Cook
- MEDI 71.** Structure of membrane bound pyrophosphatase from *Thermotoga maritima* in complex with imidodiphosphate and *N*-[(2-aminobenzo[*d*]thiazol-6-yl)methyl]-1*H*-indole-2-carboxamide. K. Vidilaseris, A. Kiriazis, A. Turku, A. Khattab, **N.G. Johansson**, T.O. Leino, P.S. Kiuru, G. Boije af Gennäs, S. Meri, J.T. Yli-Kauhaluoma, H. Xhaard, A. Goldman
- MEDI 72.** Discovery of a novel olefin derivative as a highly potent and selective acetyl-CoA carboxylase 2 inhibitor. **Y. Nishiura**, A. Matsumura, N. Kobayashi, A. Shimazaki, S. Sakamoto, N. Kitade, Y. Tonomura, A. Ino, T. Okuno
- MEDI 73.** New organic photo CORM and the PCBA polymer nanoparticle incorporating it. **A. Elgattar**, **A. Alwagdani**, **T. Khalil**, **H. Pal**, **Y. Liao**
- MEDI 74.** First-generation structure-activity relationship studies of 2,3,4,9-tetrahydro-1*H*-carbazol-1-amines as CpxRA modulators. Y. Li, **J.J. Gardner**, K.R. Fortney, S. Spinola, A.S. Duerfeldt
- MEDI 75.** Targeting glioma progression: Human heparanase inhibition by a novel class of non-anticoagulant heparinoids. **S. Nadji**, R.K. Dhar
- MEDI 76.** Azulene-based compounds targeting orexin receptors. **T.O. Leino**, A. Turku, J.T. Yli-Kauhaluoma, J.P. Kukkonen, H. Xhaard, E. Wallen
- MEDI 77.** PPE51-mutation effect the sensitivity of *Tubercle bacilli* to selected thio-sugars. **Z.J. Wiczak**, M. Korycka-Machala, A. Brzostek, P. Borowka, D. Strapagiel, J. Dziadek



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

MEDI 78. Progress towards orally bioavailable, potent, and selective small-molecule inhibitors of CD73 for immuno-oncology. R. Thomas-Tran, E. Lindsey, K. Lawson, **J. Beatty**, J. Jeffrey, J. Fournier, D. Mandal, X. Yan, S. Drew, N. Walker, S. Moschütz, N. Sträter, A. Chen, M. Reddy Leleti, J. Powers

MEDI 79. Discovery and characterization of potent and selective small-molecule inhibitors of ecto-nucleotidase CD73 for cancer immunotherapy. **E.U. Sharif**, K. Lawson, J. Kalisiak, E. Lindsey, E. Newcomb, B. Rosen, N. Walker, L. Jin, E.R. Scaletti, N. Sträter, A. Chen, M. Reddy Leleti, J. Powers

MEDI 80. Discovery of SAM competitive and non-nucleoside derivative PRMT5 inhibitors with potent antitumor activity. **X. Yang**, W. Zhou, C. Li

MEDI 81. Impact of automated supersaturation stability assay to differentiate poorly soluble compounds in Novartis drug discovery and development. **S. Skolnik**, S. Dodd, G. Geraci

MEDI 82. Phytochemical screening and antioxidant activities of *Irvingia gabonensis* and its effect on alloxan-induced diabetes rats. **O.E. Ogunjinmi**, I.A. Salaudeen, M.O. Abdulganeey

MEDI 83. *In-situ* single-step electrochemical detection of DL-methionine in human serum sample. **A.N. Kawde**

MEDI 84. Discovery of novel 6-aryl-2-benzoyl-pyridines as tubulin polymerization inhibitor with potent antiproliferative properties. **H. Chen**, S. Deng, N. Albadari, D.D. Miller, W. Li

MEDI 85. Design and development of novel selective D₄-receptor ligands as CNS-therapeutics. **U. Gonela**, S.Y. Ablordeppey

MEDI 86. Antioxidant activity of eugenol derivatives. **E. Siech**, **V. Thurman**, A. Vummenthala

MEDI 87. Discovery of a novel second-site corrector for delF508 CFTR mutations. **P. Lam**, K.D. Boss, A.K. Cheung, R. Epple, S. Espinola, A. Honda, C. Lay, W. Li, H.A. Malik, L. Whitehead, B. Wu, W.G. Barnes, S.J. Patel

MEDI 88. Discovery and SAR studies of novel 2-anilinopyrimidine-based selective inhibitors against triple-negative breast cancer cell line. **J. Jo**, S. Kim, H. Kim, M. Jeong, Y. Jung, H. Yun

MEDI 89. Efficient synthetic methods of 7-trifluoromethyl-7-deazapurine ribonucleoside analogs and their phosphoramidate prodrugs. **J. Cho**, S. Choi, J. Kim, F. Amblard, L. Bassit, R. Schinazi

MEDI 90. *In silico* discovery of new small-molecule immune checkpoint inhibitors as an innovative approach to treat cancer. **S. Ferla**, S. Lanfredini, G. Patel, A. Brancale

MEDI 91. Delivering glutathione persulfide by an esterase-sensitive donor. **Z. Yuan**, Y. Zheng, B. Yu, S. Wang, X. Yang, B. Wang

MEDI 92. Highly advanced intermediate towards a macrocyclic ketone mimic of zampanolide. **Z. Jiang**, G. Chen, Q. Chen

MEDI 93. Development of a platform for resveratrol delivery: Functionalization of resveratrol-loaded nanoparticles and hypertrophy modulation in cardiac cells. **P. Garcia**

MEDI 94. Chromatography and fractionation of *Schinus terebinthifolius* extracts which inhibit breast cancer cell migration *in vitro*. **M. Pina**, **J.M. Brown**, A. Tapanes-Castillo



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- MEDI 95.** Computational designed new inhibitors of xanthine oxidase for treatment of gout. **C. Dong**, V. Usanga
- MEDI 96.** Structure Activity Relationship (SAR) studies of a nucleotide reverse transcriptase inhibitors (NRTI) AZT (Zidovudine) analogs using Gaussian computational techniques. **S. Narayan**, K. Quirk, K. Baldwin
- MEDI 97.** Time-on-target: Easy method development for reverse phase preparative chromatography. **J.E. Silver**, C. Bailey, D. Johnson, R. Lewis
- MEDI 98.** Searching for sensitizers of bacteria toward existing antibiotics. **M. Roy Choudhury**, B. Yu, A. Kumar, M. Zhu, D.W. Boykin, B. Wang
- MEDI 99.** On-column dilution: A method to improve loading and resolution in chromatography. **J.E. Silver**, C. Bailey, D. Johnson, R. Lewis
- MEDI 100.** Optimization of structural features of the 4-anilinoquin(az)oline scaffold for chordoma utilizing an innovative toxicology profiling assay panel. **C.R. Asquith**, A.A. Bieberich, K. Maffuid, R. Fatig, G.J. Tizzard, T. Laitinen, M.P. East, C.D. Torrice, D. Drewry, G.J. Johnson, D.J. Crona, B. Calvin, D.C. Morris, W.J. Zuercher
- MEDI 101.** Biphenyl acid derivatives as APJ receptor agonists. **S. Su**, A. Clarke, Y. Han, H. Chao, J. Bostwick, W. Schumacher, T. Wang, M. Yang, M. Hsu, E. Simmons, Y. Hsiao, E.E. Luk, M. Dabros, M.A. Galella, J. Onorato, D. Gordon, R.R. Wexler, P.S. Gargalovic, M. Lawrence
- MEDI 102.** Using electrostatic complementarity to design compounds: A new approach to visualize and predict activity. **T. Cheeseright**, S. Sciammetta, M. Bauer, M.D. Mackey
- MEDI 103.** Cruentaren A analogs and their biological activities. **B. Patel**, M. Topinka, B.S. Blagg
- MEDI 104.** Potential correlation between chlorine-treated drinking water and cancer incidences. **A. Avalos**, S. Rodriguez
- MEDI 105.** Design and optimization of CDK4/6 and FLT3 dual inhibitors with a novel hinge binder. **K. Li**, L.R. McGee, J.E. Eksterowicz, D. Piper, Z. Wang, G. Alba, M. Ragains, R. Ngo, M. Lo, J. Ma, K. Keegan, C. Li, L. Liang, K. Dai
- MEDI 106.** Transporter informatics: Predicting substrates for transmembrane transporters. **G.F. Ecker**, S.M. Kohlbacher
- MEDI 107.** Discovery of a pan-mGluR PAM for the treatment of CNS disorders. **S. Mayer**
- MEDI 108.** Fisetin derivatives as anti-prostate cancer agents. **k.W. muthima**, Q. Chen, G. Chen, M. Lee
- MEDI 109.** Immuno-oncology (IO) drug conjugate concentrates at cells and tumors and enhances survival. **S. Kaulagari**, M. Doligalski, A.S. Cohen, H. Zheng, V. Estrella, A. Beg, D. Morse, M. McLaughlin
- MEDI 110.** Discovery and characterization of peptide inhibitors of RsmC function. **D.D. To**, K. GC, S. Abeyirigunawardena
- MEDI 111.** Implementation of vector analysis for the identification of potential KLK-6/PAR-1 dual inhibitors for the treatment of multiple sclerosis through molecular docking, molecular dynamics and chemoinformatic studies. **J. S. Tejada**, M.A. Loza-Mejia, S. Fuentes-Villegas, M. Salinas-Parra, V. Villegas-Gonzalez
- MEDI 112.** Molecular docking of torreyunlignans in phosphodiesterases 9A, 4B, and 8A: Computational analysis of torreyunlignan inhibition. **E.M. Bonett**, M. McEwan, K.E. Cole, J.M. Carney



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- MEDI 113.** Molecular docking and lead optimization of torreyunlignans, phosphodiesterase 9A inhibitors. **E.M. Bonett**, K.E. Cole, J.M. Carney
- MEDI 114.** Cytosine-based TET enzyme inhibitors. **H. Sun**, N. Kuzio, M.J. Bennett, G. Chua, K.L. Wassarman, J.A. Alp, E.I. Jarczyk, B.G. Malachowsky, A. Kennedy
- MEDI 115.** Comparison of native ribose and conformationally-constrained (N)-methanocarpa nucleosides for A₁ adenosine receptor agonists: Design and *in vivo* characterization. **D. Tosh**, H. Rao, A. Bitant, V. Salmaso, P. Mannes, D. Lieberman, J. Auchampach, A. Ciancetta, N. Liu, Z. Cui, Z. Gao, M. Reitman, O. Gavrilova, K.A. Jacobson
- MEDI 116.** Curcumin-metal complexes as inhibitors of beta-amyloid aggregation. **M. Dervisevic**, A. Vummenthala, **J. Brabant**
- MEDI 117.** Biochemical analysis of *Syzygium aromaticum* as potential agent in the treatment of diabetes. **G.W. Garcia**, A. Mar, H.M. Morales
- MEDI 118.** Structure-function studies of a novel allosteric site of the dopamine transporter as a target for alternative therapeutics against cocaine use disorder. **S. Aggarwal**, X. Liu, C. Rice, S. Kortagere, J. Salvino, O. Mortensen
- MEDI 119.** Cyclization-centered structure-activity relationship of a noncovalent inhibitor of the KEAP1-NRF2 interaction. **K.M. Booker**, T.W. Moore, B. David
- MEDI 120.** *In vivo* effect of PEG-tethered A_{2A} adenosine receptor agonist-alendronic acid conjugates on induced bone degeneration. **K.S. Toti**, A. Larrañaga-Vera, A. Gadiano, E. Warnick, H. Rao, Z. Gao, B.N. Cronstein, K.A. Jacobson
- MEDI 121.** Treatment of sensorimotor gating deficits in neuropsychiatric disorders using deuterated α6-GABA_AR subtype selective ligands. **D.E. Knutson**, R. Kodali, M. Treven, B. Divovic, H. Lee, J. Chou, H. Chen, L. Chiou, M. Ernst, M.D. Mihovilovic, M.M. Savić, W. Sieghart, J.M. Cook
- MEDI 122.** Anti-glycation effect and advanced glycation end-products protein cross-links breaking ability of *Psidium guajava* leaf extracts. **O.I. Adeniran**, A. Mogale, L.J. Shai
- MEDI 123.** Renoprotective effects of hypoxylonol derivatives isolated from *Hypoxylon truncatum* against cisplatin-induced cytotoxicity. **J. Ham**, K. Kang, B. Hwang, D. Lee, P. Choi, T. Kim, Y. Park, S. Choi, B. Song, K. Cho
- MEDI 124.** Incarvilleatine produces antinociceptive and motor suppressive effects via adenosine receptor activation. **J. Kim**, D.M. Bogdan, M.W. Elmes, M. Awwa, S. Yan, J. Che, G. Lee, D.G. Deutsch, R.C. Rizzo, M. Kaczocho, I. Ojima
- MEDI 125.** Study of the biochemistry of lemon grass: A widely used diabetes remedy. **N. Trejo**
- MEDI 126.** Investigation of effects of rigidity on kinase inhibitor selectivity. **C. Yu**, A. Assadieskandar, C. Zhang
- MEDI 127.** Androgen receptor degraders and transactivation domain inhibitors targeting castration-resistant prostate cancer. **D. N. G. Ralalage**, J. An, M.E. Jung, M.B. Rettig
- MEDI 128.** Discovery and SAR studies of novel non-toxic azacyclic derivatives for the treatment of type 2 diabetes mellitus. **H. Choi**, Y. Park, J. Kwak, E. Jung, M. Yang, K. Kang, H. Yun
- MEDI 129.** Optimization of 6-amino-3-methylpyrimidinones as potent, selective, and orally efficacious SHP2 inhibitors. **M.G. Palermo**, P.J. Sarver, M. Acker, J.T. Bagdanoff, Z. Chen, M. Fodor, J. Garcia-Fortanet, H. Hao, M. Kato, R. Koenig,



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

L. LaBonte, G. Liu, S. Liu, C. Liu, M. Mohseni, M. Sendzick, T. Stams, R.B. Tichkule, C. Towler, H. Wang, P. Wang, S.L. Williams, B. Yu, M.J. Lamarche

MEDI 130. Optimizing the anti-proliferative activity of CJ-15,208 in prostate cancer cells. **R. Pescatore**, J.V. Aldrich

MEDI 131. Finding new molecules for treatment of neurological and metabolic disorders by *in silico* analysis of phytoconstituents from traditional Indian and Russian medicines. N. Ionov, P. Pogodin, A. Rudik, S. Ivanov, A. Lagunin, V. Poroikov, V. Luzhanin, M. Povydysh, R. Kumar Goel, G. Sastry, **D. Druzhilovskiy**

MEDI 132. Development of tumor-targeting, light-activated chemotherapy with vitamin B₁₂-protein kinase inhibitor conjugates. **L.N. Gendron**, **C.G. Sheveland**, T.A. Shell, **J.R. Shell**

MEDI 133. Tagetnoic acid: A new lipoxygenase inhibitor peroxy fatty acid from *Tagetes minuta* growing in Saudi Arabia. **M.T. Khayat**, G.A. Mohamed, S.R. Ibrahim

MEDI 134. *In silico* assessment of cardiovascular adverse effects of drug-drug interactions. S. Ivanov, A. Lagunin, D. Filimonov, V. Poroikov, **D. Druzhilovskiy**

MEDI 135. Novel macrocyclic tetrapeptide kappa opioid receptor ligands: Cytochrome P450 metabolism and interactions. **T. Khaliq**, **J.V. Aldrich**

MEDI 136. AI-driven design of dual-pharmacophore libraries. **C.S. Bury**, J.P. Overington, A. Pannifer

MEDI 137. Development of potent and specific inhibitors for oncogenic kinase FGFR4. **R. Rezende Miranda**, C. Zhang

MEDI 138. Flexibility at different stages of mechanism of activation of the GPCR-prototype agrees with local motions explored by molecular dynamics simulations. **K. Gonzalez Ponce**, A. Madariaga, K. Martinez Mayorga

MEDI 139. Drug delivery of xanthohumol to adipocytes using ultrasmall superparamagnetic iron oxide nanoparticles. I. Khaki Najafabadi, J. Samuels, R. Dansby-Sparks, T. Fields, A. Singh, S. Raylam, R. Deshmukh, **V.V. Mody**

MEDI 140. Nonracemic prodrugs of a butyrophilin ligand. **N.A. Lentini**, C.C. Hsiao, A.J. Wiemer, D.F. Wiemer

MEDI 141. Structural optimization of pyrrolopyrimidine RET kinase inhibitors. **V. Garcia**, S. Toenjes, S.M. Maddox, G. Dawson, M.M. Cardenas, J.L. Gustafson

MEDI 142. Discovery and optimization of imidazoisoindole-based IDO/TDO dual inhibitors. **R. Pastor**, B. Parr, Y. Liu

MEDI 143. Multi-approach strategy to improve the spectrum of ClpP activators. **Q. Avila**, A.S. Duerfeldt

MEDI 144. Development and characterization of hiPSC cortical neurons and their application to drug evaluation in CNS disease models. **K. Autar**, X. Guo, A. Goswami, M. Jackson, J. Rumsey, C. Long, J.J. Hickman

MEDI 145. Effect of lithium at therapeutic and subtherapeutic doses in GSK3beta autonomous pathways at primary hippocampal neurons cell culture. **V. De-Paula**, A. Barbosa, O. Forlenza, H. Brentani

MEDI 146. Anti-diabetic activity of *Cissus rotundifolia* plant growing in Saudi Arabia. **S. Alshehri**, F.T. Halaweish

MEDI 147. Development of a thermal shift assay for evaluating inhibitor candidates targeting viral hemagglutinin and neuraminidase. **A. de Moya**, S.A. Whitney, L. Offermann, **N.L. Snyder**



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- MEDI 148.** Identifying of the molecular target for the potent antimicrobial agent TI-I-100 to treat drug resistance bacteria. **V. Tiruveedhula**, R. Kodali, L. Han, L. Arnold, J.M. Cook
- MEDI 149.** Pharmacophore generation of μ -opioid receptor biased-ligands: Uncovering structural features from molecular modeling analysis. **B. Hernández**, A. Madariaga, K. Martinez Mayorga
- MEDI 150.** Nucleic acid nano-vehicles designed form flexible tetra-U/T helix linking motif. **E.F. Khisamutdinov**
- MEDI 151.** Drug development on chemical therapeutics/antidote for chemical and biological warfare agents/toxic agents. **S.N. Olatunji**
- MEDI 152.** Next-generation bedaquiline for the treatment of tuberculosis. **P.J. Choi**, H. Sutherland, A. Tong, D. Conole, A. Blaser, C.B. Cooper, S.G. Franzblau, A.M. Upton, W.A. Denny, B.D. Palmer
- MEDI 153.** Inhibition of Dengue virus protease by chemical constituents of a clove: From food ingredient to medicine. **M. Saeed**
- MEDI 154.** Development of novel C3-analogs of galeterone for prostate cancer therapy. **P. Puranik**, F.N. Murigi, A.K. Kwegyir-Afful, S. Ramalingam, V.P. Ramamurthy, V.C. Njar
- MEDI 155.** Design, synthesis, and evaluation of quinazoline derivatives as FAK inhibitor with antiproliferative and antiangiogenic activity on cancer induced chick embryo. **A. Verma**, P. Pathak, p.K. Shukla, V. Kumar
- MEDI 156.** Pharmacoinformatic-based structural exploration, synthesis, and bioevaluation of selective Gly/NMDA antagonists: Potential ligands to treat intractable epilepsy. **V.G. Ugale**, S. Bari
- MEDI 157.** Identification of dibutyrate prodrug of antiviral deoxynojirimycin derivative IHVR-19029. **Y. Du**, H. Lu, G. Guo, H. Luo, Q. Su, N. Hwang, J. Ma, X. Zhang, S. Bixler, T. Warren, S. Bavari, J. Guo, T. Block, J. Chang
- MEDI 158.** Multiple quantitative structure-activity relationships (QSARs) analysis for γ -secretase inhibitors. **V. Patil**, N. Masand
- MEDI 159.** Potent, non-carboxylesterase-labile pro-drugs of the enolase inhibitor HEX for the treatment of ENO1-deleted glioblastoma. **V.C. Yan**, E.S. Ballato, K.L. Yang, D.K. Georgiou, K. Arthur, P. Shrestha, S. Khakha, J. Ackroyd, F.L. Muller
- MEDI 160.** Rational design, synthesis, and *in-vitro* screening of novel tankyrase inhibitors for the treatment of cancer. **B.D. Patel**, A. Patel, H.G. Bhatt
- MEDI 161.** Novel diphenylbutylpiperidine analogs to treat lung cancer. **M. Ashraf Uz Zaman**, M. Sajib, C.M. Mikelis, N. German
- MEDI 162.** Discovery of novel toll-like receptor 7 antagonists. **S. Jiang**, H. Chen, H.H. Yin
- MEDI 163.** Green synthetic approach to access thiazetid-2-imine and thiazolidin-2-imine fused pyrazolo-pyrimidine scaffold as hybrid bifunctional molecules: Structure-based optimization and evaluation of calcium dependent protein kinase1(CDPK1) inhibition. **N. Rao**
- MEDI 164.** Development of inhibitors of the pore forming protein perforin for the treatment of leukaemia. **J. Jose**, J. Spicer, C.K. Miller, P.D. O'Connor, A. Giddens, H. Akhlaghi, J. Trapani, W.A. Denny



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

MEDI 165. Design and synthesis of macrocyclic CREBBP bromodomain ligands. **M. Moroglu**, M.D. Selby, J. Reuberson, W. Pitt, J. Clayton, S.J. Conway

MEDI 166. Design and synthesis of novel benzoxazole derivatives as B-Raf kinase inhibitor for the treatment of skin cancer. **J.P. Chavda**, K.V. Shah, H.G. Bhatt

MEDI 167. Photopharmacology for GPCR receptor proteins: 1st and 2nd generation chemical biology tools. **M. Wijtmans**

MEDI 168. Inhibitors for Asp-proteases: Anchor-based virtual screening, innovative chemistry, and protein crystallography. **M. Konstantinidou**, F. Magari, F. Sutanto, M. Unver, V. Jumde, C.J. Camacho, G. Klebe, A. Hirsch, A. Doemling

MEDI 169. Designing and synthesis of novel scaffold by adopting ligand- and structure-based approaches as HIV-1 entry inhibitor specially targeting to viral glycoprotein Gp120. **K.V. Shah**, J.P. Chavda, H.G. Bhatt

MEDI 170. Developing a chemical probe: Thieno[3,2-d]pyrimidines, selective and potent inhibitors of protein kinase DRAK2/STK17B. **A. Picado**, C. Wells, D. Drewry

MEDI 171. PROTAC small-molecule degraders of AR protein. **X. Han**, C. Wang, C. Qin, W. Xiang, E. Fernandez-Salas, C. Yang, M. Wang, L. Zhao, T. Xu, J. Stuckey, S. Wang

MEDI 172. Design, synthesis, and application of GLP1 agonist-ASO conjugates to gene silencing in pancreatic beta cells. **L. Knerr**, A. Hayen, M. Ölwegård-Halvarsson, P.P. Seth, T.P. Prakash, W.J. Drury, C. ämmälä, I. Ahlstedt, P. Stillemark-Billton, C. Wennberg-Huldt, E. Andersson, E. Valeur, R. Jansson-Löfmark, D. Janzén, L. Sundström, J. Meuller, J. Claesson, P. Andersson, C. Johansson, R.G. Lee, B.P. Monia, S. Andersson, A. Björkbom, E. Cavallin, X. Li

MEDI 173. Synthetic efforts towards the preparation of 2'-dihalogenated nucleotide prodrugs. **S.P. Mengshetti**, L. Zhou, O. Sari, C. De Shutter, S. Zhou, Z. Chen, H. Zhang, A. Khalil, H. Li, R. Ovadia, M. Kasthuri, F. Amblard, R.F. Schinazi

MEDI 174. Design, synthesis, and biological evaluation of novel oxadiazole- and thiazole-based histamine H₃R ligands. **M.A. Khanfar**, H. Stark

MEDI 175. Design and optimization of a first-in-class NACK inhibitor: A novel path to notch inhibition. **T.T. Kelley**, X. Zhu, A.J. Capobianco, S. Schürer

MEDI 176. Anthrax antitoxin lead optimization via bioisosteric replacement and other *in silico* strategies. **C. McDermott**, E.A. Ambrose

MEDI 177. Radioiodinated aromatic choline analog tracers. **P. Svec**, Z. Novy, J. Kucka, M. Petrik, O. Sedlacek, M. Hajduch, M. Hruby

MEDI 178. Evolution of commercially available compounds for HTS. **D. Volochnyuk**, S. Ryabukhin, Y. Moroz

MEDI 179. Chemical tools to probe the role of bromodomains in the parasite *Trypanosoma cruzi*. **C. Laurin**, M. Schiedel, A.K. Chan, P.G. Humphreys, J.T. Seal, S.J. Conway

MEDI 180. PAMAM-half-dendron-based drug conjugates as efficient tumor-targeted drug-delivery system for a new-generation taxoid. **Y. Sun**, L. Wei, Y. Zhang, I. Ojima



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- MEDI 181.** *In-silico* designing and synthesis of novel and selective hits as Poly ADP-Ribose Polymerase 1 (PARP1) inhibitors for treatment of solid tumours. **P.G. Jain**, B.D. Patel
- MEDI 182.** Ligand-based drug design and synthesis of novel phosphoinositide 3-kinase (PI3K) beta inhibitors for the treatment of lung cancer. **S.R. Mehta**, M. Ghate, P. Parikh
- MEDI 183.** Targeting membrane-bound dimer of cRaf kinase in search of anti-cancer drugs. **P. Srivastava**, J. Hancock, A. Gorfe Abebe
- MEDI 184.** Green synthesis of a synergetic structure of tellurium nanowires and metallic nanoparticles for biomedical applications. **A. Vernet Crua**, D. Medina Cruz, T. Webster, B. Zhang
- MEDI 185.** Intracellular paired agent imaging enables personalized medicine for cancer patients. **L. Wang**, E. Schultz, A. Solanki, K. Tichauer, K.S. Samkoe, S.L. Gibbs
- MEDI 186.** Catalytic allylic oxidation of cyclic enamides and 3,4_dihydro_2H_pyran by TBHP. **R. Humeidi**, Y. Yu, M. Doyle
- MEDI 187.** Exploring novel E3 ligase binders for targeted protein degradation. **Y. Tomata**, K. Gamo, N. Kitamoto, Y. Tominari
- MEDI 188.** BD2-selective BET inhibition induces cell death in pediatric tumor cell lines. **P.J. Slavish**, N. Martinez, A. Shelat
- MEDI 189.** Development of polymer-based nanoparticulate intranasal lipopeptide vaccine constructs against group A streptococcus. **R. Nevagi**, W. Dai, Z. Khalil, W. Hussein, R. Capon, M. Skwarczynski, I. Toth
- MEDI 190.** SAR of novel anti-fungal agents targeting the synthesis of fungal GlcCer. **K. Haranahalli**, C. Lazzarini, Y. Sun, M. Del Poeta, I. Ojima
- MEDI 191.** Encapsulation and controlled release of antimetabolite drug 6-thioguanine from aluminum metal-organic framework. C. Grinnell, R. Lapidus, **A. Samokhvalov**
- MEDI 192.** Modification of hydroxynaphthoquinone scaffold in search of antimicrobial and antineoplastic agents. E. Smith, T. Maloney, M. Humphrey, C. Ray, **I.N. Nawarathne**
- MEDI 193.** Design, syntheses, and SAR studies of carbasugar SGLT2 inhibitors. **W. Ng**, H. Li, V. Lau, A.K. Chan, J. Chan, C. Lau, T.K. Shing
- MEDI 194.** Synthesis and characterization of NIR dye-doped nanoparticles for *in vivo* medical imaging. **C. Schneider**, S. Dembski, F. Miller, T. Riess, J. Jose
- MEDI 195.** Dynamic DNA-encoded library technology: Discovery of kinesin-1 activators and inhibitors. **M. Thompson**, F. Reddavid, S. Heiden, M. Cui, Y. Zhang
- MEDI 196.** Design and synthesis of quinazolinone derivatives lacking toxicity producing attributes as glucokinase activators. **S.C. Khadse**
- MEDI 197.** Novel, odorranalectin-based, opioid-like peptides: Synthesis, intranasal delivery to brain, and activity against opioid receptors. **R. Rayala**, B. Williams, S. Majumder, J.P. McLaughlin, P. Cudic



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

MEDI 198. Binary metal-containing nanoparticles for CT imaging and radiosensitization of peritoneal metastatic tumors. **R. Kashfi Sadabad**, L. Gonzalez-Fajardo, M. Jay, X. Lu

MEDI 199. Rapid screening of synergistic combinations of group IB metals and antibiotics for *E. coli* inactivation. **O. Conroy-Ben**, D.E. Novoa, S. Key, M. Tran

MEDI 200. Design and synthesis of metabolically stable endocannabinoid analogs by reversing ester and amide group. **L. Ji**, S. Nikas, Y. Liu, A. Korde, A. Ciesielski, A. Straiker, O. Benchama, A.S. Dhopeswarkar, C. Honrao, K. Mackie, L.M. Bohn, A. Makriyannis

MEDI 201. Synthesis and structure activity relationship studies of cystargolides based beta-lactones as potent proteasome inhibitors and anti-cancer agents. **D. Niroula**, R. Tello-Aburto

MEDI 202. Surface functionalization of polyethylenimine coated iron oxide nanoparticles for dual delivery of doxorubicin and ADAM10 siRNA for prostate cancer treatment. **R. Panday**, A.M. Abdalla, G. Yang

MEDI 203. Design and synthesis of peptidomimetics with attenuated reactivity for the treatment of neurodegenerative diseases. **A. Jastaniah**, R. Knopp, I. Gaisina, M. Siklos, G.R. Thatcher

MEDI 204. Design, synthesis, and biostudy of bifunctional platinum complexes: Anti-cancer activity through DNA binding and HDAC inhibition. **C. Feng**, Y. Huang, D. Chen, A. Franz, X. Guo, Y. Chen, Q. Zhao

MEDI 205. Solvent-free synthesis and activity of new derivatives of hexylarylpiperazines as 5-HT₇ receptors ligands. **J.M. Jaskowska**, P. Sliwa, P. Zareba, D. Kulaga, A. Drabczyk

MEDI 206. Development of a new structural family of microbial choline trimethylamine lyase inhibitors for the treatment and prevention of cardiovascular disease. **A. Duzan**

MEDI 207. Search of the sirtuin 2 inhibitor as antichagasic candidate by structure-based drug design. **G.H. Trossini**, G.M. Ferreira, V.M. Almeida, S.R. Marana, F.D. Emery

MEDI 208. Phytochemical screening, metal concentration determination, and antibacterial evaluation of *Drymaria diandra* plant. **A. Phuyal**

MEDI 209. Efforts in redesigning the antileukemic drug 6-thiopurine: Decreasing toxic side effects while maintaining efficacy. **A.X. Torres Hernandez**, C.J. Weeramange, P. Desman, A. Fatino, O. Haney, R. Rafferty

MEDI 210. Biological and structural studies of some new Schiff's bases: Computational and experimental approach. **A. Altaf**, A. Badshah

MEDI 211. Total synthesis of a potent antimicrobial compounds griseoleuteins, pelagiomicins and alanylgriseoluteic acid. **S. Dighe**, P. Katavic, T. Collet

MEDI 212. Targeting Alzheimer's disease: A virtual screening protocol to discover new central-acting BACE1 inhibitors. **J. Coimbra**, S.J. Baptista, A.E. Santos, P.I. Moreira, M.M. Silva, T.C. Dinis, J.A. Salvador

Metal-Mediated Reactions & Syntheses



TECHNICAL PROGRAM

Sponsored by ORGN, Cosponsored by MEDI†

MONDAY MORNING

Section A

Orange County Convention Center
Room W414AB

Synthetic Technologies to Enable Medicinal Chemistry

A. El Marrouni, L. M. Suen, J. Tucker, Y. Wang, *Organizers, Presiding*

8:15 Introductory Remarks.

8:20 **MEDI 213.** Leveraging high-throughput experimentation and cutting-edge synthetic chemistries to improve the quality and speed of the drug discovery design cycle. **S.W. Krska**

9:05 **MEDI 214.** Acceleration of medicinal chemistry research enabled by high-throughput technologies. **Y. Wang**

9:50 **MEDI 215.** Development of flow reactions to enable synthesis and medicinal chemistry. **A.B. Beeler**, G. Fleming, R. Telmesani, A.L. Courtney, Y. Corre

10:35 **MEDI 216.** Going faster and leaner: Automated microscale reaction screening in flow. **P. Richardson**, N. Sach, J. Tucker, W.P. Farrell, C.J. Helal, D. Perera

11:20 **MEDI 217.** Mapping reaction space with machine learning. **A.G. Doyle**

12:05 Concluding Remarks.

Section B

Orange County Convention Center
Room W331A

Therapeutic Developments in Health Disparities

S. Y. Ablordeppey, K. K. Bagga, *Organizers, Presiding*

8:30 **MEDI 218.** Current status of drug development for health disparity diseases: Cryptococcal meningitis. **S.Y. Ablordeppey**

9:10 **MEDI 219.** Development of drugs for the treatment of tuberculosis. **J.K. Sello**

9:40 **MEDI 220.** Developing peptides and peptidomimetics as potential treatments for substance abuse. **J.V. Aldrich**, J.P. McLaughlin



TECHNICAL PROGRAM

10:10 MEDI 221. Current approaches to anticancer drug development. **J.K. Buolamwini**

10:40 MEDI 222. Prostate cancer health disparities in African-American men: Possible targets for race specific drug development. **S. Khan**

11:10 MEDI 223. New approach to regenerative cartilage tissue engineering using temperature-sensitive therapeutic hydrogels. **J. Mendenhall**

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Sponsored by PROF, Cosponsored by AGFD, ANYL, BIOL, BIOT, CARB, CELL, CHED, CMA, COLL, COMP, ENVR, GEOC, I&EC, MEDI, MPPG, NUCL, ORGN, PHYS, PMSE, POLY, PRES, WCC and YCC

Nucleic Acids-Based Therapeutics

Sponsored by CARB, Cosponsored by BIOL and MEDI

MONDAY AFTERNOON

Section A

Orange County Convention Center
Room W414AB

Small Molecule Therapeutics for Neuro-oncology

T. P. Heffron, *Organizer, Presiding*

2:00 Introductory Remarks.

2:10 MEDI 224. Brain-penetrant kinase chemotherapeutics: Learning from CNS space. **M. Mader**, Y. Shi

2:40 MEDI 225. Mechanisms of ALK acquired resistance and the discovery of lorlatinib (PF-06463922), a macrocyclic ALK/ROS1 inhibitor for the treatment of resistant and metastatic NSCLC. **T.W. Johnson**

3:10 MEDI 226. Discovery of the clinical candidate AZD1390: A high-quality, potent and selective inhibitor of ATM kinase with the ability to cross the blood-brain barrier. **K. Pike**

3:40 MEDI 227. Discovery of entrectinib: A novel and potent inhibitor of ALK, ROS1, and Pan-TRKs kinases active in multiple molecularly defined cancer indications. **P. Orsini**

4:10 MEDI 228. Discovery of GDC-0084: A BBB penetrating PI3K/mTOR inhibitor. **T.P. Heffron**

Section B



TECHNICAL PROGRAM

Orange County Convention Center
Room W331A

Besides Off Rate: The Importance of On Rate & Target Rebinding

Y. Pan, *Organizer, Presiding*

2:00 Introductory Remarks.

2:05 **MEDI 229.** Drug-target residence time: A misleading concept. **R. Folmer**

2:35 **MEDI 230.** *In vitro* and *in vivo* target life for immucillin transition-state analogs. **V.L. Schramm**

3:05 **MEDI 231.** Kinetic profiling in drug discovery: A case study with EED hit-to-lead program. **Y. Wang**

3:35 **MEDI 232.** Importance of binding kinetics on *in vivo* target occupancy. **E. de Lange**

4:05 **MEDI 233.** Role of free ligand conformations in ligand binding kinetics: AstraZeneca case studies. **A. Balazs**

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Sponsored by PROF, Cosponsored by AGFD, ANYL, BIOL, BIOT, CARB, CELL, CHED, CMA, COLL, COMP, ENVR, GEOC, I&EC, MEDI, MPPG, NUCL, ORGN, PHYS, PMSE, POLY, PRES, WCC and YCC

Chemistry in Space: Future Directions

Sponsored by YCC, Cosponsored by AGFD, ANYL, BIOT, BMGT, CHAS, ENVR, FLUO, GEOC, HIST, I&EC, MEDI, POLY and PROF

Nucleic Acids-Based Therapeutics

Sponsored by CARB, Cosponsored by BIOL and MEDI

Undergraduate Research Posters

Medicinal Chemistry

Sponsored by CHED, Cosponsored by MEDI and SOCED

MONDAY EVENING



TECHNICAL PROGRAM

Section A

Orange County Convention Center
West Hall C

Sci-Mix

J. B. Schwarz, *Organizer*

8:00 - 10:00

43, 52, 54, 59, 69, 72, 80-81, 97, 100, 105, 127, 130, 134, 142, 152, 160, 167, 170-171, 176, 178, 187, 195, 203, 205, 219. See previous listings.

313, 330, 340, 344, 351, 355, 357, 360, 362, 364, 378, 381. See subsequent listings.

TUESDAY MORNING

Section A

Orange County Convention Center
Valencia Ballroom A

MEDI Awards Symposium

Cosponsored by BIOL
J. B. Schwarz, *Organizer*
A. Stamford, *Presiding*

8:30 MEDI 234. Design of antibiotics for tuberculosis. **C.C. Aldrich**

9:05 MEDI 235. Award Address (ACS Award for Creative Invention sponsored by the ACS Corporation Associates). Antimalarial ozonides. **J.L. Vennerstrom**

9:50 MEDI 236. Modulating host proteostasis to restrict viral adaptation. **M. Shoulders**

10:25 MEDI 237. Small-molecule modulation of HSP60/10 chaperonin systems: A therapeutic strategy over 100 years in the making? M. Stevens, S. Abdeen, A. Ray, A. Washburn, S. Chitre, J. Sivinski, Y. Park, Q. Hoang, E. Chapman, **S. Johnson**

11:00 MEDI 238. Targeting protein-protein interactions to treat misfolding diseases. **J.E. Gestwicki**

11:35 MEDI 239. Award Address (E. B. Hershberg Award for Important Discoveries in Medicinally Active Substances sponsored by the Merck Research Laboratories). Adapting the chemistry and/or biology of proteostasis to ameliorate aggregation-associated degenerative diseases. **J.W. Kelly**

Section B



TECHNICAL PROGRAM

Orange County Convention Center
Room W331A

Recent Advances in Targeting Oncogenic KRAS

E. Altmann, V. Cee, *Organizers, Presiding*

9:00 Introductory Remarks.

9:05 MEDI 240. Ras proteins in normal cells and in human disease. **F.P. McCormick**

9:40 MEDI 241. Small-molecule inhibitors of mutant RAS-effector protein interactions derived using an intracellular antibody fragment. **T. Rabbitts**

10:15 MEDI 242. Discovery of small-molecule inhibitors of GTP bound KRAS^{G12C}. **A.L. Gill**

10:50 MEDI 243. Use of chemotype evolution to discover novel, potent, irreversible inhibitors of the oncogenic G12C mutant form of KRAS. **D.A. Erlanson**, T. Arvedson, V. Cee, R. Fucini, S. Hansen, J. Iwig, J. Jeong, J. McCarter, S. Sabet, A. Sawayama, S. Sethofer

11:25 MEDI 244. Structure-based drug discovery of MRTX1257: A selective, covalent KRAS G12C inhibitor with oral activity in animal models of cancer. **M.A. Marx**, B.R. Baer, J.K. Ballard, J.F. Blake, K. Bouhana, D. Briere, L.E. Burgess, M. Burkhard, H. Chiang, M.J. Chicarelli, J.G. Christensen, J.P. Fischer, J. Hallin, M.J. Mejia, P. Olson, P. Savechenkov, N. Sudhakar, T.P. Tang, G.P. Vigers, J.B. Fell

TUESDAY AFTERNOON

Section A

Orange County Convention Center
Room W414AB

Ions Count: Acids, Bases & Zwitterionics in Drug Design (Medicinal Chemists' Toolbox Series)

N. A. Meanwell, *Organizer*

P. M. Scola, K. Yeung, *Organizers, Presiding*

2:00 Introductory Remarks.

2:05 MEDI 245. Utility of acidic and basic compounds in medicinal chemistry. **P. Walters**, P. Charifson

2:35 MEDI 246. Toxicity arising from amine-containing drugs: Where do we draw the line? **A.S. Kalgutkar**

3:05 MEDI 247. Use of a pH-dependent conformational switching mechanism to enable the discovery of potent, selective and orally bioavailable CCR2 antagonists. M. Yang, Z. Xiao, R.J. Cherney, A.J. Tebben, D.G. Batt, G.D. Brown, J. Chen, M.E. Cvijic, M. Dabros, J.V. Duncia, M.A. Galella, D.S. Gardner, P. Khandelwal, S.S. Ko, M.F. Malley, R. Mo, J. Pang, A.V. Rose, J.B. Santella, H. Shi, A. Srivastava, S.C. Traeger, R. Vuppugalla, B. Wang, S. Xu, R. Zhao, J.C. Barrish, S. Mandlekar, Q. Zhao, **P.H. Carter**



TECHNICAL PROGRAM

3:35 MEDI 248. Carboxylic acids and their isosteres. **D.M. Huryn**

4:05 MEDI 249. Design and evaluation of surrogate structures of the carboxylic acid and other acidic functional groups as possible candidates for isosteric replacements. **C. Ballatore**

4:35 MEDI 250. Challenges with zwitterions: Discovery of zwitterionic CCR3 antagonist clinical candidates. **M.W. Perry**

Section B

Orange County Convention Center
Room W331A

Academic Drug Discovery

E. A. Ambrose, C. Haskell-Luevano, *Organizers, Presiding*

1:30 MEDI 251. *In vitro* selection assays: On-DNA medicinal chemistry optimization of peptidomimetic ligands to chromodomains. **C.J. Krusemark**, S. Wang, K. Denton

2:05 MEDI 252. Development of novel transformations and structural templates to fuel medicinal chemistry discovery and optimization. **J.E. Golden**

2:40 MEDI 253. Allosteric targeting of the Parkinson's-related protein LRRK2. **E.J. Kennedy**

3:15 MEDI 254. Molecule-driven discovery for the identification of therapeutic leads. **J.G. Pierce**

3:50 MEDI 255. Caspase-2 inhibitors for the treatment of tauopathy-related cognitive decline. **K.M. Nelson**, J. Strasser, G. Singh, B. Smith, K. Ashe, M.A. Walters

4:25 MEDI 256. Novel genetically encoded cyclic and bicyclic architectures: Towards *de novo* discovery of bioavailable drugs. **R. Derda**

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Sponsored by PROF, Cosponsored by ENVR, GEOC, I&EC, MEDI, MPPG, NUCL, ORGN, PHYS, PMSE, POLY, WCC and YCC

WEDNESDAY MORNING

Section A

Orange County Convention Center
Valencia Ballroom A

First Time Disclosure of Clinical Candidates



TECHNICAL PROGRAM

E. F. DiMauro, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 MEDI 257. Discovery of AB680: A potent and selective CD73 inhibitor for cancer immunotherapy. **K.V. Lawson**, J. Kalisiak, E. Lindsey, E. Newcomb, E.U. Sharif, D. Miles, J. Jeffrey, M. Reddy Leleti, A. Chen, L. Jin, J. Tan, U. Schindler, S. Young, J. Jaen, J. Powers

9:55 MEDI 258. Identification and characterization of LHC165, a TLR7 agonist designed for localized intratumoral therapies. **G. Cortez**, S. Bender, J. Deane, N. Eifler, S. Kasibhatla, C. Li, S. Pan, N. Parikh, T. Wu

10:35 MEDI 259. Discovery of VNRX-7145: A broad-spectrum orally bioavailable beta-lactamase inhibitor (BLI) for highly resistant bacterial infections ("superbugs"). **C.J. Burns**, R. Trout, A. Zulli, E. Mesaros, R. Jackson, S. Boyd, B. Liu, L. McLaughlin, C. Chatwin, J. Hamrick, D. Daigle, D. Pevear

11:15 MEDI 260. Discovery of TAK-981, a first-in-class inhibitor of Sumo Activating Enzyme (SAE) in phase 1 clinical trials. **S.P. Langston**, D. England, X. He, D. Huszar, P.D. Greenspan

11:55 Concluding Remarks.

Section B

Orange County Convention Center
Room W331A

Exploring Cryptic Pockets

K. K. Liu, *Organizer, Presiding*

9:00 Introductory Remarks.

9:05 MEDI 261. Exploring cryptic pockets formation in targets of pharmaceutical interest with enhanced sampling simulations. **F. Gervasio**

9:40 MEDI 262. Identifying and exploiting protein shape-shifting. **G. Bowman**

10:15 MEDI 263. Development of drug design methods and applications in first-in-class drug discovery. **J. Zhang**

10:50 MEDI 264. Remote control of a dynamic enzyme by leveraging small-molecule fragments. T. Skaist, S.M. Azeem, **D.A. Keedy**

11:25 MEDI 265. Selective FKBP51 inhibitors enabled by transient pocket binding. **F. Hausch**

Section C

Orange County Convention Center
Room W414AB



TECHNICAL PROGRAM

Covalent Inhibition beyond Cysteine

E. Altmann, R. Finlay, K. K. Liu, *Organizers, Presiding*

8:45 Introductory Remarks.

8:50 MEDI 266. Targeted covalent inhibition: Review of the field and recent advances. **C.N. Rowley**

9:25 MEDI 267. Novel, boronic-acid-based, covalent lysine inhibitors. **T.A. McTeague**, N. Grimster, A. Hird, Q. Su

10:00 MEDI 268. Transition-metal-free, tryptophan-selective bioconjugation of proteins. **M. Kanai**

10:35 MEDI 269. Mapping of immunomodulatory receptor protein interactions via photocatalytic-based proximity labeling of the cell surface. **O. Fadeyi**

11:10 MEDI 270. Protein functionalization platform based on selective reactions at methionine residues. **M. Gaunt**

WEDNESDAY AFTERNOON

Section A

Orange County Convention Center
Valencia Ballroom A

First Time Disclosure of Clinical Candidates

E. F. DiMauro, *Organizer, Presiding*

2:00 Introductory Remarks.

2:05 MEDI 271. Discovery of AMG 510, a first-in-human covalent inhibitor of KRAS^{G12C} for the treatment of solid tumors. **V. Cee**

2:45 MEDI 272. Discovery of ABBV-951 to enable continuous subcutaneous infusion of levodopa for the treatment of Parkinson's disease. **P. Kym**, E.A. Voight, R. Klix, P. Mayer, B. Enright, X. Lou, T. Moldovan, D. Stolarik, M.A. Matulenko, A. Hutters, J. Ji, M. Facheris, M. Rosebraugh, J. Benesh

3:25 MEDI 273. Structure guided discovery of S64315 (MIK665): a potent and selective MCL1 inhibitor. **A. Kotschy**, Z. Szlavik, O. Geneste, J. Murray, J. Davidson, R.E. Hubbard, M. Wood, M. Csekei, A. Paczal, Z.B. Szabo, S. Sipos, A. Proszenyak, B. Balint, A.L. Maragno, D. Demarles, G. Le Toumelin-Braizat, M. Chanrion, A. Bruno, A. Claperon, A. Surgenor, P. Dokurno, N. Matassova, I. Chen, B.J. Davis, H. Simmonite, A. Studeny, G. Lysiak-Auvity, A. Girard, F. Grave, G. Guasconi, N. Cauquil, F. Colland, J.A. Hickman

4:05 MEDI 274. Discovery of PF-06882961: A potent, orally bioavailable small molecule agonist of the GLP-1 receptor. **D.J. Edmonds**, D.A. Griffith, S.W. Bagley, C. Buckeridge, E.L. Conn, J.M. Curto, D.R. Derksen, H. Eng, M.E. Flanagan, J. Fortin, M.C. Griffor, M.V. Jackson, A.S. Kalgutkar, J.B. Kuzmiski, M.S. Landis, D.J. Lettiere, C. Limberakis, S. Liras, P.M. Loria, A.M. Mathiowetz, D.W. Piotrowski, D. Price, L. Stevens, T.P. Rolph, R.B. Ruggeri, A.R. Saxena, A.H. Smith, D.A. Tess, L. Wei



TECHNICAL PROGRAM

4:45 Concluding Remarks.

Section B

Orange County Convention Center
Room W331A

General Orals

J. B. Schwarz, *Organizer*
C. Am Ende, *Presiding*

1:30 **MEDI 275.** Chemical biology impacting drug discovery. **C. Am Ende**

1:50 **MEDI 276.** Biological activity of ferrocenyl derivatives: Study of the effect of different core moieties and substituents on anticancer and antioxidant activity. **S.M. Delgado-Rivera**, S.A. Henriquez Lopez, G.E. Pérez-Ortiz, A. Baerga-Ortiz, I. Montes-Gonzalez, D.M. Pinero Cruz

2:10 **MEDI 277.** Structure-activity relationship of non-electrophilic naphthalene and isoquinoline based inhibitors of the KEAP1-NRF2 protein-protein interaction. **P. Lazzara**, B. Richardson, B. David, H.R. Potteti, K. Dye, S. Reddy, T.W. Moore

2:30 **MEDI 278.** Evolution-guided design of phosphatase inhibitors. M. Hjortness, L. Riccardi, A. Hongdusit, A. Ruppe, E. Kim, M. Zhao, P. Zwart, B. Sankaran, H. Arthanari, M. Sousa, M. Devivo, **J.M. Fox**

2:50 **MEDI 279.** Chemical tools to probe the function of TRIM33. **A. Scorah**, L. See, J. Bluck, J. Reynolds, W. McCoull, S.J. Conway

3:10 **MEDI 280.** Effects of phosphate linker modifications on 2',3'-cyclic dinucleotide STING agonists. **S.P. Walsh**, M.D. Altman, B.M. Andresen, W. Chang, A. Donofrio, T.J. Henderson, J.P. Jewell, C. Lesburg, J. Lim, H. Liu, M. Lu, R. Otte, J. Presland, D. Steinhuebel, B. Taoka, Q. Truong, W. Wu, S. Perera, S. Cemerski, W. Trotter, J. Cumming

3:30 **MEDI 281.** 2NDEP highlights allosteric activation of the $\alpha 7$ nicotinic acetylcholine receptor. A. Gulsevin, C. Stokes, R.L. Papke, **M. Quadri**, N. Horenstein

3:50 **MEDI 282.** Discovery of selective FactorD inhibitors targeting the alternative complement pathway. **R.G. Karki**, J.J. Powers, D. Belanger, D. Liu, N. Ji, K. Jendza, C. Gelin, S. Flohr, E. Lorthiois, A. Vulpetti, A. Mac Sweeney, K. Anderson, M. Mogi, N. Mainolfi

4:10 **MEDI 283.** Multi-parameter optimization of isoform-selective dual Nav1.6/1.2 antagonists to balance CNS penetration with PK and *in vivo* efficacy in mouse models for epilepsy. **C.M. Dehnhardt**, K. Buford, J. Andrez, M.E. Grimwood, A. Zenova, M. Taron, W. Gong, S. Decker, S. Chowdhury, C. Higgs, P. Tari, R. Kwan, L. Sojo, R.J. Devita, C. Cohen, J. Johnson, S. Wesolowski, J. Empfield, T. Focken

4:30 **MEDI 284.** Enzymatic late-stage oxidation of lead compounds with solubilizing biomimetic docking/protecting groups. **U.E. Lange**

4:50 **MEDI 285.** Development and characterization of LHC165, a TLR7 agonist designed for localized intratumoral injection. **N. Eifler**



TECHNICAL PROGRAM

5:10 MEDI 286. Versatile C-H methylation reaction for late-stage functionalization. **S.D. Friis**, L. Ackermann, M.J. Johansson

Section C

Orange County Convention Center
Room W414AB

The Messy Business of Target (In)Validation: Chemistry's Role & Challenges in Early Discovery

M. Herold, B. A. Knapp-Reed, J. Shotwell, *Organizers*
J. Shotwell, *Presiding*

1:30 Introductory Remarks.

1:35 MEDI 287. Enzyme target pre-clinical (in)validation: The value of rational exploration of the unknown, and how application of target engagement principles can address key pharmacology questions. **T.B. Durham**

2:05 MEDI 288. Promoting illiteracy: Development of chemical probes for epigenetic reader domains to explore untapped targets. **L.I. James**

2:35 MEDI 289. Lessons learnt from the discovery of CDK8/19 protein kinase inhibitors: From phenotypic screen to selective chemical probes. **P.A. Clarke**

3:05 Intermission.

3:15 MEDI 290. Small molecules from phenotypic screens: Looking for “a” target? **S. Patnaik**

3:45 MEDI 291. Discovery of a novel kinetoplastid inhibitor for the treatment of human African Trypanosomiasis. **J. Jiricek**, S. Rao, S. B. Lakshminarayana, C. Sarko, N. Aziz, F. Gu, T. Diagana

4:15 MEDI 292. SMYD3 target (in)validation from a medicinal chemistry perspective. **B.A. Knapp-Reed**

WEDNESDAY EVENING

Section A

Orange County Convention Center
West Hall C

General Posters

Cosponsored by ORGN[†]
J. B. Schwarz, *Organizer*

7:00 - 9:00



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- MEDI 293.** Discovery of KAG-308: A potent and orally available EP4 agonist for the treatment of inflammatory bowel disease. **Y. Ishibashi**, Y. Matsumura, Y. Miyake
- MEDI 294.** Synthesis and evaluation of linear and macrocyclic dolastatin 10 analogues containing heteroatoms on the amino acid side chains. **M. Akaiwa**, T. Martin, B.A. Mendelsohn
- MEDI 295.** Design, synthesis, and biological evaluation of bisphenol Z derivatives. **L.M. Stitzlein**, C.T. Stang, L.R. Inbody, R.A. Schneider, R.W. Dudley
- MEDI 296.** Saturated bioisosteres of benzene with improved solubility. **P. Mykhailiuk**, V. Levterov, O.O. Stepaniuk
- MEDI 297.** Conformationally restricted pyrrolidines for drug discovery. **P. Mykhailiuk**, V. Levterov, A. Cherepakha
- MEDI 298.** Synthesis and evaluation of thalassotalic acid A and analogs. J. Schulz, **J. Patrone**
- MEDI 299.** Synthesis of prodrugs from a quinazoline derivative to optimize its behavior against cancer cells. **L.C. Arenas Corona**, F. Hernández Luis
- MEDI 300.** Design and synthesis of a novel series of highly potent RAF kinase-inhibiting triarylpyrazole derivatives with potential antiproliferative activity against melanoma. **M. El-Gamal**, M. Khan, H. Tarazi, H. Choi, C. Oh
- MEDI 301.** Design, synthesis, and evaluation of biological properties of new 5-cyanopyrimidine-based compounds. **A.S. Bunev**, D. Khochenkov, Y. Khochenkova, E. Stepanova
- MEDI 302.** Novel imidazo[2,1-*B*]thiazoles as potential EGFR tyrosine kinase inhibitors: Synthesis and *in vitro* evaluation. **A.S. Bunev**, D. Khochenkov, Y. Khochenkova, E. Stepanova
- MEDI 303.** 4-Amino-5-(thiazol-2-yl) pyrimidine derivatives: New effective inhibitors of EGFR-dependent signal cascades. **A.S. Bunev**, D. Khochenkov, Y. Khochenkova, E. Stepanova
- MEDI 304.** Inhibition of pancreatic acinar ductal metaplasia by a novel STAT3 inhibitor LLL12B. L. Da Silva, **J. Song**, J. Matthews, J. Jiang, H. Luesch, C. Li, T. Schmittgen
- MEDI 305.** Structure-activity relationships of UDEPs as caseinolytic protease activators. **Y. Zhao**, E. Griffith, A. Arya, M. LaFleur, R.E. Lee
- MEDI 306.** Design, synthesis, and biological evaluation of flavones showing inhibitory effects on aurora kinases. J. Lee, **D. Koh**
- MEDI 307.** Synthesis and evaluation of novel multifunctional opioid peptidomimetics. **M.A. Baber**, D. Montgomery, J.P. Anand, L. Delong, J.R. Traynor, H.I. Mosberg
- MEDI 308.** Trifluoromethyl thiazine-based BACE1 Inhibitors: Synthesis, *in vivo* efficacy, cardiovascular side effects, and covalent binding burden. **T. Oguma**, K. Nakahara, K. Anan, Y. Isou, S. Suzuki, T. Yamamoto, Y. Kido, N. Kanegawa, T. Fukushima, Y. Tonomura, H. Ito, G. Sakaguchi, F. Bischoff, H. Gijsen, K. Kusakabe
- MEDI 309.** Medicinal chemistry and chemical biology approach in order to design and synthesize of TBK1/IKK- ϵ small molecules inhibitors. **A. Assadieskandar**, C. Zhang



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- MEDI 310.** Development of a new series of bacterial topoisomerase inhibitors for antibiotic-resistant infections. **L. Li**, S. Dellos-Nolan, A. English, J.C. Yalowich, D. Wozniak, M.J. Mitton-Fry
- MEDI 311.** Hydrazolyl linked hybrids of sulfonate esters and 4-thiazolidinone: Design, synthesis, and biological evaluation as potent α -glucosidase inhibitors. **R. Kaur**, M. Kumar
- MEDI 312.** Design, synthesis, and antimicrobial evaluation of substituted urea derivatives containing alkyl/aryl moieties. M. Patil, N. Poyil, A. Bugarin, S. Joshi, S. Patil, **S. Patil**
- MEDI 313.** Recombinant expression of xenobiotic and steroidogenic cytochrome P450 enzymes. **L. Sanchez**, S. Brixius-Anderko, E. Scott
- MEDI 314.** Exploratory synthesis of novel cyclic and straight-chain 1,3-azaborines as potential HIV-1 protease inhibitors. **K. Hawley**, **R. Latsis**, **C. Suarez**, K. Norris, **A. Vulcano**, **S. Dawson**, **A. Williams**, A. Lanin, J. Murray, **L. Fabry-Asztalos**
- MEDI 315.** Examination of aminophenol-containing compounds designed as antiproliferative agents and potential atypical retinoids. **S. Altman**, M. Imai, N. Takahashi, T.R. Burke
- MEDI 316.** Synthesis and biological evaluation of 1,2,3-triazole analogs of CFTR corrector VX-809. **J. Brace**, S.J. Post, N.L. Thacker, L. Tang, S.M. Rowe, S.G. Aller, M.L. Turlington
- MEDI 317.** Discovery of novel anti-tubercular agent for the treatment of MDR/XDR TB. **J. Choi**, S. kang, Y. Kim, I. Choi, A. Lee, G. Jin, V. Delorme, **K. Park**
- MEDI 318.** Development of novel treatments against inherited blinding diseases *Retinitis pigmentosa* and Leber's congenital amaurosis. **E. Pileggi**, G. Pasqualetto, M. Rozanowska, A. Brancale, M. Bassetto
- MEDI 319.** Synthesis and biological activity of a new saccharine derivatives as a dual D₂/5-HT_{1A} receptor ligands. **D. Kulaga**
- MEDI 320.** New long-chain derivatives of 1-(1,2-benzisothiazol-3-yl)piperazine with high affinity for selected serotonin receptors. **P. Zareba**, J. Jaskowska, A. Drabczyk
- MEDI 321.** Structure-activity relationships of fragment-based inhibitors of *Trichomonas vaginalis* uridine nucleoside ribohydrolase. **J.K. Persaud**, S.F. Thuilot, S. Auletta, W. Caravan, A. Leonardo, T. Li, Z. Dulloo, N. Kabir, D.G. Brown, D.W. Parkin, M.A. Vanalstine-Parris, B.J. Stockman
- MEDI 322.** Novel applications of biocatalysis to late stage derivatization and stereochemistry determination of 2'3'-cyclic dinucleotide bisphosphorothioates. **J. Lim**, L. Nogle, H. Kim, J. Sauri, Y. Chen, J. Piesvaux, J. Cumming, W. Trotter
- MEDI 323.** (1-4)-S-thiodisaccharides induction of ER stress as possible mechanism of glioblastoma cells death. J. Sarnik, A. Maciejaja, **Z.J. Witczak**, T. Poplawski
- MEDI 324.** Synthesis of 1,2,3-triazole analogs of CFTR potentiator VX-770. **B. Ody**
- MEDI 325.** Design, synthesis, and antimicrobial evaluation of dibenzothiophene sulfones derivatives. **S. Alelaiwi**
- MEDI 326.** Discovery of *in situ* click chemistry compatible analogs of F508del-CFTR corrector VX-809. **O.R. Brown**, M.L. Turlington



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- MEDI 327.** Design, synthesis, and structural activity relationships of styrylquinoline derivatives as potent antimalarial agents. **G. Huang**, C. Solano, J. Kreisel, A.K. Arshadi, D. Chakrabarti, Y. Yuan
- MEDI 328.** NMR-based counter screens of fragment inhibitors of *Trichomonas vaginalis* uridine nucleoside ribohydrolase confirm reversible, target-specific inhibition. **S.F. Thuilot**, J.K. Persaud, D.G. Brown, D.W. Parkin, B.J. Stockman
- MEDI 329.** Molecular modeling and NMR-based counter screens of fragment inhibitors of *Trichomonas vaginalis* adenosine/guanosine nucleoside ribohydrolase. **A. Kaur**, J. Gonzalez, D.G. Brown, D.W. Parkin, B.J. Stockman
- MEDI 330.** Novel class of STING agonists that self-assemble into nanostructures are potent anti-cancer immunotherapeutic agents. **A. Sheri**, S. Padmanabhan, G. Meher, R.H. Gimi, D. Cleary, S. Khedkar, S. Challa, S. Zhou, V. Nair, L. Suppiah, D. Schmidt, N. Afdhal, R. Iyer
- MEDI 331.** Synthesis of novel functionally selective and long-acting muscarinic antagonists. **L. Mesa**, **C. Martin**, J. Boulos
- MEDI 332.** Cyclooxygenase-2 inhibitory activity of metal-curcumin complexes. **J. Harder**, **A. Vummenthala**, **M. Vazquez**
- MEDI 333.** Synthesis of new β -benzyloxy-*N*-phenethylamines as biogenic amine neurotransmitter transporter blockers. S. Almendras, A. Fierro, J. Campusano, J. Eltit, **E.G. Pérez**
- MEDI 334.** Synthesis of ω -hydroxy isoprenoid bisphosphonates as potential GGDPs inhibitors. **N. Bhuiyan**, M. Varney, S.A. Holstein, D.F. Wiemer
- MEDI 335.** Design, synthesis, and biological evaluation of water-soluble amino acid prodrugs of a rhein-derived anti-cancer agent. **A. Anifowose**, Z. Yuan, X. Yang, Y. Zheng, Z. Pan, Z. Zhang, B. Wang
- MEDI 336.** Synthesis and biological evaluation of selective tubulin inhibitors as anti-trypanosomal agents. **V. Bobba**
- MEDI 337.** Synthesis of triclosan derivatives that function as azo dyes. **S. Desmond**, P. Sibbald
- MEDI 338.** Synthesis and design of CRB, a resveratrol analog, reduces cell injury caused by surgery mimicking deep brain stimulation. **M. Lee**, S. Gallemore, A. Linberg, Z. DeBruine, B. Babu, K.A. Brien, G. Fraley
- MEDI 339.** Synthesis, optimization, and analysis of hexavalent sulfoglycodendrimers as anti-viral agents. **C. Vierra**, K.D. McReynolds
- MEDI 340.** Synthesis and biological evaluation of nitrogen containing marine natural products. **C. Martinez-Brokaw**, K.R. Robinson, J.G. Pierce
- MEDI 341.** 2-Amino-quinolin-4(1*H*)-ones as novel anti-coronavirus agents. **C. Park**, J. Song, J. Lee, J. Lee, S. Kim, H. Kim
- MEDI 342.** Translation of ^1H and ^{19}F NMR-based activity assays to *in vitro* characterization of nucleoside hydrolase activity in cell extracts and whole cells. **M. Canestrari**, M. Mahmood, S.F. Thuilot, B.J. Stockman
- MEDI 343.** Design, synthesis, and biological evaluations of next-generation taxoids, bearing *m*-OCF₃ and *m*-OCF₂H groups at the C2 benzoate moiety. **L. Chen**, C. Wang, W. Guo, X. Wang, Y. Jing, Y. Sun, I. Ojima
- MEDI 344.** Improved synthetic approach to CA IX selective inhibitors featuring one-pot cyclization/deprotection. **H. Li**, A.B. Murray, M. Quadri, R. McKenna, N. Horenstein



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- MEDI 345.** Synthesis, evaluation, and *in silico* study of structural analogs of colchicine as potential anticancer agents. **S. Yoganathan**, N. Karadkhelkar, P. Gupta, Z. Chen
- MEDI 346.** Synthesis of inhibitors of 1-deoxyulose- 5-phosphate reductoisomerase. **G. Mancini**, J.W. Tomsho
- MEDI 347.** Studies toward an amide core for zampanolide mimics as potential anti-prostate cancer agents. **M. Gonzalez**, G. Chen, Q. Chen
- MEDI 348.** Structure-based design, synthesis and evaluation of D-3,3-diphenylalanine-based tetrapeptides inhibitors of thrombin-activated platelets aggregation and potent anticoagulants. **C.C. Clement**, J. Gonzalez, A. Babinska, M.R. Gil
- MEDI 349.** Synthesis of 2-aminocyclobutanones as potential serine- and metalloprotease inhibitors. **T. Habeeb Mohammad**, C. Reidl, D.P. Becker
- MEDI 350.** Synthesis, *in silico*, and *in vitro* evaluation of long chain alkyl amides from 2-amino-4-quinolone derivatives as biofilm inhibitors. M.A. Loza-Mejia, **S. Borbolla-Alvarez**, **A.E. Delgado**, **M.P. Espinosa Valdes**, J. S. Tejada, A. Cerón-Nava, O. Quintana-Romero, A. Ariza-Castolo, D. García-del Río
- MEDI 351.** Synthesis of small molecules based on novobiocin and the biphenylcyclohexane system that inhibit the Hsp90 molecular chaperone. **A. Zuo**, P.N. Meka, B. Keegan, B.S. Blagg
- MEDI 352.** Synthesis of oxindole derivatives via C-H alkylation and intramolecular cyclization: Access to Hit compound for anti-tumor agent. **S. Han**
- MEDI 353.** Design, synthesis, and evaluation of resveratrol-NSAID hybrids as potential antioxidants and anti-inflammatories. **M.A. Enriquez-Pichardo**, **S.S. Medina-Rosas**, **G. Sánchez-Tejeda**, I. Rodríguez-Nuño, J. García-Ibarra, H. Mancilla-Díaz, J.R. Salazar, M.A. Loza-Mejia
- MEDI 354.** Design, synthesis, and structure-activity relationship studies of phthalimide-based sphingosine kinase inhibitors. **F. Afrin**, K. Obuch, Y. Kharel, W. Santos, K. Lynch, S. Pashikanti
- MEDI 355.** Design, synthesis, and biological evaluation of truxillic acid-based fatty acid binding protein 5 (FABP5) inhibitors as anti-nociceptive and anti-inflammatory agents. **T.S. Clement**, M. Awwa, A. Taouil, A. Maharaj, J. Kim, Y. Sun, A. Pepe, H. Li, D.G. Deutsch, M.W. Elmes, M. Kaczocha, I. Ojima
- MEDI 356.** TB or not TB? That is not the only question. **J. Trant**, **N. Milligan**, A. Ford, Z. Hodge, I.N. Nawarathne
- MEDI 357.** Pharmacology and modeling of methcathinone (MCAT) isomers and achiral analogs at the monoamine transporters (MATs). **R.A. Davies**, F. Sakloth, B. Ruiz, J. Eltit, R.A. Glennon
- MEDI 358.** Design, synthesis, and evaluation of the anthranilic acid derivative HGA-01 as a potential multitarget drug for the management of metabolic syndrome. **H. González Álvarez**, **M. Bravo Jimenez**, **M.A. Loza-Mejia**, R. Pinto-Almazán, K. Gallardo-Ignacio, L.A. González-Hernández, E. Chávez-Gutiérrez
- MEDI 359.** Synthesis and bioevaluation of new pyrazino[2,3-*b*]quinolinones as potential antitumorals: Effect of the nature of alkyl substituents in position 5. **D.G. Juan Guadarrama**, **L.J. Jimenez Sanchez**, J. Villalobos, J. Solano, A. Lira, L. Martino, M.A. Loza-Mejia
- MEDI 360.** Synthesis of small molecules for protein control. **E. Bray**, C. Alvarez, J. Leahy, M.W. White



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

MEDI 361. Development of a selective phosphatase inhibitor for neurodegenerative disorders. **J. Nunziata**, B.J. Eduful, Y. Chen, D. Kang, J. Leahy

MEDI 362. Synthesis of rhodacyanine derivatives as Hsp70 inhibitors for improved tau degradation in tauopathies. **A. Lemus**, S. Patel, R. Swonger, R. Blackburn, J. Koren, C. Dickey, L. Blair, J. Leahy

MEDI 363. Design, synthesis, and SAR of matrix metalloprotease 9 inhibitors as anti-metastasis agents. **M. Awwa**, V.M. Alford, X. Ren, J. Cao, N.S. Sampson, I. Ojima

MEDI 364. Conformational constraint of aromatic residues of the kappa opioid receptor antagonist arodyn using ring closing metathesis. **S.A. Gisemba**, J.V. Aldrich, T. Murray

MEDI 365. Synthesis and QSAR study of novel NSAID hybrid conjugates as potential anti-inflammatory agents. **H.H. Honkanadavar**, S.S. Panda

MEDI 366. Design, synthesis, and characterization of new modulators of the leukotriene A₄ hydrolase aminopeptidase activity. **G. Petruncio**, K. Lee, L. Jansen, S. Noble, Y. Shim, M. Paige

MEDI 367. Structure-activity relationship-guided synthesis and identification of the GATA4 and NKX2-5 protein-protein interaction modulators. **M. Jumppanen**, S. Kinnunen, M. Välimäki, S. Auno, G. Boije af Gennäs, H. Xhaard, V. Talman, H. Ruskoaho, J.T. Yli-Kauhaluoma

MEDI 368. Atypically substituted carbapenem antibiotics with improved activity against OXA-23-producing *Acinetobacter baumannii*. N.M. Al-Kharji, **M. Alqurafi**, T. Nguyen, W. Chai, N.K. Stewart, M. Toth, J. Kim, N. Nformi, S. Solanki, K. Wong Wirth, M. Ardesna, A. Mehta, A. Jakubowski, B. Meshram, C. Varner, A. He, M. Pan, S.B. Vakulenko, J.D. Buynak

MEDI 369. Synthesis of new β -heteroarylmethoxy-*N*-phenethylamines as possible monoamine neurotransmitter transporter blockers. **I. Almodovar**, E.G. Perez, M. Madrid

MEDI 370. Identification, validation, and synthesis of small molecule inhibitors of the Lin28b/pre-Let-7 interaction in pancreatic ductal adenocarcinoma. **H. Ahamed**, **T. Aramburu**, R.L. Broadrup, R. Mostoslavsky

MEDI 371. Evaluation of the effects of differentially sulfated heparin/heparan sulfate analogs on MCF-7 cell migration. **A.M. Brown**, **N.L. Snyder**

MEDI 372. Synthesis and biological screening of praziquantel derivatives for use as pharmacological chaperones of arylsulfatase B. **K. Terpstra**, T.A. Russell

MEDI 373. Synthesis and computational study of pyrazinoic acid conjugates as potential anti-infective agents. **W.F. Littlefield**, S.S. Panda

MEDI 374. Design and synthesis of quinolone-based hybrid conjugates as potential anticancer agents. **R.M. Bokhtia**, T.S. Ibrahim, A.M. Al-Mahmoudy, E.H. Abdel-Aal, S.S. Panda

MEDI 375. Synthesis of indoles-based Schiff base complexes and spiro compounds as potential anticancer agents. **I. Seliem**, T.S. Ibrahim, A.M. Al-Mahmoudy, Z.K. Abdel-Samii, S.S. Panda

MEDI 376. Synthesis of carbon nitride dots for target-specific biomedical applications. **P. Liyanage**, R. Graham, C.C. Chusuei, K.J. Mintz, Y. Zhou, J. Harper, R.M. Leblanc



TECHNICAL PROGRAM

MEDI 377. Heterocycle libraries based on natural anti-inflammatories. **B. Maki**

MEDI 378. New tools for targeting the asialoglycoprotein receptor. **N.L. Snyder, A. Strasser,** N. Fendler

MEDI 379. Trehalose-based photosensitizers targeting *Mycobacterium tuberculosis*. **L.A. Russell,** R.C. Steffens, M.B. Burch, D.G. Dennis, M. Parris, J.V. Ruppel, **N.L. Snyder**

MEDI 380. *In silico* models for predicting metabolism by Flavin-Containing Monooxygenases (FMOs). **G. KC,** M. Hassan, S. Sirimulla

MEDI 381. Synthesis, characterization and reactivities of a new HDAC inhibitor. **D. Shao,** E.S. Guo, C. Feng, Q. Zhao

MEDI 382. Design, synthesis, and structure-activity relationship of novel 1,2,4-triazine-3-one derivatives as multimodal compounds intended to treat schizophrenia. **B. Narasimha,** V.R. Middekadi, M. Rasheed, D.S. Sisodaya, V.R. Mekala, S. Petlu, R. Nirogi

MEDI 383. Design, synthesis, and structure-activity relationship of novel pyrazolo-pyrimidine carboxamides as Muscarinic₁ Positive Allosteric Modulators (M₁ PAM). **S.R. Gagginapally,** D.M. Kancharla, M. Dasoju, N.R. Mudanna, R. Subramanian, R. Nirogi

MEDI 384. Design, synthesis, and pharmacological characterization of novel series of 4,5,6,7-tetrahydro-thiazolo[5,4-c]pyridine derivatives as H3 receptor antagonists. **P.K. Achanta,** S.K. Saraf, R.K. Badange, R. Subramanian, N.R. Mudanna, P. Jayarajan, R. Nirogi

MEDI 385. Design, synthesis, and pharmacological characterization of novel carboxamides as 5-HT₄ receptor agonists. **R.K. Badange,** P.K. Achanta, K.K. Kandukuri, V. Bhatta, V. Reballi, V.R. Mekala, G. Bhyrapuneni, V. Benade, R. Nirogi

Asymmetric Reactions & Syntheses

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CH Activation

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Heterocycles & Aromatics

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Peptides, Proteins & Amino Acids



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

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Total Synthesis of Complex Molecules

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NUCL

Division of Nuclear Chemistry and Technology

A. Hixon, *Program Chair*

SUNDAY MORNING

Section A

Orange County Convention Center
Room W330C

Computational Methods in Lanthanide & Actinide Chemistry

Cosponsored by COMP and INOR
D. A. Penchoff, C. C. Peterson, *Organizers, Presiding*
A. Shields, *Presiding*

8:30 Introductory Remarks.

8:35 NUCL 1. Predictive practical approaches to heavy-element computational chemistry for nuclear security. **R.J. Harrison**, D.A. Penchoff, H.L. Hall

9:05 NUCL 2. Separation of americium-241 and plutonium-238. **J. Auxier**

9:35 Intermission.

9:50 NUCL 3. Coupled cluster studies of actinyl interactions in the gas phase. R. Feng, **K.A. Peterson**

10:20 NUCL 4. Understanding selectivity of lanthanide and actinide compounds by computational techniques. **C.C. Peterson**, D.A. Penchoff, H.L. Hall, R. Harrison

10:50 Intermission.

11:05 NUCL 5. Electronic structure and chemical bonding of f-element coordination complexes with N,O,S-donor ligand. **E.R. Batista**, J. Su, P. Yang



TECHNICAL PROGRAM

11:35 NUCL 6. Covalency of actinides (An^{III} , An^{IV}) with chelating agents across the actinide series. **P. Yang**, M. Kelley, J. Su, E.R. Batista

12:05 Concluding Remarks.

SUNDAY AFTERNOON

Section A

Orange County Convention Center
Room W330C

Glenn T. Seaborg Award for Nuclear Chemistry: Symposium in Honor of Thomas E. Albrecht-Schmitt

K. N. Raymond, *Organizer, Presiding*

1:10 Introductory Remarks.

1:20 NUCL 7. **Award Address** (Glenn T. Seaborg Award for Nuclear Chemistry sponsored by the ACS Division of Nuclear Chemistry and Technology). I wonder: A journey into the outer reaches of the periodic table. **T.E. Albrecht-Schmitt**

2:00 NUCL 8. New uranyl chemistry mediated by redox-active ligands. E. Coughlin, Y. Qiao, E. Lapsheva, M. Zeller, E.J. Schelter, **S.C. Bart**

2:20 NUCL 9. Spectroscopic and binding constant studies of actinium chelation for targeted alpha therapy applications. **B.W. Stein**, A. Morgenstern, M. Kerlin, L. Lilley, S.A. Kozimor, E.R. Batista, P. Yang

2:40 NUCL 10. Structural chemistry of tetravalent metal ion complexes and clusters: Assessing the impact of non-bonding interactions. **K.E. Knope**

3:00 NUCL 11. ARIES: From pits to plutonium oxide. **J.T. Stritzinger**, D.J. Garcia

3:20 Intermission.

3:40 NUCL 12. Targeted radionuclide therapy: The promise of short-lived alpha-emitting actinides. **R.J. Abergel**, d. An, A. Lakes, G. Deblonde, J. Rees, S. Gauny, D. Sridharan

4:00 NUCL 13. ^{119m}Te production for ^{119}Sb radiopharmaceuticals. **S.A. Kozimor**, A. Akin, K. Bennett, E. Birnbaum, A. Blake, S. Bone, M. Brugh, J. Engle, L. Lilley, M. Fassbender, V. Mocko, F. Nortier, B.W. Stein, S. Thiemann, C. Vermeulen

4:20 NUCL 14. Kinetics in f-element separations. **M.P. Jensen**, G.A. Picayo, M.A. Eddy

4:40 NUCL 15. Lanthanide-based single-molecule magnets with high blocking temperatures. C.A. Gould, P.C. Bunting, S. Demir, R.R. McClain, L.E. Darago, K. Chakarawet, M. Gonzalez, K.R. Meihaus, J. Zadrozny, M. Nippe, J.D. Rinehart, S.J. Teat, B.G. Harvey, W.J. Evans, **J.R. Long**



TECHNICAL PROGRAM

5:00 NUCL 16. Organometallic neptunium chemistry and the importance of spontaneous reduction reactions. **P.L. Arnold**, T. Ochiai, J. Shephard, V. Berryman, M. Dutkiewicz, O. Walter, R. Caciuffo, N. Kaltsoyannis, S. Parsons

Section B

Orange County Convention Center
Room W311H

Computational Methods in Lanthanide & Actinide Chemistry

Cosponsored by COMP and INOR
D. A. Penchoff, C. C. Peterson, *Organizers, Presiding*
A. Shields, *Presiding*

2:00 Introductory Remarks.

2:05 NUCL 17. Actinides on surfaces. **G. Schreckenbach**

2:35 NUCL 18. Exploiting crystal structure–property relationships to characterize uranium materials. **A. Shields**, A. Miskowiec, M.C. Kirkegaard, J. Niedziela, R. Kapsimalis, B. Anderson

2:55 NUCL 19. Understanding the polymorphism of $A_4[(UO_2)_3(PO_4)_2O_4]$ (A=alkali metals) uranyl phosphate framework structures using density functional theory. **V. Kocovski**, T. Besmann

3:15 Intermission.

3:30 NUCL 20. Evaluation of van der Waals interactions in uranium phases using density-functional theory (DFT) using the exchange-hole dipole moment (XDM) dispersion correction. **M. Christian**, E.R. Johnson, T. Besmann

3:50 NUCL 21. Role of extractant structure in the self-association and phase behavior of uranyl nitrate complexes in organic solvents. **M. Servis**, D. Wu, J. Shafer, A.E. Clark

4:10 NUCL 22. Computational design of actinium-225 chelators for use in targeted alpha therapy. **A. Morgenstern**, L. Lilley, B.W. Stein, S.A. Kozimor, E.R. Batista, P. Yang

4:30 Concluding Remarks.

MONDAY MORNING

Section A

Orange County Convention Center
Room W330C

Glenn T. Seaborg Award for Nuclear Chemistry: Symposium in Honor of Thomas E. Albrecht-Schmitt



TECHNICAL PROGRAM

K. N. Raymond, *Organizer*
D. L. Clark, *Presiding*

8:20 NUCL 23. Bonding in the actinide series: Using EXAFS to systematically probe coordination compound structures of Th through Cf. **C. Booth**, G. Deblonde, L.M. Moreau, J. Rees, R.J. Abergel

8:40 NUCL 24. Plutonium physics and chemistry highlights from Los Alamos National Laboratory: Neutron and NMR spectroscopy. **E.D. Bauer**

9:00 NUCL 25. How f-block atoms behave in intermetalloid clusters: [Ln@Zintl] and [Ac@Zintl]. **S. Dehnen**

9:20 NUCL 26. Californiums moving to Colorado. N. Bessen, M. Kelley, J. Su, E.R. Batista, P. Yang, **J. Shafer**

9:40 NUCL 27. Soft X-ray synchrotron radiation studies of actinide materials. **D.K. Shuh**

10:00 Intermission.

10:20 NUCL 28. Protactinium and the intersection of actinide and transition metal chemistries. **R. Wilson**

10:40 NUCL 29. Selective separation of Zr(IV) from Pu(IV) for used nuclear fuel reprocessing applications. **N.A. Wall**, M. Friend

11:00 NUCL 30. Trans-uranic organometallic chemistry: Oxidation states, bonding, and electronic structure. **C.A. Goodwin**, N. Lichtenberger, S.A. Kozimor, W.J. Evans, A. Gaunt

11:20 NUCL 31. Analytical chemistry in support of plutonium production. **J.N. Cross**, A.C. Olson, L. Tandon

11:40 NUCL 32. Actinide chemistry at the most fundamental and comprehensible level: Gas-phase reactions. **J.K. Gibson**

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

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MONDAY AFTERNOON

Section A

Orange County Convention Center
Room W330C

Glenn T. Seaborg Award for Nuclear Chemistry: Symposium in Honor of Thomas E. Albrecht-Schmitt



TECHNICAL PROGRAM

K. N. Raymond, *Organizer*
A. P. Sattelberger, *Presiding*

1:40 NUCL 33. Recent advances in actinide ligand multiple bonding. **S.T. Liddle**, J. Du, L. Chatelain, M. Dutkiewicz, O. Walter

2:00 NUCL 34. Differentiating f-elements from ion-specific electronics and coordination environments. **E.J. Schelter**, T. Cheisson, B.E. Cole, Y. Qiao, J. Nelson, R. Higgins

2:20 NUCL 35. Oak Ridge National Laboratory's Isotope Program: Unique and dynamic. **J. Ezold**, S. Hogle

2:40 NUCL 36. From actinides to superheavies and to the stars. **C. Duellmann**

3:00 NUCL 37. From trivalent actinide borate complexes to cationic materials. **M. Polinski**

3:20 Intermission.

3:40 NUCL 38. Recent developments in uranium(V) chemistry. **M. Mazzanti**

4:00 NUCL 39. Efficient removal of radionuclides from aqueous solutions using carbon nanomaterials. **X. Wang**

4:20 NUCL 40. Actinide polyrotaxane compounds: From structural diversity to inclusion effect. **W. Shi**, L. Mei, Z. Chai

4:40 NUCL 41. Efficient separation and remediation of $^{99}\text{TcO}_4^-$ under extreme conditions using advanced cationic porous materials. **S. Wang**

5:00 NUCL 42. Recent advances in low oxidation state actinide chemistry. **W.J. Evans**

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

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TUESDAY MORNING

Section A

Orange County Convention Center
Room W330C

Glenn T. Seaborg Award for Nuclear Chemistry: Symposium in Honor of Thomas E. Albrecht-Schmitt

K. N. Raymond, *Organizer*
D. E. Hobart, *Presiding*



TECHNICAL PROGRAM

8:00 NUCL 43. Review of synthesis, spectroscopy, and structural characterization of the intrinsic Pu(IV) colloidal polymer. **D.L. Clark**, D.E. Hobart

8:20 NUCL 44. Exploring the actinide series from periodic trends to electronic structure and bonding. **S.K. Schrell**, J. Su, S. Galley, T.E. Albrecht-Schmitt, E.R. Batista, M. Ferrier, S.A. Kozimor, V. Mocko, B. Scott, C. Van Alstine, F.D. White, P. Yang

8:40 NUCL 45. From Glenn T. Seaborg via the transuranium elements to Thomas E. Albrecht-Schmitt. **T. Schleid**

9:00 NUCL 46. Exploring *in-situ* hydrothermal redox chemistry with the *f*-elements. **E.M. Villa**

9:20 NUCL 47. Chelation strategies and applications for large s-, p-, and f-block metal ions. **J.J. Wilson**, N.A. Thiele, A. Hu

9:40 NUCL 48. Actinide endohedral fullerenes: Molecular structures and unique bindings. **N. Chen**

10:00 Intermission.

10:20 NUCL 49. Synthesis of rare-earth chalcogenide nanomaterials. **S.L. Stoll**, R. Atif, D. Asuigui, P. Glaser

10:40 NUCL 50. Design and synthesis of 3,2-HOPO-grafted chitosan oligosaccharide nanoparticles for the removal of uranium and reactive oxygen species (ROS) *in vivo*. **J. Diwu**

11:00 NUCL 51. Fundamental differences of the lanthanides and later actinides in non-aqueous conditions. **F.D. White**, M. Marsh, C.A. Celis-Barros, A. Gaiser, D. Dan, T.E. Albrecht-Schmitt

11:20 NUCL 52. Preparation of Tc-doped TiO₂ by simple aqueous chemistry and leaching behavior of Tc. **W.W. Lukens**

11:40 NUCL 53. 5f-Electron behavior of actinide nanoparticles embedded in porous frameworks. **S.G. Minasian**, A. Braun, S. Alayoglu, C. Booth, A. Herve, Y. Liu, T.D. Lohrey, L.M. Moreau, D. Olive, M. Straub

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TUESDAY AFTERNOON

Section A

Orange County Convention Center
Room W330C

Young Investigators in Nuclear & Radiochemistry



TECHNICAL PROGRAM

Cosponsored by YCC
M. A. Deri, A. L. Tamasi, *Organizers, Presiding*

1:15 Introductory Remarks.

1:20 NUCL 54. Binding preference determination of lanthanum and ytterbium with beta-diketones. **E.S. Auxier**, D.A. Penchoff, G.K. Schweitzer, H.L. Hall

1:35 NUCL 55. Exploring the speciation and redox chemistry of technetium-99 using polyoxometalates as highly controlled metal oxide mimics. **S. Pollozi**, R. Salcedo, E. Valencia, D.M. McGregor, G. Lopez, L.C. Francesconi

1:50 NUCL 56. Covalency in heavy actinide dithiophosphinates. **R. Greer**, T.E. Albrecht-Schmitt

2:05 NUCL 57. Evaluation of N-donor ligands for selective minor actinide separations. **M.L. Brown**, J.D. Carrick, C.A. Hawkins

2:20 Intermission.

2:40 NUCL 58. Dissolution and stability of the bismuthate species in the presence of fission products. **J. Einkauf**, J. Burns

2:55 NUCL 59. Reduction of uranium hexafluoride with a room temperature ionic liquid (1-methyl-1-propylpiperidinium bis(trifluoromethylsulfonyl)imide). **C.J. Higgins**, K.I. Luebke, K.R. Czerwinski, D.W. Hatchett

3:10 NUCL 60. Metal flux syntheses of actinide silicide intermetallics. **W. Potter**, T.E. Albrecht-Schmitt, S.E. Lattner

3:25 NUCL 61. Oxoamide and thioamide ligands for solvent extraction applications from used nuclear fuel: Investigating actinide vs lanthanide extraction selectivity. **I. Lehman-Andino**, T.S. Grimes, J.R. McLachlan, C.J. Dares, K. Kavallieratos

3:40 NUCL 62. Effects of metal flux composition on the growth of uranium silicide intermetallics. **A.S. Jayasinghe**, Y. Lai, R.E. Baumbach, S.E. Lattner

3:55 Intermission.

4:15 NUCL 63. Spectroscopic studies of novel N-donor ligand metal ion complexation. **K. Lawson**, J.D. Carrick, C.A. Hawkins

4:30 NUCL 64. Oxygen isotopes in uranium oxides measured by NanoSIMS: Refining a technique for nuclear forensics. **I. Weisman**, J. Matzel, P. Weber, M. Singleton

4:45 NUCL 65. Structural and spectroscopic investigation of aged plutonium oxalate species. **J.F. Corbey**, S.I. Sinkov, L.E. Sweet, C. Delegard

5:00 NUCL 66. Neural networks for removal of background matrix peaks from optical emission spectra. **J. Starks**, A. Braatz, P. Taylor, M. Cook

Exploring the Frontiers of Chemistry through NASA Research



TECHNICAL PROGRAM

Living There: Science for the Future of Manned Space Exploration

Sponsored by COMSCI, Cosponsored by ANYL, BIOL[‡], BIOT, CELL, COLL, ENFL[‡], I&EC[‡], INOR[‡], NUCL[‡], PHYS[‡], PMSE[‡] and POLY[‡]

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Sponsored by PROF, Cosponsored by ENVR, GEOC, I&EC, MEDI, MPPG, NUCL, ORGN, PHYS, PMSE, POLY, WCC and YCC

WEDNESDAY MORNING

Section A

Orange County Convention Center
Room W330C

Crosscutting Research in Environmental Radiochemistry & Nuclear Forensics

A. E. Hixon, *Organizer*
L. W. McDonald, *Organizer, Presiding*

8:00 NUCL 67. Role of surface hydroxyls on the radiolysis of gibbsite and boehmite nano-platelets. **Z. Wang**, X. Zhang, W. Cui, Y. Chen, E. Walter, A. Winkelman, A. Tuladhar, Z. Chase, M. Sassi, C. Pearce, H. Wang, S.B. Clark, K. Rosso

8:30 NUCL 68. Simulating uranium(VI) diffusion in sodium-montmorillonite as a function of chemical solution conditions. **R.M. Tinnacher**, J.C. Pistorino, C. Tournassat

8:50 NUCL 69. Rare-earth element interactions with uranium oxides. **R. Carter**, A.E. Hixon

9:10 NUCL 70. Dissolution studies of technetium sulfide under oxidizing and reducing conditions: Effect of pH and ionic strength. J. Stanberry, A. Anda, R.K. Gudavalli, N.P. Qafoku, **V. Anagnostopoulos**

9:30 Intermission.

9:50 NUCL 71. Nuclear forensic measurement impacts of uranium hexafluoride sampling methods. **J.M. Richards**, L.R. Martin, D. Simmons, L.D. Trowbridge, G.A. Fugate

10:10 NUCL 72. U-He age dating of uranium hexafluoride. **M. Singleton**, W.S. Cassata, W.C. Beaumont, R.M. Cox, D. Simmons, L.D. Trowbridge, G.A. Fugate

10:30 NUCL 73. Oxygen isotope fractionation in the processing of uranium oxides relevant to the nuclear fuel cycle. **M. Klosterman**, L.W. McDonald



TECHNICAL PROGRAM

10:50 Intermission.

11:10 **NUCL 74.** Characterizing uranium isotopic heterogeneity in nuclear fuel pellets using nanoscale secondary ion mass spectrometry. **R. Kips**, P. Weber, E. Ramon, B. Jacobsen, M. Kristo

11:40 **NUCL 75.** Variation of oxygen isotopes in uranium oxide fuel pellets. M. Singleton, **J. Matzel**, E. Oerter, A. Deinhart, N. Marks, M. Kristo

WEDNESDAY AFTERNOON

Section A

Orange County Convention Center
Room W330C

Crosscutting Research in Environmental Radiochemistry & Nuclear Forensics

L. W. McDonald, *Organizer*
A. E. Hixon, *Organizer, Presiding*

1:30 **NUCL 76.** Characterization of uranyl hydroxide hydrates and the formation of uranyl peroxide. **M.C. Kirkegaard**, J. Niedziela, A. Miskowicz, M. Ambrogio, A. Shields, B. Anderson

1:50 **NUCL 77.** Multiscale microscopy study of plutonium(III)-oxalate crystal growth. **T. Meadows**, J.A. Soltis, E. Buck, S.B. Clark, C. Parker

2:10 **NUCL 78.** Supporting legal aspects of forensic cases involving illegal trafficking and the use of radionuclides. **K.M. Elkins**, B. Kiesel

2:30 Intermission.

2:50 **NUCL 79.** Visualizing chemical and isotopic perturbations in heterogeneous nuclear material with direct, uncorrected isotope imaging. **E. Groopman**, D.G. Willingham, A. Meshik, O. Pravdivtseva

3:20 **NUCL 80.** Morphological and elemental characterization of environmental actinide bearing fuel particles formed by non-nuclear weapons accidents. **G. Varshney**, J. Cezeaux, A.A. Bickley, J. Petrosky

3:40 **NUCL 81.** Ensuring radiological emergency preparedness: EPA-NAREL's efforts in developing metrologically-traceable performance testing samples for environmental laboratories. **J. Burns**, C. Tutson, Z. Chambers, R. Stiles, A.L. Tamasi, J. Griggs

4:00 Intermission.

4:20 **NUCL 82.** Direct, uncorrected, molecule-free analysis of actinides from glassy nuclear materials. **D.G. Willingham**, E. Groopman, D. Weisz, K. Knight

4:50 **NUCL 83.** Development of synthetic nuclear melt glass representative of an urban, post-detonation environment for forensic analysis. **N. Kaminski**, G. Bull, R.B. Gilbreath, J. Alexander



TECHNICAL PROGRAM

5:10 NUCL 84. Synthesis of debris samples in controlled environments to understand the effects of mixing on radionuclide fractionation in fallout particles. **B. Koroglu**, Z. Dai, J.C. Crowhurst, D. Weisz, M. Armstrong, H. Radousky, J.M. Zaug, K. Knight, T. Rose

THURSDAY MORNING

Section A

Orange County Convention Center
Room W231B

General Topics in Nuclear Chemistry & Technology

J. Shafer, *Organizer, Presiding*

8:20 Introductory Remarks.

8:40 NUCL 85. Schiff-base coordination complexes with the *f*-elements. **B.E. Klamm**, C.J. Windorff, C.A. Celis-Barros, M.L. Marsh, D.S. Meeker, T.E. Albrecht-Schmitt

9:00 NUCL 86. Characterization of several new ternary actinide fluorides. **A.T. Chemey**, C.A. Celis-Barros, K. Huang, J.M. Sperling, C.J. Windorff, R.E. Baumbach, D.E. Graf, D. Páez-Hernández, D.E. Hobart, T.E. Albrecht-Schmitt

9:20 NUCL 87. Explorations of high-pressure behavior of lanthanide and actinide complexes. **E. Warzecha**, T.E. Albrecht-Schmitt

9:40 NUCL 88. Homoleptic dithiocarbamate complexes of transuranium elements. **J.M. Sperling**, T.E. Albrecht-Schmitt

10:00 NUCL 89. Probing plutonium redox behavior with cyclooctatetraene. **C.J. Windorff**, J.M. Sperling, B.E. Klamm, C.A. Goodwin, D.N. Huh, A. Gaiser, D.E. Hobart, S.A. Kozimor, A. Gaunt, W.J. Evans, T.E. Albrecht-Schmitt

10:20 Intermission.

10:40 NUCL 90. Computational study of binding preferences across the actinide series. **D.A. Penchoff**, C.C. Peterson, M.S. Quint, J.D. Auxier, G.K. Schweitzer, R. Harrison, H.L. Hall

11:00 NUCL 91. Functional hybrid molecules for the visualization of cancer: Dimeric BBN₇₋₁₄ dendroids combined with a bimodal molecular probe for positron emission tomography (PET) and optical imaging (OI) suited for tracking of GRPR-positive malignant tissue. **R. Hübner**, C. Wängler

11:20 NUCL 92. Application of PET neuroimaging probes targeting epigenetics. Y. Xu, P. Bai, S. Fiedler, B. Ntaganda, Y. Lan, Z. Chen, S. Bai, **C. Wang**

11:40 NUCL 93. Synergistic biosorption and bioprecipitation strategy for *Shewanella putrefaciens* and *Kocuria* sp. to immobilizing U(VI) from aqueous solution under aerobic conditions. **x. Nie**, Y. Wang, W. Huang, C. Ding, W. Cheng, M. Liu, F. Dong



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

12:00 NUCL 94. Exploring ionophore interaction with lanthanides and actinides. **A. Gaiser**, T.E. Albrecht-Schmitt

THURSDAY AFTERNOON

Section A

Orange County Convention Center
Room W231B

General Topics in Nuclear Chemistry & Technology

J. Shafer, *Organizer, Presiding*

1:30 NUCL 95. Investigation on complexation of uranyl with Raman spectroscopy: Coordination mode, intensity, and related Raman shift. **G. Tian**, Q. Liu, S. Yang, Q. Zhang, D. Li, Y. Zhang

1:50 NUCL 96. Alcohol clustering mechanisms in supercritical carbon dioxide using diffusion NMR and network analysis. **S.R. Saunders**, T.R. Graham, D. Pope, Y. Ghaadrghadr, A.E. Clark

2:10 NUCL 97. Computational assistance in the supramolecular assembly of actinide hybrids. **C.L. Cahill**, R.G. Surbella, K. Carter, N. Byrne, L. Colucci Ducati, J. Autschbach

2:30 NUCL 98. Revisiting the recovery of plutonium from chloride salt wastes by solvent extraction. **R.M. Chamberlin**, D.L. Decker, C.H. Helma, D.R. Porterfield, D.P. Montoya, S.P. Aragon, N. Xu, K.R. Weisbrod, D.B. Kimball

2:50 NUCL 99. Cation exchange applications for processing plutonium-238. **L.H. Delmau**, L.F. Mora, B. Tinker, D.E. Benker, D.W. DePaoli

3:10 Intermission.

3:30 NUCL 100. Real-time adjustment of Pu:U ratios in the CoDCon (modified PUREX) flowsheet. **G.B. Hall**, J.R. Allred, A.M. Lines, S.I. Sinkov, F.D. Heller, S.A. Bryan, G.J. Lumetta

3:50 NUCL 101. What is old is new: production and purification of polonium from bismuth using TBP and TBP resin. **A. Younes**, C. Alliot, A. Bonraisin, M. Mokili, F. Haddad, G. Montavon

4:10 NUCL 102. Chemistry of the strong force. **G.L. Smith**

4:30 NUCL 103. Uranium chemistry in condensing laser-induced plasmas. **D. Weisz**, J.C. Crowhurst, B. Koroglu, H. Radosky, T. Rose, M. Finko, D. Curreli

4:50 NUCL 104. Analysis of synthetic nuclear melt glass (urban) using x-ray fluoroscopy. **G. Bull**, D.E. Riegner, K. Onaka, N. Kaminski, R.B. Gilbreath

ORGN



TECHNICAL PROGRAM

Division of Organic Chemistry

S. Silverman and E. McLaughlin, *Program Chairs*

SUNDAY MORNING

Section A

Orange County Convention Center
Room W230A

New Reactions & Methodology

S. M. Silverman, *Organizer*
T. J. Henderson, *Presiding*

8:00 ORGN 1. Visible-light-promoted, regioselective C(sp²)-H bond selenylation of indoles, imidazoles, and arenes: A Metal-Free Approach. **J.R. Khan, A.L. Braga, S. Saba**

8:20 ORGN 2. Novel approach to conduct electronically mismatched Diels-Alder reactions. **Z. Wang**, J.C. Lake, K. Chiba, Y. Okada, I. Yasushi, A. Ozaki, Y. Yamaguchi, S.R. Hussaini

8:40 ORGN 3. Synthesis of novel bicyclic amines and their application for drug design. **P. Mykhailiuk**, B. Chalyk, O. Kirichok, T. Druzenko, E. Skalenko, O. Denisenko, A. Cherepakha

9:00 ORGN 4. Sustainable *p*-hydroxycinnamic acids synthesis through proline-mediated Knoevenagel reaction. **C. Peyrot**, A. Peru, L. Mouterde, F. Allais

9:20 ORGN 5. Nickel-catalyzed conjunctive cross-coupling of 9-BBN borates and acyl electrophiles. **C.M. Law**, Y. Meng, S. Koo, J.P. Morken

9:40 ORGN 6. Synthesis of styryl carboxylates and highly substituted esters: A unique application of RCOOPdH and ArCOPdCl species. **M. Al-Masum**, M. Aman, S.L. Chrisman, N. Nguyen, A. Hira

10:00 ORGN 7. Unusual products from the thionation of bicyclic ketones. **T. Nguyen**, J.D. Williams

10:20 ORGN 8. Utilization of cyclic amides as masked aldehyde equivalents in reductive amination reactions. **R.J. Prince**, F. Gao, J.E. Pazienza, I.E. Marx, J. Schulz, B.T. Hopkins

10:40 ORGN 9. Am I a chemist, an engineer, or an architect? How to redesign natural porphyrins as organocatalysts. **M. Kielmann**, M. Roucan, S. Connon, M.O. Senge

11:00 ORGN 10. Electrode material selective functionalization of styrenes with oxygen: Olefin cleavage and synthesis of tetrahydrofuran derivatives. **Y. Imada**, Y. Okada, K. Chiba



TECHNICAL PROGRAM

11:20 ORGN 11. Regioselective substitution of the Baylis-Hillman (BH) adducts with indoles and its applications towards synthesis of heterocyclic derivatives. **Z. Shafiq**, L. Liu

Section B

Orange County Convention Center
Room W230B

Metal-Mediated Reactions & Syntheses

S. M. Silverman, *Organizer*
T. Diao, *Presiding*

8:20 ORGN 12. (Cyclopentadienone)iron-catalyzed lactonizations of symmetrical and unsymmetrical diols. **T.W. Funk**

8:40 ORGN 13. Taming rhodium(II) carbenes with tethered, axial coordination. **A. Darko**, W. Sheffield, D. Cressy, A. Abshire, C. Zavala

9:00 ORGN 14. Transition-metal catalyzed synthesis of unsymmetrically substituted triazolium salts. **J.L. Bolliger**

9:20 ORGN 15. Continuing mechanistic study of gold catalyzed alkene hydroamination. **A.C. Jones**, B. Yager, W. Zhou, Y. Zhu, Y. Jee

9:40 ORGN 16. Complexities of carbonyl-Lewis acid interactions in catalytic systems. **C. Hanson**, M. Psaltakis, S. Siddiqi, J. Cortes, J.J. Devery

10:00 ORGN 17. Novel design and preparation of a triazole-based tridentate ligand. **Q. Xing**, X. Shi

10:20 ORGN 18. Palladium/copper cooperative-catalysis for the synthesis of aryl boronic esters. **S. Laulhe**, J. Floreancig, A. Spencer

10:40 ORGN 19. Synthetic utility of boracarboxylated styrene derivatives. **T.M. Perrone**, B.V. Popp

11:00 ORGN 20. Iron-based catalysts for the Suzuki-Miyaura cross coupling reaction. **J.A. Byers**, M. Crockett, C. Tyrol, A. Wong, N. Yone

Section C

Orange County Convention Center
Room W230C

CH Activation

S. M. Silverman, *Organizer*
K. Olsen, *Presiding*

8:20 ORGN 21. Surprising differences of alkane C-H activation catalyzed by ruthenium nanoparticles. **D. Bouzouita**, N. Rothermel, I. De Rosal, S. Tricard, R. Poteau, T. Gutmann, B. Chaudret, H. Limbach, G. Buntkowsky



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

8:40 ORGN 22. Reactivity of hypercoordinated iodanes in C-H functionalization. **A. Stirling**

9:00 ORGN 23. Newly discovered ruthenium Formate catalyst MCAT-53 for versatile and practical synthesis of biaryls through C-H activation. **A. Mehta**, B. Saha, A. Koohang, M. Chorghade

9:20 ORGN 24. *closo*-Borate anions activate C-H bonds in hydrocarbons in the gas phase. **X. Ma**, J. Liu, J. Warneke, J. Laskin, H.I. Kenttamaa

9:40 ORGN 25. Mild and efficient palladium-catalyzed fluoroalkylation and fluoroalkenylation of (hetero)aromatic systems by directed ortho-C-H activation. **B. Tóth**, S. Kovács, O. Egyed, A. Bényei, A. Stirling, Z. Novák

10:00 ORGN 26. Selective synthesis of mono-functionalized naphthalenediimides by copper-catalyzed C-H activation. **J.J. Reczek**

10:20 ORGN 27. Tunable, catalyst-controlled syntheses of β - and γ -amino alcohols enabled by silver complexes. **M. Ju**, M. Huang, L. Vine, M. Dehghany, J.M. Schomaker

10:40 ORGN 28. Desymmetrization of cyclohexanes by site- and stereoselective C-H functionalization. **J. Fu**, Z. Ren, J. Musaev, H.M. Davies

11:00 ORGN 29. Palladium-catalysed C(sp³)-H arylation of primary amines using a catalytic alkyl acetal to form a transient directing group. **S. St John-Campbell**, A.K. Ou, J.A. Bull

11:20 ORGN 30. Adventures in C-H activation with carbon dioxide. **M. Young**, M. Kapoor, P. Chand-Thakuri, J.M. Maxwell

Section D

Orange County Convention Center
West Hall F3

Opportunities & Challenges in Carbohydrates

Cosponsored by CARB†
H. M. Nguyen, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 ORGN 31. Chemical probes of immunity. **L.L. Kiessling**

9:05 ORGN 32. Radical SAM enzymes in the biosynthesis of sugar-containing natural products. **H. Liu**

9:35 ORGN 33. Carbohydrate probes for chemoproteomics. **S.D. Townsend**

10:05 Intermission.

10:20 ORGN 34. Synthesis as an enabling technology for understanding glycan function and assembly. **T.L. Lowary**



TECHNICAL PROGRAM

10:50 ORGN 35. Opportunities and challenges in automating chemistry in batch and flow: The case of carbohydrates. **N.L. Pohl**

Section E

Orange County Convention Center
West Hall F4

James Flack Norris Award in Physical Organic Chemistry

M. Jeffries-El, *Organizer, Presiding*
S. Wiskur, *Presiding*

8:00 Introductory Remarks.

8:05 ORGN 36. Diarenoindacenes and diindenoarenes: From quinoidal electron-accepting materials to stable organic diradicals. **M.M. Haley**

8:35 ORGN 37. Probing and harnessing the hydrophobic and Hofmeister effects. **B.C. Gibb**

9:05 ORGN 38. Application of supramolecular sensing to epigenetics. **M. Waters**

9:35 ORGN 39. Bifunctional foldamer catalysis. **S.H. Gellman**

10:05 Intermission.

10:20 ORGN 40. Autocatalytic models for symmetry breaking and the emergence of biological homochirality. **D.G. Blackmond**

10:50 ORGN 41. Integrating data science with physical organic chemistry. **M.S. Sigman**

11:20 ORGN 42. Award Address (James Flack Norris Award in Physical Organic Chemistry sponsored by the ACS Northeastern Section). Physical organic chemistry in the analytical sciences. **E.V. Anslyn**

Wolfrom Award

Sponsored by CARB, Cosponsored by CELL, MEDI, ORGN and PROF

Horton Award

Sponsored by CARB, Cosponsored by CELL, MEDI, ORGN and PROF

SUNDAY AFTERNOON



TECHNICAL PROGRAM

Section A

Orange County Convention Center
Room W230A

New Reactions & Methodology

S. M. Silverman, *Organizer*
C. Brindle, *Presiding*

1:00 ORGN 43. Multidirectional desymmetrization of pluripotent building block *en route* to the asymmetric/diastereoselective synthesis of complex nature-inspired scaffolds. **T.H. Altel**

1:20 ORGN 44. α -Keto- β -diimines: Straightforward synthesis and applications. **M. Tripathi, D. Martin**

1:40 ORGN 45. Stereoselective one-pot deconjugation, aldol, and stabilized Peterson olefination of α -trialkylsilyl- β -alkyl- α , β -unsaturated esters. **M. Probasco**, D. Johnson, M.P. Jennings

2:00 ORGN 46. Light-driven intermolecular charge transfer induced reactivity of ethynylbenziodoxol(on)e and phenols. **B. Liu**, C. Lim, G. Miyake

2:20 ORGN 47. Bioactive components of marine brown macroalgae from the south coast of Peru. **X. Solis**, R. Fernandez, S. Zevallos, L. Quispe, V. Dianderas, J.J. Fernandez, M. Norte, C. Areche, T. Cano

2:40 ORGN 48. Flow electrochemical cyclizations via sulfur radicals: Easy access of thiazolidines. **M. Islam**

3:00 ORGN 49. [^{18}F]Fluorobenziodoxole, an electrophilic ^{18}F -fluorination reagent: Synthesis and application to labeling reactions. **M.A. Cortes Gonzalez**, P. Nordeman, A. Bermejo Gomez, D.N. Meyer, G. Antoni, M. Schou, K.J. Szabo

3:20 ORGN 50. Direct substitution of alcohols to form new C-X and C-C bonds. **L. Geary**

3:40 ORGN 51. Difunctionalization of ketone via *gem*-bis(boronates). **P. Zheng**

4:00 ORGN 52. Recent advances in nickel-catalyzed amide C–N bond activation. **J.E. Dander**, N.K. Garg

4:20 ORGN 53. Vicinal C-H di-functionalization via radical-polar crossover. **A. Prusinowski**, R.K. Twumasi, E. Wappes, D.A. Nagib

4:40 ORGN 54. Bisulfite removal of aldehydes using liquid-liquid extraction and the effect of salt age. **C. Brindle**, W. Patterson, M. Furigay, M.M. Boucher

Section B

Orange County Convention Center
Room W230B

Asymmetric Reactions & Syntheses



TECHNICAL PROGRAM

S. M. Silverman, *Organizer*
J. Zbieg, *Presiding*

1:00 ORGN 55. Copper(I)-catalyzed [3 + 3]-cycloaddition of enoldiazocarbonyl compounds: An efficient tool for the synthesis of chiral oxazines and pyrazines. **K. Marichev**, M. Doyle

1:20 ORGN 56. Phase transfer-catalyzed phospho-Michael additions: An asymmetric approach to phosphinate esters. **K. Yadavalli**, S.D. Lepore

1:40 ORGN 57. Recent studies on Lewis base catalyzed carbon-heteroatom bond formation. **s. sun**

2:00 ORGN 58. Catalytic asymmetric synthesis of cyclopentanones and furans from ketenes. **N. Kerrigan**, M. Mondal, M. Panda

2:20 ORGN 59. Catalyst optimisation for asymmetric synthesis by ligand chirality element addition. **C.J. Richards**, R.A. Arthurs

2:40 ORGN 60. Metal-catalyzed hydrofunctionalizations. **N. Shaozhen**, R. Davison, V.M. Dong

3:00 ORGN 61. Synergistic palladium/enamine catalysis for asymmetric hydrocarbon functionalization of inactive alkene with ketone/aldehyde. **C. Wei**, X. Ye, X. Shi

3:20 ORGN 62. Excited-state reactivity of chiral iminium ions to perform enantioselective cascade reactions. **C.M. Holden**, P. Bonilla, M. Bernús, G. Magagnano, Y. Rey, K. Ling, P. Melchiorre

3:40 ORGN 63. Enantioselective carbofunctionalization of alkenes. **T. Diao**

4:00 ORGN 64. Discovery of a chiral amphiphilic iridium catalyst for carbon-heteroatom bond formation: Reactions of amines, anilines, indoles, and other various nucleophiles. **J. Zbieg**

Section C

Orange County Convention Center
Room W230C

CH Activation

S. M. Silverman, *Organizer*
G. Hughes, *Presiding*

1:20 ORGN 65. Amino acid ligands accelerate enantioselective C-H functionalization via di-palladium catalysts. **J. Gair**, J. Lewis

1:40 ORGN 66. Iridium-catalyzed silylation of the C-H bonds of un-activated arenes: Faster catalysis enable new reactivity. **Z. Chen**, C. Karmel, J.F. Hartwig

2:00 ORGN 67. δ C-H (hetero)arylation via Cu-catalyzed radical relay. **Z. Zhang**, L.M. Stateman, D.A. Nagib



TECHNICAL PROGRAM

2:20 ORGN 68. Overcoming the limitations of γ , and σ -C–H arylation of amines through ligand development. **Y. Chen**, J. Yu

2:40 ORGN 69. Accelerated asymmetric δ -lactam synthesis with a monomeric streptavidin artificial metalloenzyme. **I. Hassan**, A. Ta, M. Danneman, N. Semakul, M. Burns, B. Mcnaughton, T. Rovis

3:00 ORGN 70. Aliphatic C–H oxidation for late-stage functionalization. **J. Zhao**, E. de Lucca, Jr., T. Nanjo, M. White

3:20 ORGN 71. Enabling and accelerating C–H functionalization through continuous-flow chemistry. **T. Noel**

3:40 ORGN 72. Asymmetric allylic C–H alkylation via palladium(II)/sulfoxide-oxazoline catalysis. **W. Liu**, S. Ali, S.E. Ammann, M. White

4:00 ORGN 73. Evidence for a distinct C–H activation mechanism for mild dehydrogenative coupling: *Electrophilic Concerted Metalation-Deprotonation* (eCMD). **B.P. Carrow**

4:20 ORGN 74. Advances in platinum-catalyzed C_{sp^3} -H oxidation reactions. **N. Laloo**, M.S. Sanford

Section D

Orange County Convention Center
West Hall F3

Opportunities & Challenges in Carbohydrates

Cosponsored by CARB[†]
H. M. Nguyen, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 ORGN 75. Studies toward catalytic site-selective alterations of glycopeptide antibiotics and other carbohydrates. **S.J. Miller**

1:35 ORGN 76. Using reversible covalent bonding to enhance site selective catalysis. **K.L. Tan**

2:05 ORGN 77. Catalytic stereoselective 1,2-cis glycosylations. **H.M. Nguyen**

2:35 Intermission.

2:50 ORGN 78. Streamlined methods for the synthesis of heparan sulfate oligosaccharide libraries. **L.C. Hsieh-Wilson**

3:20 ORGN 79. Stereoselective reactions of oxocarbenium ions: Conformational analysis, stereoelectronic effects, and reactivity. **K.A. Woerpel**

3:50 ORGN 80. Influence of side-chain configuration and conformation on reactivity and selectivity in glycosylation. **D. Crich**

Section E



TECHNICAL PROGRAM

Orange County Convention Center
West Hall F4

ACS Award for Encouraging Disadvantaged Students into Careers in the Chemical Sciences

K. N. Maloney, *Organizer*
D. E. Figueroa, *Presiding*

1:00 Introductory Remarks.

1:05 **ORGN 81.** Role of heparan sulfate in prion replication and cell targeting. **P. Aguilar Calvo**, J. Bapat, N. Williams, A. Sevellano, K. Soldau, D.R. Sandoval, H. Altmepfen, L. Linsenmeier, D. Pizzo, S. Edland, M. Glatzel, K. Nilsson, J. Esko, C. Sigurdson

1:40 **ORGN 82.** Towards *Mycobacterium tuberculosis* detection at the point-of-care: solvatochromic probes permits the detection of mycobacteria within minutes. **M. Kamariza**, C.R. Bertozzi

2:15 **ORGN 83.** Regulation of mTOR dependent entry and exit from diapause-like state. **A. Hussein**, H. Ruohola-Baker

2:50 Intermission.

3:05 **ORGN 84.** Development of small molecule inhibitors of IKK2. **S.J. Hotchkiss**, G. Ghosh

3:40 **ORGN 85.** National Institute of General Medical Sciences undergraduate and predoctoral grant programs. **S. Singh**

4:15 Introduction of Awardee.

4:20 **ORGN 86. Award Address** (ACS Award for Encouraging Disadvantaged Students into Careers in the Chemical Sciences sponsored by The Camille and Henry Dreyfus Foundation, Inc.). My success in encouraging disadvantaged students into careers in the chemical sciences using mentoring and research in organic chemistry. **E.C. Alexander**

Hudson Award

Sponsored by CARB, Cosponsored by CELL, MEDI, ORGN and PROF

Isabell Award

Sponsored by CARB, Cosponsored by CELL, MEDI, ORGN and PROF

Gin New Investigator Award

Sponsored by CARB, Cosponsored by CELL, MEDI, ORGN and PROF



TECHNICAL PROGRAM

SUNDAY EVENING

Section A

Orange County Convention Center
West Hall C

Metal-Mediated Reactions & Syntheses

Cosponsored by MEDI⁺
E. C. McLaughlin, *Organizer*

5:30 - 7:30

ORGN 87. Borylation of aryl iodides using a Pd/Cu dual catalysis. **J. Floreancig**, A. Spencer, S. Laulhe

ORGN 88. Stereoselective oxyamidation of glycals: Exploration of N-acyloxycarbamates and azidoformates as metallanitrene and metalloradical precursors. **I. Rocroi, K. Song**, A. Banerjee, E. Latif, C.M. Rojas

ORGN 89. Applications of conjunctive cross-coupling towards the synthesis of β -hydroxy ketones. **C.M. Law**, Y. Meng, S. Koo, J.P. Morken

ORGN 90. Gold alkene pi-complexes: Ligand effects on structure, formation and reactivity. **A.C. Jones**, D. Hodges, B. Yager, C. Griebel, J. Piedad, F. Liu

ORGN 91. Method development of air-free techniques with samarium diiodide. **G. Rojas**

ORGN 92. Substituent effects in intramolecular palladium-catalyzed oxyarylation reactions. **M.C. Maust**, W.E. Brenzovich, Z.L. Croft

ORGN 93. Enantioselective hydroalkoxylation of 1,3 dienes via metal hydride catalysis. **R. Le Tourneau**, X. Yang, V.M. Dong

ORGN 94. Base-metal-catalyzed hydrofunctionalization. **A. Jiu**

ORGN 95. Transition-metal mediated cycloisomerizations of allenes to afford highly substituted cyclopentenes. **R.D. Reeves**, J.M. Schomaker

ORGN 96. Deprotonative zincation for the generation and functionalization of organozinc pivalate reagents. **K. Bitting**

ORGN 97. Scope and limitation on the preparation of isoquinolin-4(3H)-ones and tetrahydro-1H-benzo[d]azepin-1-ones via Parham cyclization chemistry. **S. Shoeb, Z. St. John**, D.A. Hunt

ORGN 98. Quinoline-oxazoline ligand synthesis for bimetallic catalysis. **A. Noonikara Poyil**

ORGN 99. Synthesis of 2-substituted benzo[b]thiophenes via gold(I)-IPr hydroxide-catalyzed cyclization of 2-alkynyl thioanisoles. **C.C. Dillon**, B. Keophimphone, **M. Sanchez**, P. Kaur, H. Muchalski



TECHNICAL PROGRAM

- ORGN 100.** Supramolecular ensemble of PBI derivative and metal NPs: Potential application in various organic transformations. **G. Singh**, V. Bhalla
- ORGN 101.** Application of allenylboronic acids for the synthesis of homopropargylic alcohols with vicinal quaternary carbon stereocenters. J. Zhao, S. Jonker, **D.N. Meyer**, G. Schulz, C. Tran, L. Eriksson, K.J. Szabo
- ORGN 102.** Synthesis of cyclobutanones and 1,4-diketones via low-valent titanium intermediates. **A. Rodriguez**, N.N. Le, J.R. Alleyn, M.R. Gesinski
- ORGN 103.** Bulky bipyridine/pyridine-oxazoline ligands: Synthesis and catalytic reactivity study. **Z. Zheng**, P.J. Walsh
- ORGN 104.** Development of a novel gold(I)-cleavable protecting group. **S.N. Cantu**, C. Lacker, M.R. Gesinski
- ORGN 105.** Ni-catalyzed C-O bond cleavage of 3-phenoxy acrylic acid derivatives and subsequent intramolecular C-C bond formation to give benzofurans. **O. Shohei**, K. Murai, H. Fujioka, M. Arisawa
- ORGN 106.** Synthesis of ortho-substituted benzamides through nickel mediated cross-coupling. **R.L. Johnson**, **E.M. Heyboer**, J.B. Johnson
- ORGN 107.** Examination of the reaction mechanism of the rhodium-catalyzed decarbonylation of pyridyl ketones. **E.J. Schoonover**, C.J. Wagner, G.J. Campbell, **J.B. Johnson**
- ORGN 108.** Synthesis of aryl boronic esters from aryl bromides Using Pd/Cu dual catalysis. **A. Spencer**, J. Floreancig, S. Laulhe
- ORGN 109.** Transition-metal catalyst development for alkyne coupling reactions. **S. Acharya**, P. Zhao
- ORGN 110.** Safer solvents for alkyllithium reagents. **T. Malinski**, D.E. Bergbreiter
- ORGN 111.** Palladium-catalyzed hydrodefluorination: A robust and operationally convenient procedure. **J. Gair**, R. Grey, S. Giroux
- ORGN 112.** Highly diastereoselective synthesis of (*Z*)-trisubstituted alkenes containing phenyl and (1,3-dioxan-2ylethyl) moieties via organoboranes. **N.G. Bhat**
- ORGN 113.** Highly diastereoselective synthesis of (*E*)-trisubstituted alkenes containing phenyl and biphenyl moieties via organoboranes. **N.G. Bhat**

Section A

Orange County Convention Center
West Hall C

New Reactions & Methodology

E. C. McLaughlin, *Organizer*

5:30 - 7:30



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- ORGN 114.** Mild intramolecular ring opening of oxetanes. **L. DeRatt**, S.D. Kuduk
- ORGN 115.** Simplified system for glycosylation of nucleosides and beta-glycosylation of peptides. **Y. Zhang**, S.A. Knapp, J.J. Hale
- ORGN 116.** Mild and efficient synthesis of amides from acid chlorides and amines using Cs_2CO_3 & TBAI. **J. Shamp**, E. Carey, D. Orlando, R.N. Salvatore
- ORGN 117.** Acid-promoted synthesis of cyclic imides from carboxylic acids and isocyanates. **S. Kennedy**, M.N. Schaeff, D.A. Klumpp
- ORGN 118.** Synthesis of medchem-relevant Dimethylphosphine Oxide (DMPO) containing building blocks. Y. Dmytriv, S. Ryabukhin, **D. Volochnyuk**, A.A. Tolmachev
- ORGN 119.** One-step synthesis of functionalized pyridines by reaction of propargylamine and ketones catalyzed by Cu(II) compounds. S.A. Sotnik, A.I. Subota, S. Ryabukhin, S.V. Kolotilov, **D. Volochnyuk**
- ORGN 120.** Unexpected macrocycles formation in a synthesis of fused aza-cycloalkyl oxazoles. **D. Volochnyuk**, S. Ryabukhin, O. Grygorenko, E.Y. Slobodyanyuk
- ORGN 121.** Efficient synthesis of drug-like tetrahydropyridoazepines. A.I. Subota, O. Grygorenko, S. Ryabukhin, **D. Volochnyuk**
- ORGN 122.** New frontiers in Castagnoli–Cushman reaction. **S. Ryabukhin**, D. Volochnyuk, M. Adamovskyi, O. Grygorenko
- ORGN 123.** Stereospecific connective synthesis of allenes by eliminative cross-coupling of stereodefined sp^3 - and sp^2 -hybridized carbenoids. **Y. Cao**, P.R. Blakemore
- ORGN 124.** Synthesis and purification of [^{18}F]fluorobenziodoxole: A no-carrier-added electrophilic ^{18}F -fluorination reagent. **M.A. Cortes Gonzalez**, P. Nordeman, A. Bermejo Gomez, D.N. Meyer, G. Antoni, M. Schou, K.J. Szabo
- ORGN 125.** Vinylation and acetylenylation of N,O-acetal TMS ethers derived from medium-sized lactams. M. Kim, **J. Mun**, S. Jo, G. Choi, Y. Suh, S. Kim, J. Jung
- ORGN 126.** Selective microwave heating of organic reaction systems. **M. Vincent**, H. Fulo, G.B. Dudley
- ORGN 127.** Transition-metal-catalyzed synthesis of 2-substituted alpha-carbolines. **F. Edioma**, K.M. Medas, R.M. Lesch, **S.P. Mulcahy**
- ORGN 128.** Fluorination of alkynes using keteniminium ion intermediates. **G.J. Rainone**, **S.P. Mulcahy**
- ORGN 129.** Regioselective synthesis of isoxazoles by hypervalent iodine(III) reagent mediated oxidative cyclization. **M. Jarvi**, G. Rohde, V. Nemykin, V.V. Zhdankin, A. Yoshimura
- ORGN 130.** Metal-free imidation of sulfides and phosphines using iminoiodane reagents. **C.L. Makitalo**, S. Larson, G. Rohde, V. Nemykin, A. Saito, V.V. Zhdankin, A. Yoshimura
- ORGN 131.** Preparation, structure, and reactivity of bicyclic benziodazole: A new hypervalent iodine heterocycle. **M. Shea**, C. Huss, Y. Vlasenko, P. Postnikov, G. Rohde, V. Nemykin, A. Yoshimura, V.V. Zhdankin



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- ORGN 132.** Synthetic access to sterically enhanced *N*-aryl amines and progress toward a novel, tunable carbene scaffold. **J.P. Moerdyk**, D. Martin, M. Kline, B. Mayro, Z. Herman
- ORGN 133.** Base-catalyzed isomerization of dienyl alcohols and ethers. N. Molleti, **S. Martinez Erro**, A. Sanz-Marco, B. Martín-Matute
- ORGN 134.** Metal-free amino-oxidation of alkenes mediated by *N*-oxoammonium salts. **A. Millimaci**, J.D. Chisholm
- ORGN 135.** Fluorine as an oxygen transfer agent. **S. Rozen**
- ORGN 136.** Remote C-H functionalization enabled by imidate radicals. **A. Prusinowski**, R.K. Twumasi, E. Wappes, D.A. Nagib
- ORGN 137.** Synthesis of indolizidines from L-pyroglutamic acid using the Ireland–Claisen rearrangement and ring-closing metathesis. **D. Essayan**, J. Cannon
- ORGN 138.** Photoredox-catalyzed alkene hydroalkylation and dialkylation. **A. Crooke**, K.C. Forbes, J. Cannon
- ORGN 139.** Development of a reductive enyne Cope rearrangement for synthesis of allenyl malonates. **K. White**, S. Scott, A.J. Grenning
- ORGN 140.** Accessing functionalized beta-hydroxyboronate esters via a diboration/homologation sequence with aldehydes. **M. Nistler**, **G. Meyer**, **A.M. DePaul**, A.V. Samoshin, T. Thane, C.J. Ferber, G.W. O'Neil, T.B. Clark
- ORGN 141.** Simple, tunable synthetic routes to cannabinoid natural product analogues. **P.V. Navaratne**, A.J. Grenning
- ORGN 142.** Synthesis of terpenoid natural product frameworks via [3,3] sigmatropic rearrangements. **O. Lahtigui**, A.J. Grenning
- ORGN 143.** Decarboxylative heptannulations via divinylcyclopropane Cope rearrangements: Access to terpenoid-like polycycloalkane scaffolds. **R. Schroeder**, A.J. Grenning
- ORGN 144.** Towards scalable terpenoid synthesis: Multifunctionalization of Knoevenagel adducts. **P. Vertesaljai**, A.J. Grenning
- ORGN 145.** Stereodivergent total synthesis of hapalindoles, fischerindoles, hapalonamide H, and ambiguine H alkaloids by developing a biomimetic, redox-neutral, cascade Prins-type cyclization. **S. Sahu**, B. das, M.S. Maji
- ORGN 146.** Toward the synthesis of radicinin, an inhibitor of Pierce's disease and citrus greening disease. **C.A. Brandenburg**, J.W. Lockner, K.N. Maloney, C. Castro, A. Blacutt, C. Roper, P. Rolshausen
- ORGN 147.** "Anion pool"-driven organic transformations. **M.M. Dissanayake**, A.K. Vannucci
- ORGN 148.** Facile conversion of hydroxyfluorophores to aminofluorophores via Smiles rearrangement. **Y. Ahmed**, **O. Elghawy**, R.R. Walvoord
- ORGN 149.** Copper-catalyzed silyl-additions to imines using a disilane as the silicon source. **T.S. Carpenter**, R. Van Hoveln
- ORGN 150.** Accessible synthesis of organofluorosilicates. **S.R. Harruff**, R. Van Hoveln



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- ORGN 151.** Progress toward synthesis of an acylsilane via copper catalysis. **B.M. Thomas**, R. Van Hoveln
- ORGN 152.** New methodology for the preparation of 3,4-dihydroxybenzenesulfonamide chelators for iron complexation. **A.S. Gopalan, T.T. Pham**
- ORGN 153.** Synthesis of sulfoximines and sulfonimidamides by highly chemoselective NH and O transfer. **S. St John-Campbell**, E.L. Briggs, S. Chawner, L. Degennaro, R. Doran, G. Romanazzi, A. Tota, M. Zenzola, R. Luisi, J.A. Bull
- ORGN 154.** Synthesis of highly substituted aryl(trifloxyvinyl)iodonium triflate salts. **F. Béke**, B. Tóth, O. Egyed, A. Bényei, Z. Novák
- ORGN 155.** Terpenoid synthesis via the reductive Cope rearrangement. **R. Serrano**, P. Vertesaljai, A. Grenning
- ORGN 156.** Catalytic C–C bond silylation with hydrosilyl acetals. **T. Avullala**, P. Asgari, A. Bokka, J. Jeon
- ORGN 157.** Hydrosilyl acetal-directed catalytic exo-syn hydrosilylation of propargylic alcohols. **U. Dakarapu**, T. Avullala, J. Jeon
- ORGN 158.** Direct acyl amide synthesis from carboxylic acids using *N*-haloimide reagents. **C.D. Irving**, S. Walker, M. Gasonoo, S. Lualhe
- ORGN 159.** Deoxyamination of activated alcohols using *N*-haloimides and triphenylphosphine. **M. Gasonoo**, C.D. Irving, Z. Thom, S. Lualhe
- ORGN 160.** Facile synthesis of aromatic 1,2-azaborine derivatives through oxidation of 1,2-BN-3-cyclohexene. **Q. Xing**, X. Shi
- ORGN 161.** Chiral benzamidine formation by reaction of nucleophilic alkylquinazolinones with chiral electrophiles and subsequent regioselective rearrangement. **S. Rozema**, J.N. Fitz-Henley, J.E. Golden
- ORGN 162.** Reductive Nef reaction mediated by CS₂ and amidine/guanidine bases. **w. guan**, M. Ju, J.M. Schomaker, K. Harper
- ORGN 163.** Visible-light-assisted and catalyst-free intramolecular hydroamidation of allenyl amides. **L. Liu**, R. Ward, J.M. Schomaker
- ORGN 164.** Synthesis of *anti*- and *syn*-hydroxymethyl 1,3-diol motifs based on the regioselective cleavage of 2,3-epoxy alcohols using Grignard and organoaluminum reagents: application to the polypropionate synthesis. **R.R. Rodriguez Berrios, J.A. Prieto**
- ORGN 165.** Investigation of methods for introducing structural complexity into cyclic carbonate monomers. **E. Whitman**, M.L. Turlington
- ORGN 166.** Organocatalyzed domino reactions of cannabinoid and anthracene derivatives. **A. Kelley, E. Wolf**, L. Davis
- ORGN 167.** Investigation of coupling reagents for esterification reactions of carboxylic acid-containing cyclic carbonate monomers. **B. Marx**, C. Howard, E. Whitman, C. Hanger, M.L. Turlington
- ORGN 168.** Making the precursors to β -heteroatom-stabilized carbenes. **L.J. Bitsko**, J. Unger



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- ORGN 169.** Direct access to lactam-fused lactones by chemo-, regio-, and stereoselective halolactonization of lactam-bearing alkenoic acids. **M.J. Rodriguez**, K. Hovenkotter, T.K. Beng
- ORGN 170.** Distal C-H functionalization via an interrupted HLF mechanism. **L.M. Stateman**, Z. Zhang, D. Nagib
- ORGN 171.** Bioorthogonal cross-metathesis reaction of allenes. **C. Hanger**
- ORGN 172.** Desilylative Ullmann reaction. **G. Petruncio**, M. Girgis, M. Paige
- ORGN 173.** Synthesis of ethyl and propyl fatty acid esters in nano-reactors. **D. Welborn**, N.N. Shaw
- ORGN 174.** Mechanistic studies of Lewis base catalyst-controlled regioselective chlorination of arenes and heterocycles. A. Dinh, S.M. Maddox, **L.S. Janke**, B. Addison, J.L. Gustafson
- ORGN 175.** Microwave-assisted sustainable entry to 6*H*-chromeno[4,3-*b*]quinolin-6-ones. **D. Bandyopadhyay**, C. Pena, V.M. Cano
- ORGN 176.** Reaction of organotrifluoroborates with benzyne in tandem with coupling chemistry. **T. Choi**, **W. Yang**, P. Persichini
- ORGN 177.** Enantioselective conjugate addition of aldehydes to nitroolefins catalyzed by chiral bifunctional non-natural amino acid derivatives. **E. Westemeier**, D. Just, U. Jahn
- ORGN 178.** Light-induced coupling reactions through electron transfer of electron donor-acceptor complexes. **B. Liu**, C. Lim, G. Miyake
- ORGN 179.** Friedel-Crafts acylations with unusual bench-stable *N*-quaternized ketene-*N,O*-acetals. **D. McConnell**, **D.G. Rodrigues**, **A.M. Blades**, C.E. Anthony, J. Sonberg, **P.V. Keyes**, S. Rachad, C.C. Williams, **O.M. Simone**, **M.M. Majireck**
- ORGN 180.** One-step synthesis of biflavones mediated by peroxyxynitrite oxidative coupling of flavone monomers. **X. Yang**, D. Huang
- ORGN 181.** Direct primary electrophilic amination of alkylmetals with *NH*-oxaziridine. **N. Behnke**, R. Kielawa, L. Kurti
- ORGN 182.** Divergent reductive ketyl radical couplings. **S.M. Rafferty**, J. Rutherford, D. Nagib
- ORGN 183.** Vinyl cation reaction with aromatic system. **J. Fang**, M. Brewer
- ORGN 184.** Cleavage of C–C bonds through transfer hydroformylation. **A. Lu**, F.A. Cruz, X. Wu, V.M. Dong
- ORGN 185.** Titanium catalyzed coupling reactions of triazoles and alkynes: An unexpected synthesis of halovinyl sulfides. **A. Nguyen**, A.N. Desnoyer, I. Tonks

Section A

Orange County Convention Center
West Hall C



TECHNICAL PROGRAM

Photoredox Chemistry

E. C. McLaughlin, *Organizer*

5:30 - 7:30

ORGN 186. Illuminating science of photochemistry: The formation of disubstituted aniline derivatives via photoinitiation. **J. Gulliver**, N. Zheng, D.L. Jacobs

ORGN 187. Catalytic, cross-selective aza-pinacol reaction. **J. Rutherford**, S. Rafferty, D. Nagib

ORGN 188. Applications of amino modified metal organic frameworks in photocatalytic organic reactions. **K. Bobek**, Y. Yuan, F. Uribe, D.A. Vazquez-Molina

ORGN 189. Photo-induced direct C(sp²)-H bond azo coupling of imidazo-heteroarenes with aryl diazonium salts. **A.L. Braga, J.R. Khan**, S. Saba, M.S. Franco, B.R. Zavarise, C.R. Santos

MONDAY MORNING

Section A

Orange County Convention Center
Room W230A

New Reactions & Methodology

S. M. Silverman, *Organizer*
C. Yeung, *Presiding*

8:20 ORGN 190. Investigation the scope and reaction pathway of oxidopyrylium-alkene [5+2] cycloaddition conjugate addition cascade (C³) sequences. R.H. Kaufman, C.M. Law, J. Simanis, E. Woodall, C.R. Zwick, H. Wedler, P. Wendelboe, C.G. Hamaker, J.R. Goodell, D.J. Tantillo, **T. Mitchell**

8:40 ORGN 191. Impact of increased CO₂ pressure on substrate scope and boracarboxylation reaction efficiency. **S.W. Knowlden**, B.V. Popp

9:00 ORGN 192. Decarboxylative amination of redox-active esters using diazirines. **P.P. Chandrachud**, J.M. Lopchuk

9:20 ORGN 193. Cyanide-mediated nitrile-to-nitrile cyclocondensation towards efficient synthesis of polysubstituted pyrroles. **S. Sisodiya**, M. Saini, Y.V. Shah, G. Kumar, D.P. Daniel, N. Hura, V. Chaudhary, S.K. Guchhait

9:40 ORGN 194. Boron cluster-based approach to nucleophilic borylation. **A.M. Spokoyny**

10:00 ORGN 195. Room-temperature palladium-catalyzed C-S cross-couplings: Synthetic chemistry innovations from the Merck Co-op Program and the importance of academia-industry partnerships. **C. Yeung**



TECHNICAL PROGRAM

10:20 ORGN 196. Metal-catalyzed cyclotrimerization reactions of alkynes tethered to vinyl sulfones. **A. Martin**, G.B. Dudley, B.V. Popp

10:40 ORGN 197. Palladium-catalyzed imine formation from acetylenes and anilines. **M. Mihelac**, J. Kosmrlj, M. Gazvoda

11:00 ORGN 198. Synthesis of medchem-relevant gem-difluorocycloalkane building blocks. **S. Ryabukhin**, D. Volochnyuk, P. Nosik, K. Melnykov, O. Grygorenko

11:20 ORGN 199. Multigram scale synthesis of spirocyclic pyrrolidines. **S. Ryabukhin**, D. Volochnyuk, K. Melnykov, E. Ostapchuk

11:40 ORGN 200. Synthesis of functionalized cyclobutanes as a conformational restriction tool for the medicinal chemistry. D. Radchenko, O. Grygorenko, I.S. Kondratov, I. Komarov, **D. Volochnyuk**

Section B

Orange County Convention Center
Room W230B

Physical Organic Chemistry: Calculations, Mechanisms, Photochemistry & High-Energy Species

S. M. Silverman, *Organizer*
A. S. Petit, *Presiding*

8:20 ORGN 201. Gas-phase reactivity and mechanism study of charged quinoline-based σ -type tri- and tetradicals. **D. Ding**, R.R. Kotha, H.I. Kenttamaa

8:45 ORGN 202. Control of reaction mechanism and reactivity and by photoswitchable *N*-heterocyclic carbene ligands in Rh-catalyzed hydroboration of styrene: A computational investigation. **H. Shao**, C. Bielawski, P. Liu

9:10 ORGN 203. Modulation of photogenerated radicals in self-assembled methylene urea tethered triphenylamine dimers. **A. Sindt**, B. DeHaven, M. Smith, L.S. Shimizu

9:35 ORGN 204. Chemical characterization of boron-centered radical anion. **J. Liu**, X. Ma, E. Johnson, J. Warneke, R. Kumar, J. Laskin, H.I. Kenttamaa, M. Rohdenburg

10:00 ORGN 205. Effects of linkers between coumarin units on determination of sodium and potassium. **D. Tan**, A. Akdag

10:25 ORGN 206. Selective microwave heating in thermal Friedel-Crafts benzylations. **H. Fulo**, M. Vincent, A. Tavakoli, G.B. Dudley

10:50 ORGN 207. Probing the mechanism of the Prins and related reactions *via* a combined experimental and computational study. **L.C. Evans**, A. Dobbs, J. Pang

11:15 ORGN 208. Computational investigation of the formation and intramolecular cyclization of 2'-arylbenzaldehyde oxime ether radical cations. S. Kong, L. Ulloa, A. Vigil, **A.S. Petit**

Section C



TECHNICAL PROGRAM

Orange County Convention Center
Room W230C

Biologically Related Molecules & Processes

S. M. Silverman, *Organizer*
S. Choi, *Presiding*

8:20 ORGN 209. Reactivity and dual mechanism of action of α -nucleophile scaffolds for the protection of acetylcholinesterase. S. Tang, P.T. Wong, S. Bhattacharjee, J. Cannon, K. Yang, S. Bowden, **S. Choi**

8:40 ORGN 210. Natural product inspired bridged bicyclic compounds as neuroprotective agents. **S. Maki**, N. Sial, E. St. Germain, W. Bollinger, K. Dawson-Scully, S.D. Lepore

9:00 ORGN 211. Total synthesis of 9-CD₃-9-cis-retinal for studying vision. **M. Navidi**, s. yadav, A.V. Struts, M.F. Brown, N. Nesnas

9:20 ORGN 212. Conformational preference and chemical stability of 6-nitrochrysene modified 2'-deoxynucleosides. **B.V. Powell**, A.K. Basu, M. Guberman-Pfeffer, J. Gascon

9:40 ORGN 213. Kinetic dearomatization strategy for an expedient biomimetic route to the Bielschowskysin skeleton. **P.D. Scesa**, S. Roche, L.M. West

10:00 ORGN 214. Design, synthesis, and evaluation of novel azapeptide carbonyls as inhibitors of the 20S proteasome. **O. Dogan Ekici**, T.S. Corrigan, K.Q. Kasper, L.M. Lotti Diaz, D. Ciarlariello, D. Benson, C.M. Hadad

10:20 ORGN 215. Preparation, characterization, and COX activity of novel boron-containing ibuprofen derivatives. **R. Abeyasinghe**, B.V. Popp

10:40 ORGN 216. Improved, efficient synthesis of the calmodulin antagonist TAPP. J.W. Johnson, K. Cain, T. Dunlap, **G.R. Naumiec**

11:00 ORGN 217. Small-molecule ion channel restores host defenses in cystic fibrosis airway epithelia. **R. Chorghade**, M.D. Burke

11:20 ORGN 218. Design, synthesis, characterization, and structural studies of modulators of bacterial cell-to-cell signaling illuminate a secondary conformation of the *Pseudomonas aeruginosa* receptor LasR. **M.C. O'Reilly**, S. Dong, H.E. Blackwell, S.K. Nair

Section D

Orange County Convention Center
West Hall F3

Innovative Green Chemistry: Striving toward Zero Waste API Manufacturing

Financially supported by Green Chemistry Institute
G. R. Humphrey, K. M. Maloney, *Organizers, Presiding*



TECHNICAL PROGRAM

8:00 Introductory Remarks.

8:05 ORGN 219. Translational chemistry. **P.S. Baran**

9:00 ORGN 220. Innovative green chemistry: Striving towards zero-waste API manufacturing. **M. Faul**

9:55 ORGN 221. Towards a fully biocatalytic manufacturing route for MK-8591. **C.C. Nawrat**

10:50 ORGN 222. Innovation by evolution: Bringing new chemistry to life. **F.H. Arnold**

Section E

Orange County Convention Center
West Hall F4

Ernest Guenther Award in the Chemistry of Natural Products

S. M. Sieburth, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 ORGN 223. Art, craft, logic, and the unforeseen in natural product synthesis. **S. Hanessian**

8:55 ORGN 224. From natural product to unnatural product: Seeking for better biological activity. **M. Sodeoka**

9:45 ORGN 225. Therapeutic function through synthesis-informed design: Approaches to HIV/AIDS eradication, Alzheimer's disease, and enhanced cancer immuno-therapy. **P.A. Wender**

10:35 Introduction of Awardee.

10:45 ORGN 226. **Award Address** (Ernest Guenther Award in the Chemistry of Natural Products sponsored by Givaudan). Exploration of the exceptional potential of taxane-class diterpenes at the interface of chemistry, biology and medicine. **I. Ojima**

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Sponsored by PROF, Cosponsored by AGFD, ANYL, BIOL, BIOT, CARB, CELL, CHED, CMA, COLL, COMP, ENVR, GEOC, I&EC, MEDI, MPPG, NUCL, ORGN, PHYS, PMSE, POLY, PRES, WCC and YCC

MONDAY AFTERNOON

Section A

Orange County Convention Center
Room W230A



TECHNICAL PROGRAM

New Reactions & Methodology

S. M. Silverman, *Organizer*
J. McCabe Dunn, *Presiding*

1:00 ORGN 227. C-H arylation via Cu-catalyzed radical relay. **L.M. Stateman**, Z. Zhang, D. Nagib

1:20 ORGN 228. Development of novel methods for homologation of protected α -oxyboronate esters. **A. Samoshin**, G. Meyer, M. Nistler, A.M. DePaul, T.B. Clark, G.W. O'Neil

1:40 ORGN 229. Controlled α -halogenation of alkyl sulfones using reagent-solvent halogen bonding. C. Poteat, **V. Lindsay**

2:00 ORGN 230. Water mediated benzyne reactions using arylbenziodoxaboroles. **A. Yoshimura**, J. Fuchs, G. Rohde, V. Nemykin, A. Saito, M. Yusubov, V.V. Zhdankin

2:20 ORGN 231. Palladium-catalyzed dearomative *syn*-1,4-oxyamination and carboamination. **C. Tang**, M. Okumura, Y. Zhu, D. Sarlah

2:40 ORGN 232. Harnessing the reactivity of strained heterocyclic allenes. **M. Yamano**, N.K. Garg

3:00 ORGN 233. HFIP and the development of an interrupted Schmidt reaction. **J. Aube**, M. Charaschanya, K. Li, H. Motiwala

3:20 ORGN 234. Reductive ketyl radical couplings via atom transfer catalysis. **S.M. Rafferty**, J. Rutherford, D. Nagib

3:40 ORGN 235. Direct electrochemical carboxylation of benzylic C-N bonds with carbon dioxide. **D. Yang**, M. Zhu, R. Ye, Z. Schiffer, K. Manthiram

4:00 ORGN 236. Gold-catalyzed oxidative coupling of alkynes toward the synthesis of cyclic conjugated diynes and its application on polymer post-functionalization. **J. Wei**, X. Ye, X. Shi

4:20 ORGN 237. Synergistic, Au-Fe-catalyzed, directed aldol reaction. **t. yuan**, X. Shi

4:40 ORGN 238. Catalytic enantioselective approaches to allenes. **S. Ma**

Section B

Orange County Convention Center
Room W230B

Physical Organic Chemistry: Calculations, Mechanisms, Photochemistry & High-Energy Species

S. M. Silverman, *Organizer*
M. Jaramillo, *Presiding*

1:00 ORGN 239. Fundamental studies of the singlet oxygenation of melanin model compounds: Reaction products and pathways. **M. Jaramillo**, K.E. O'Shea



TECHNICAL PROGRAM

- 1:25 ORGN 240.** Stereoelectronic effects in bicyclo[1.1.1]pentanes: Radical chlorination and hydrodechlorination. **J. Kaleta**, I. Roncević, I. Cisarová, M. Dracínský, V. Solínová, V. Kasicka, J. Michl
- 1:50 ORGN 241.** Substituent effects on ultrafast photochemistry: ethylene, butadiene and larger polyenes. **R.J. MacDonell**, M. Schuurman
- 2:15 ORGN 242.** Understanding the connection between cation- π interactions and reaction selectivity. **S.L. Wiskur**
- 2:40 ORGN 243.** Computational mechanistic study of a P_4 -catalyzed anti-Markovnikov alcohol addition to styrene derivatives. **J. Alegre Requena**, R.S. Paton
- 3:05 ORGN 244.** Computational modeling of substituent effect on the frontier orbitals of conjugated molecules. **Y. Shao**, Y. Mao, V. Satalkar
- 3:30 ORGN 245.** *trans*-Hydroboration-oxidation products. Revisiting the reaction mechanism in Δ^5 -steroids. **M.A. Fernandez-Herrera**, J. Sandoval-Ramírez, M. Muñoz-Hernández, L. Kürti, G. Merino
- 3:55 ORGN 246.** Copper-catalyzed difunctionalization of alkenes with boron and CO_2 : Evidence for a cooperative carboxylation transition-state. **B.V. Popp**, N.N. Baughman

Section C

Orange County Convention Center
Room W230C

Successful Products & Models of Undergraduate-Based Research: Good Science, Better Scientists

J. J. Reczek, K. A. Wheeler, *Organizers, Presiding*

1:00 Introductory Remarks.

1:05 ORGN 247. Fluorogenic polymer synthesis for biological detection. **C.B. Cooley**

1:30 ORGN 248. Design of undergraduate organic synthesis research projects with a high probability of success. **E. Bosch**

1:55 ORGN 249. Internship experiences at Biogen: Chemical process development. **W. Liang**

2:20 ORGN 250. One click away from products: Click chemistry as a powerful tool for the synthesis of ionic liquids for undergraduate chemistry students. **A. Mirjafari**

2:45 Intermission.

2:55 ORGN 251. Undergraduate research at the University of Texas: What's unique with us? **E.V. Anslyn**

3:20 ORGN 252. SPR biosensors based on guided-wave plasmon-polariton modes. **J. Leger**

3:45 ORGN 253. Research opportunities for undergraduate students and educators at Eli Lilly. **M.S. Zia Ebrahimi**



TECHNICAL PROGRAM

4:10 ORGN 254. Polymer chemistry with undergraduate women: Reactive, azlactone-functionalized polymers for the fabrication of multifunctional biomaterials. **M.E. Buck**, A. Mineo, E. Fitzgerald, R. Yan

4:35 ORGN 255. Development of functional organic charge-transfer materials: Diverse on-ramps to the undergraduate research highway. **J.J. Reczek**

Section D

Orange County Convention Center
West Hall F3

Innovative Green Chemistry: Striving toward Zero Waste API Manufacturing

Financially supported by Green Chemistry Institute
G. R. Humphrey, K. M. Maloney, *Organizers, Presiding*

1:00 Introductory Remarks.

1:05 ORGN 256. Transitioning organic synthesis to a water world: Faster, better, cheaper, & environmentally responsible chemistry. **B.H. Lipshutz**

1:50 ORGN 257. Use of continuous flow technology towards more sustainable API manufacturing. **C. Kappe**

2:35 ORGN 258. New catalysts for carbonyl-olefin metathesis. **C. Schindler**

3:20 ORGN 259. Platform for automated nanomole scale reaction screening and micromole scale synthesis in flow. **D. Perera**, J.W. Tucker, S. Brahmbhatt, C.J. Helal, A. Chong, W.P. Farrell, P. Richardson, N. Sach

4:05 ORGN 260. Chemistry in water for highly selective reaction pathways. **S. Handa**

Section E

Orange County Convention Center
West Hall F4

ACS Award for Creative Work in Synthetic Organic Chemistry

K. B. Hansen, *Organizer*
S. Paradine, *Presiding*

1:00 Introductory Remarks.

1:05 ORGN 261. Metalloenzyme discovery in the microbial world. **E.P. Balskus**

1:45 ORGN 262. Single electron processes enabling organic synthesis. **G.A. Molander**

2:25 ORGN 263. Nucleophilic substitution reactions: A radical alternative to S_N1 and S_N2 reactions. **G.C. Fu**



TECHNICAL PROGRAM

3:05 ORGN 264. Chrial H-bond donor/Lewis acid cooperativity. **E.N. Jacobsen**

3:45 Introduction of Awardee.

3:55 ORGN 265. **Award Address** (ACS Award for Creative Work in Synthetic Organic Chemistry sponsored by MilliporeSigma). Molecular surgery. **M. White**

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Sponsored by PROF, Cosponsored by AGFD, ANYL, BIOL, BIOT, CARB, CELL, CHED, CMA, COLL, COMP, ENVR, GEOC, I&EC, MEDI, MPPG, NUCL, ORGN, PHYS, PMSE, POLY, PRES, WCC and YCC

MONDAY EVENING

Section A

Orange County Convention Center
West Hall C

Sci-Mix

E. C. McLaughlin, *Organizer*

8:00 - 10:00

102, 104, 106, 109-110, 123, 130-131, 137-138, 141, 144, 146, 150, 162, 168, 170, 173, 176. See previous listings.

347, 349, 352, 354, 361, 365, 372, 382-383, 385, 390, 394, 397, 404, 408, 409, 411, 417, 421, 425, 430, 435, 450, 452, 454, 465, 555, 571-573, 575, 578, 587, 594, 596-597, 600-601, 617-618, 629, 633, 637, 643-644, 648, 657, 659, 665, 667. See subsequent listings.

TUESDAY MORNING

Section A

Orange County Convention Center
Room W230A

Molecular Recognition & Self-Assembly

S. M. Silverman, *Organizer*
J. Jung, *Presiding*



TECHNICAL PROGRAM

- 8:20 ORGN 266.** Pillar[5]arene-functionalized silver nanoclusters: Synthesis and host-guest induced vast PL enhancement. **N.M. Khashab**
- 8:40 ORGN 267.** Structure-property relationship in self-assembling [n.n]paracyclophanes. **W.R. Henderson**, Y. Zhu, D.E. Fagnani, K.A. Abboud, R.K. Castellano
- 9:00 ORGN 268.** Can self-assembly into wormlike micelles occur in polar solvents at sub-zero temperatures? **N. Agrawal**, S.R. Raghavan
- 9:20 ORGN 269.** Conversion of a weak DAD-ADA H-bond dimer to a much stronger DDD-AAA dimer via proton-coupled electron transfer. **D.K. Smith**, H. Choi
- 9:40 ORGN 270.** Supramolecular boronic acids: Gelator and receptor design. **K. Dannaher**
- 10:00 ORGN 271.** Hierarchical and anion-templated organization of macrocycles. **J. Dobscha**, A.H. Flood
- 10:20 ORGN 272.** Towards switchable anion receptors. **D. Van Craen**, A.H. Flood
- 10:40 ORGN 273.** Anion recognition with π -acids and Lewis acids. **S. Saha**
- 11:00 ORGN 274.** Enhancing the stability of photogenerated benzophenone triplet radical pairs through supramolecular assembly. B. DeHaven, D. Goodlett, **L.S. Shimizu**
- 11:20 ORGN 275.** Dramatic enhancement of electron donor/acceptor ability by complementary hydrogen bonding. **C. Liu**, D.F. Perepichka
- 11:40 ORGN 276.** Residual copper detection by molecular probe: Applications by coupling with HPLC system. **J. Jung**, J. Jo, A. Purohit

Section B

Orange County Convention Center
Room W230B

Peptides, Proteins & Amino Acids

S. M. Silverman, *Organizer*
J. Iegre, *Presiding*

- 8:00 ORGN 277.** Development of novel CK2 inhibitors: From small molecules to conformationally constrained peptides targeting allosteric binding sites. **J. Iegre**, P. Brear, D.R. Spring
- 8:20 ORGN 278.** Synthesis of malformin C and analogs for targeted anti-cancer drug delivery. **F. Hossain**, S. Nishat, P.R. Andreana
- 8:40 ORGN 279.** Reaction design for highly efficient chemical protein synthesis. G. Hayashi, **A. Okamoto**
- 9:00 ORGN 280.** Reinvention of peptide synthesis through utilization of nano-reactors. **C. Chapman**, N.N. Shaw



TECHNICAL PROGRAM

- 9:20 ORGN 281. 3- ^{18}F fluoropropane-1-thiol and ^{18}F PEG4-1-thiol: Versatile prosthetic groups for radiolabeling maleimide functionalized peptides. **D.O. Kiesewetter**, O. Jacobson
- 9:40 ORGN 282. *N*-amino peptides: From natural products to protein mimics. **J.R. Del Valle**
- 10:00 ORGN 283. Thioenamide synthesis inspired by peptide macrocycles. **J.A. Lutz**, C.M. Taylor
- 10:20 ORGN 284. Aerobic oxidation of *N*-phenylglycyl peptides for catalyst-free oxime ligations. Q. Guthrie, **C. Proulx**
- 10:40 ORGN 285. Spectroscopic study of methyl salicylate hydrolysis in the presence of amino acids. **L. Pan**, T. Brinzari, C. Cheng, Z. Hao, X. Wang
- 11:00 ORGN 286. Structural revision and total synthesis of the bacterial siderophore madurastatin C1. **M.J. Hall**
- 11:20 ORGN 287. Highly parallelized single-molecule sequencing and identification of proteins. **J. Bachman**, E.V. Anslyn, E.M. Marcotte, J. Swaminathan, A. Bardo

Section C

Orange County Convention Center
Room W230C

Heterocycles & Aromatics

S. M. Silverman, *Organizer*
H. Ren, *Presiding*

- 8:00 ORGN 288. Operationally simple approach to indole derivatives from 2-alkenylanilines utilizing an oxidation-transannulation-elimination sequence. **C.J. Monceaux**, R.M. Chapman, J.R. King
- 8:20 ORGN 289. Ketone Pictet-Spengler routes to spiro-, C1-methyl, and azepane analogs of an antimalarial tetrahydro- β -carboline. **S. Ding**, M. Ghavami, J.H. Butler, E.F. Merino, C. Slebodnick, M.B. Cassera, P.R. Carlier
- 8:40 ORGN 290. Use of microwaves for synthesis of propargylic ethers as precursors of 1,2,3-triazoles in click reactions. L.C. García, M.A. García-Eleno, E. Cuevas-Yañez, **A.F. Becerra**
- 9:00 ORGN 291. Development of a green and sustainable commercial manufacturing process. **H. Ren**
- 9:20 ORGN 292. Phosphorus ligand-coupling for cross-electrophile coupling of pyridines and diazines. **B. Boyle**, M. Hilton, A. McNally
- 9:40 ORGN 293. Direct and regioselective difluoromethylation of azines and pharmaceuticals via phosphorus ligand-coupling. **K. Nottingham**, C. Patel, A. McNally
- 10:00 ORGN 294. Revisiting the gamma-gauche effect: A ^1H NMR method for stereochemical assignment of 1,3-disubstituted-1,2,3,4-tetrahydro- β -carbolines. **K. Cagasova**, M. Ghavami, Z. Yao, P.R. Carlier
- 10:20 ORGN 295. Photochemistry of (4+3)-cycloadducts: Formation of rigid tropane alkaloid derivatives. C. Fu, **M. Harmata**



TECHNICAL PROGRAM

10:40 ORGN 296. Incorporation of fused heterocycles to the macrocyclic ring of calix[4]arene by reactions at the methylene bridge. **J.L. Fantini**

11:00 ORGN 297. Donor-acceptor thiazolothiazole dyes exhibiting solvatofluorochromism, high quantum yields, and large electronic dipole changes. **N. Sayresmith**, J. Sailer, K. Sandor, S.M. Patberg, M.G. Walter

11:20 ORGN 298. Developing the chemistry of boroles to access larger boracycles. **C. Martin**

11:40 ORGN 299. Iminoquinones as a source of electrophilic nitrogen for heterocycle synthesis. **L.M. Mori Quiroz**, M.D. Clift, C. Comadoll, J. Super

Section D

Orange County Convention Center
West Hall F3

Process Chemistry: New Developments in Pharmaceutical Process Development

Cosponsored by I&EC
R. Vaidyanathan, *Organizer*
J. A. Pesti, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 ORGN 300. Process development of merestinib. **Y. Lu**, K.P. Cole, J. Fennell, M.O. Frederick, N.J. Kallman, J.L. Burt

8:40 ORGN 301. Development of a crystallization-induced dynamic resolution to IDO inhibitor, Navoximod. **D.E. Carrera**, H. Hou, K. Piechowicz, J. Xu, F. St-Jean, R. Angelaud, F. Gosselin

9:20 ORGN 302. Development of active pharmaceutical ingredients for clinical development: Synthesis of a gamma secretase modulator. **S. Caron**

10:00 ORGN 303. Journey from early- to late-stage development at Merck. **J. McCabe Dunn**

10:40 ORGN 304. Impact of remnants from reactions on subsequent transformations. **R. Vaidyanathan**

11:20 ORGN 305. Early phase process development and scale up of novel APJ agonist AMG 986. **R.P. Farrell**, S.M. Mennen, S.J. Hedley, J.S. Tedrow, T. Judd

11:55 Concluding Remarks.

Section E

Orange County Convention Center
West Hall F4

Elias J. Corey Award for Outstanding Original Contribution in Organic Synthesis by a Young Investigator



TECHNICAL PROGRAM

J. G. Pierce, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 ORGN 306. Organic and organometallic reactions mediated by water-soluble host-guest supramolecular systems. **R.G. Bergman**

8:45 ORGN 307. Unleashing the supramolecular potential of strained carbon nano hoops. **M. von Delius**

9:25 ORGN 308. Innovation at Merck Process R&D via discovery and development of new catalytic reactions. **R. Ruck**

10:05 Intermission.

10:15 ORGN 309. New photoredox reactions. **D.W. MacMillan**

10:55 ORGN 310. **Award Address** (Elias J. Corey Award for Outstanding Original Contribution in Organic Synthesis by a Young Investigator sponsored by the Pfizer Endowment Fund). Make it or break it with metal-hydrides. **V.M. Dong**

Opportunities and Challenges in Carbohydrate Synthesis B

Sponsored by CARB, Cosponsored by CELL and ORGN

GSSPC: Artificial Molecular Machines & the Next Generation of Molecular Control

Sponsored by CHED, Cosponsored by COLL, I&EC, ORGN‡, PHYS, POLY and PRES

TUESDAY AFTERNOON

Section A

Orange County Convention Center
Room W230A

Molecular Recognition & Self-Assembly

S. M. Silverman, *Organizer*
M. von Delius, *Presiding*

1:20 ORGN 311. Rapid optical determination of *ee*, *de*, and total concentration: A demonstration using 2-aminocyclohexanol. **B.T. Herrera**, E.V. Anslyn, F. Marini

1:40 ORGN 312. Discovery of novel TLR8 antagonists via structure-based rational design. **S. Jiang**, S. Zhang, Z. Hu, H. Tanji, T. Shimizu, H.H. Yin



TECHNICAL PROGRAM

- 2:00 ORGN 313.** Programmed assembly of near-infrared fluorescent molecular probes. **J.M. Dempsey**, C. Zhai, H. McGarraugh, C. Schreiber, B. Smith
- 2:20 ORGN 314.** Co-assembled protein mimicking peptide immunofibers for affinity precipitation of monoclonal antibodies. **Y. Li**, L. Lock, J. Mills, S. Ou, D. Stern, M. Morrow, X. Xu, S. Ghose, H. Cui
- 2:40 ORGN 315.** Bioinspired artificial nanoparticle esterases for effective stabilization of the tetrahedral anionic transition state. **M. Arifuzzaman**, Y. Zhao
- 3:00 ORGN 316.** Dynamic covalent self-assembly based on oxime condensation. **H. Li**
- 3:20 ORGN 317.** Molecularly Imprinted Nanoparticles (MINP) as fluorescent sensors for Nonsteroidal Anti-Inflammatory Drugs (NSAIDs). **L. Duan**
- 3:40 ORGN 318.** Construction of linked G-octamer via monomer conformational control stabilized in MeOH and DMSO. **m. liu**, X. Shi
- 4:00 ORGN 319.** New approach to gold recovery: Supramolecular co-precipitation of square-planar gold complexes. **C. Shaffer**, W. Liu, B.D. Smith
- 4:20 ORGN 320.** Tessellation of shape-persistent donor-acceptor cyclophanes for the creation of two-dimensional porous materials. **M. Cetin**, Y. Beldjoudi, J.F. Stoddart
- 4:40 ORGN 321.** Self-assembly of adaptive orthoester architectures. **M. von Delius**

Section B

Orange County Convention Center
Room W230B

Metal-Mediated Reactions & Syntheses

S. M. Silverman, *Organizer*
G. Howell, *Presiding*

- 1:20 ORGN 322.** Straightforward α -amino nitrile synthesis through $\text{Mo}(\text{CO})_6$ -catalyzed reductive functionalization of carboxamides. **P. Trillo**
- 1:40 ORGN 323.** Catalytic hydroamination of unactivated internal alkenes. **Y. Xi**, J.F. Hartwig
- 2:00 ORGN 324.** Allyl- and allenylboronic acids: Preparation and application in organic synthesis. **K.J. Szabo**
- 2:20 ORGN 325.** Development of palladium-catalyzed cross-coupling reactions for carbon-carbon and carbon-heteroatom bond forming reactions of aryl chlorides. **Z. Novák**, B. Petho, D. Vangel, M. Zwillinger, J. Csenki, G. Tolnai, L. Ondi
- 2:40 ORGN 326.** Copper-catalyzed synthesis of sterically encumbered allenylboronic acids using $\text{B}_2(\text{OH})_4$ as boron source. J. Zhao, S. Jonker, **D.N. Meyer**, G. Schulz, C. Tran, L. Eriksson, K.J. Szabo



TECHNICAL PROGRAM

3:00 ORGN 327. Aqueous Atom Transfer Radical Polymerization (ATRP) of commonly used vinyl monomers with *N*-heterocyclic carbene (NHC) containing homogeneous Ru catalyst. **S. Kim, H. Chung**

3:20 ORGN 328. Metal–hydride catalysis in organic synthesis. **R. Davison**

3:40 ORGN 329. Short stories from the pharmaceutical industry: A new Suzuki-Miyaura procedure for the synthesis of Savolitinib. **G. Howell**, N. Adlington, L. Agnew, A. Campbell, R. Cox, A. Dobson, M. Gall, W. Hicks, A. Jawor-Baczynska, M. Pilling, L. Miller-Potucka, K. Shepherd, B. Taylor, A. Williams

Section C

Orange County Convention Center
Room W230C

Chemistry for New Frontiers

S. M. Silverman, *Organizer*
M. Straub, *Presiding*

1:00 ORGN 330. Synthesis and circularly polarized luminescence of chiral boron-chelated dipyrromethene fluorophores. **M.J. Hall**

1:20 ORGN 331. Sustainable route to bio-based terephthalic acid from crude sulfate turpentine. **J. Tibbetts**, P. Plucinski, S. Bull

1:40 ORGN 332. Visible-light-induced dearomative spirocyclization of non-phenolic biaryl carboxylic acids. **E. Subbotina**, H. Li, A. Bunrit, F. Wang, J.S. Samec

2:00 ORGN 333. Bioorthogonal catalysis: Overview, applications, and state-of-the-art. **A. Unciti-Broceta**

2:20 ORGN 334. From fuzzy to functionally smart molecules: Orchestrated asymmetric synthesis of indolo[2,3-*a*]quinoline scaffolds as novel motifs for cancer immunotherapy. **T.H. Altel**

2:40 ORGN 335. Ring distortion of vincamine produces complex and diverse molecules for drug discovery. **C.M. Norwood, R. Huigens**

3:00 ORGN 336. Organocatalytic enantioselective synthesis of α -fluoro- β -amino acid derivatives. **M. Straub**, V. Birman

3:20 ORGN 337. Lewis base-catalyzed rearrangement of *S*-phenacyl thioesters. **M. Straub**, D. Leace, B. Matz, V. Birman

3:40 ORGN 338. Synthesis and anti-microbial activity of 1,2,3-triazoles-coumarin hybrids from chalcones. **T. Moodley**, N. Koorbanally

4:00 ORGN 339. New frontiers of difluorocyclopropanation of alkenes using Ruppert–Prakash reagent. **S. Ryabukhin**, P. Nosik, D. Volochnyuk, O. Grygorenko

4:20 ORGN 340. Expanding the boundaries of water tolerant frustrated Lewis hydrogenation via size-exclusion catalyst design. **T. Soos**



TECHNICAL PROGRAM

Section E

Orange County Convention Center
West Hall F4

Herbert C. Brown Award for Creative Research in Synthetic Methods

A. K. Franz, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 ORGN 341. Functionalizations of C-H bonds in a flask and a cell. **J.F. Hartwig**

1:45 ORGN 342. Radical reactions for control freaks: New synthetic methods involving aryl radicals and strong C-F bonds. **N. Jui**

2:25 ORGN 343. Break-it-to-make-it strategies for complex molecule synthesis. **R. Sarpong**

3:05 ORGN 344. Enantioselective and remote C-H activation reactions. **J. Yu**

3:45 Introduction of Awardee.

3:50 ORGN 345. Award Address (Herbert C. Brown Award for Creative Research in Synthetic Methods sponsored by the Purdue Borane Research Fund and the Herbert C. Brown Award Endowment). Catalyst-controlled site-selective and enantioselective C-H functionalization. **H.M. Davies**

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Sponsored by PROF, Cosponsored by ENVR, GEOC, I&EC, MEDI, MPPG, NUCL, ORGN, PHYS, PMSE, POLY, WCC and YCC

ACS Award in Industrial Chemistry: Symposium in Honor of Guy R. Humphrey

Sponsored by I&EC, Cosponsored by ORGN

Opportunities and Challenges in Carbohydrate Synthesis B

Sponsored by CARB, Cosponsored by CELL and ORGN

GSSPC: Artificial Molecular Machines & the Next Generation of Molecular Control



TECHNICAL PROGRAM

Sponsored by CHED, Cosponsored by COLL, I&EC, ORGN[‡], PHYS, POLY and PRES

TUESDAY EVENING

Section A

Orange County Convention Center
West Hall C

Biologically Related Molecules & Processes

E. C. McLaughlin, *Organizer*

5:30 - 7:30

ORGN 346. Development of photoactivatable (2-quinolinyl)methyl-based nitroxyl (HNO)-releasing compounds. **M.S. Rahman**, N.E. Brasch, A.J. Seed, P. Sampson

ORGN 347. Synthesis of near-infrared emitting fluorescent dyes and their application in organelle specific labelling studies. **J. Jose**, P. Choi, K. Noguchi, M. Ishiyama, W.A. Denny

ORGN 348. Synthesis of folate-appended β -cyclodextrin for cancer-targeting drug delivery. **N. Russel**, P. Paul, M.R. Karim, B. Song

ORGN 349. Synthesis of mixed, hypoxia-activated phosphoramidate esters for the inhibition of enolase in *ENO1*-deleted glioblastoma. **V.C. Yan**, E.S. Ballato, K.L. Yang, D.K. Georgiou, K. Arthur, P. Shrestha, S. Khakha, J. Ackroyd, F.L. Muller

ORGN 350. New small, rigid nitroxide for site-directed spin labeling of proteins. **N. Richards**, Z. Yang, A. Rajca, S. Rajca

ORGN 351. Green synthesis of potential anticancer drugs NUK-1. **H. Cheng, H. Yu, Y. Huang**

ORGN 352. Synthesis and analysis of 1-benzazepines derivatives as potential therapeutic drugs for the treatment of Alzheimer's disease. **C. Nieves**, L.E. Pinero-Santiago, S. Espinosa-Díaz, M. Ortiz Marciales

ORGN 353. Recyclable solid-support for the synthesis of boronic acid-modified peptides. **R. Ulrich**, A. Emig, P. Jervis, A.G. Glenn, T.A. Nile, S. Flower

ORGN 354. Iterative deconjugative alkylation/Cope rearrangement and ring-rearrangement metathesis for the synthesis of 5-6-5-n scaffolds. **E. Semenova**

ORGN 355. Design, synthesis, and biological evaluation of novel spiro-isoxazoline-peroxides as potent inhibitors of human-cytomegalovirus (HCMV) and glioblastoma cell (GBM6). **P. Das**, M.H. Hasan, D. Mitra, R.K. Bollavarapu, E.J. Valente, R. Tandon, D. Raucher, A.T. Hamme II

ORGN 356. Synthesis of 4-(methylsulfinyl)benzyl and 3-pyridylmethyl glucosinolate via the nitronate pathway. **M.A. Anderson, E. Ronning, A.A. Snyder**, S. Fisher, J.R. Mays



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- ORGN 357.** Extraction of some triterpenoid saponins from *Tetraena qatarense* (*Zygophyllum qatarense*) and their biological activities. **S. Yousuf**, H. Nimir, H. Hassan, H. Al Easa
- ORGN 358.** Flavins as enophiles in ene reactions and catalysts for retro-ene reactions. **A.W. Jensen**
- ORGN 359.** Investigation of new benzoate-1,2-dioxygenase substrates using quantitative ¹H-NMR spectroscopy. **Z. Clark**, S.Q. Erickson, D.K. Pawar, J.A. Collins
- ORGN 360.** Effect of selenium nutrition, temperature, and photoperiod on gibberellic acid accumulation in spinach plants. A. Malkawi, **C. True**, A. Bailey
- ORGN 361.** Development of bisphosphonate conjugates for molecular imaging of natural bone restoration processes. **E. Marris**, A. Trice, K. Ha, J.G. Schoenecker, J. McCarthy
- ORGN 362.** Synthesis, characterization, and conformational investigation of partially saturated menaquinone derivatives. **J.T. Koehn**, D.C. Crick, D.C. Crans
- ORGN 363.** Synthesis and spectroscopic characterization of fluorescent labeling inhibitor for C.diff. binary toxins. **H.F. Sobhi**, N. Clayton, P. Puranik, P. Wilder, D. Weber
- ORGN 364.** Inhibition of ribonucleolytic activity of RNase A by triazolylated thymidines. **P. Mondal**, **S. Dasgupta**, T. Pathak
- ORGN 365.** Fluorescent probe for carbapenemase detection. **C. Ma**, D. Yang
- ORGN 366.** Synthetic studies on K204, a potent new SHIP1 agonist. **O.M. Dungan**, L. Chen, S. Fernandes, W.G. Kerr, J.D. Chisholm
- ORGN 367.** Utilizing triazole-based compounds as potential inhibitors active against gram-negative bacteria. **R. Roldan**, C. Embry, L. Peterson, M.L. Cafiero
- ORGN 368.** Development and synthesis of conjugated cyclic diyne as a novel beta strand mimic strategy. **S. Zhang**, X. Ye, X. Shi
- ORGN 369.** Development and synthesis of conjugated cyclic diyne as a novel alpha-helix structure constraining strategy. **X. LI**
- ORGN 370.** Synthesis of 5-bromo-benzo[b]naphtho[2,1,d]thiophene S-oxide and its ability to cause oxidative stress in cells. **E. Currens**, A. Isor, S. Chintala, R.D. McCulla
- ORGN 371.** Investigating metallocene-based multiQACs as novel amphiphilic antiseptics. **B. Bentley**, R. Kontos, **J. Feliciano**, W.M. Wuest, K.P. Minbiole
- ORGN 372.** Synthesis of piperidinol-based inhibitors of KasA: A novel treatment for *Mycobacterium tuberculosis* infection. **L. Jones**, D. Oldham
- ORGN 373.** Synthesis of the enantiomers of the environmental contaminant diethylhexylphthalate (DEHP) and its metabolites. **D. Oldham**, L. Harris, C. Amurrio, K. Bempong



TECHNICAL PROGRAM

ORGN 374. Synthesis of substituted heterocycles to inhibit a pro-metastatic cytokine. **J. Tuccinardi**, K. Skluzacek, T. Muhammed, C. Ashton, C. Wolf, M. King, C. Jorcyk, D.L. Warner

ORGN 375. Design, modeling, and synthesis of potential LpxC inhibitors. **C.P. Embry**, R. Roldan, A.O. Pajarillo, J.D. Greenberg, M.L. Cafiero, L. Peterson

ORGN 376. Synthesis of small molecule derivatives of CK-666 as potential inhibitors of the Arp2/3 complex. **A. Sripeng**, **N. Wade**, **Z. Cournia**, B. Nolen, A. Baggett

ORGN 377. Synthesis of highly substituted 5-aryl-3-oxo-delta-lactones and their agonistic quorum sensing activity. **M. Peterson**, A. Champion, D. Ewald, B.J. Andersh, M.R. Fry

ORGN 378. Synthesis of 4-thiazolidinone small molecules as potential inhibitors of the Arp2/3 complex. **H. Smith**, A. Baggett, B. Nolen, Z. Cournia

ORGN 379. *In vitro* determination of potency of small molecule inhibitors of Arp2/3 complex. **K. Andersen**, B. Nolen, Z. Cournia, A. Baggett

ORGN 380. Synthesis, characterization, and chromic properties of thio-ether derivatives of 1,4-naphthoquinones. **C.A. Arias**, A.L. Perez, G. Lamoureux, A. Bella Cruz, V. Cechinel Filho

Section A

Orange County Convention Center
West Hall C

Carbon Allotropes & Nanomaterials

E. C. McLaughlin, *Organizer*

5:30 - 7:30

ORGN 381. Selective oxidation of olefins to ketones over palladium supported on weak acidic graphene oxide. **X. Gao**

ORGN 382. Analytical method to measure surface area of graphene materials in solution. **I.V. Kalinina**, G. Tamas, D. Meyers

Section A

Orange County Convention Center
West Hall C

Chemistry for New Frontiers

E. C. McLaughlin, *Organizer*

5:30 - 7:30



TECHNICAL PROGRAM

ORGN 383. Catalyzed degradation of organic contaminants in produced water by biomimetic riboflavin derivatives. **A. Taiclet**, M.M. Abu-Esba, F.W. Foss

ORGN 384. ^{13}C NMR spectroscopic studies of intra- and intermolecular interactions of amino acid derivatives in solutions. **Y. Hiraga**, Y. Uyama, **S. Niwayama**

ORGN 385. Microwave synthesis and characterization of acridine-triazole derivatives. **C. Kannigadu**, N. Koorbanally

ORGN 386. Oxygen-18 enrichment of alcohols by a modified Mitsunobu esterification reaction. **R. Beddoe**, H. Sneddon, R. Denton

ORGN 387. Catalytic epoxidation of olefins over transition metal ferrite nanoparticles. **A.I. Mohamadi**, M.S. Eldous, K. Salih

ORGN 388. Catalytic oxidation of aldehydes over transition metal oxide nanoparticles. **R.a. Al-Awabdeh**, A. Khatib, K. Salih

ORGN 389. Synthesis of photoresponsive derivatives derived from maleonitrile. **H. Ayoub**

ORGN 390. Green, sustainable, nanocatalysed, synthetic route for an exploration of Knoevenagel condensation. **D. Madan**

ORGN 391. Synthesis and characterization of the zinc and manganese complexes of 5,10,15,20-tetra[3,4-dibenzyloxyphenyl]porphyrin. **P. Bharara**, C.P. Tidwell, K. Belmore, Q. Liang, A. Ezell, T. Hudson, E. Hutchens, H. Palacio, T. Tidwell

ORGN 392. Phytochemical investigation of *Magnolia grandiflora* green seed cones. **D. Bandyopadhyay**, B. Garza, A. Echeverria, F. Gonzalez

Section A

Orange County Convention Center
West Hall C

Flow Chemistry & Continuous Processes

E. C. McLaughlin, *Organizer*

5:30 - 7:30

ORGN 393. Impact of flow turbulence in narrow capillaries on the nucleation rate of small organic molecules. R. Debuyschère, **B. Rimez**, B. Scheid

ORGN 394. Applications of flow chemistry in undergraduate research. A. Schroeder, J.A. Shea, C. Ford, **Z. Matesich**

ORGN 395. Improving multiphase catalytic microreactor productivity using a tube-in-tube membrane contactor. **M. Burkholder**, S.E. Gilliland, A. Luxon, C. Tang, F. Gupton

Section A



TECHNICAL PROGRAM

Orange County Convention Center
West Hall C

Materials, Devices & Switches

E. C. McLaughlin, *Organizer*

5:30 - 7:30

ORGN 396. Synthesis and characterization of extended viologens for advanced functional materials. H.D. Mandal, **E. Padilla**, R. Cortez, E.A. Macias, P.K. Bhowmik, E.J. Dizon, S.T. Killarney, J. Kim, H. Han

ORGN 397. Thieno[2,3]pyrrole containing organic small molecules for organic electronics applications. **R. Gunawardhana**, M.C. Stefan, M.C. Biewer, P.L. Gamage, C. Bulumulla

ORGN 398. Synthesis and electronic properties of alkylated spirobifluorene derivatives. **R. Kundu**

ORGN 399. Viologens for advanced functional materials: Synthesis, thermal, and optical properties. H.D. Mandal, **R. Cortez**, E. Padilla, E.A. Macias, P.K. Bhowmik, E.J. Dizon, S.T. Killarney, J. Kim, H. Han

ORGN 400. NIR-responsive metastable-state photoacid. **O.Z. Alghazwat**, T. Khalil, A. Elgattar, Y. Liao

ORGN 401. Synthesis and characterization of liquid-crystalline and light-emitting properties of several 1,3,4-oxadiazole diamines-based azomethine compounds. H.D. Mandal, **R. Cortez**, J. Gutierrez, P. Quach, P.K. Bhowmik, S.L. Chen, H. Han

ORGN 402. Electron acceptors based on cyclopentannulated tetracenes. **G.C. Kulkarni**, J.L. Morales-Cruz, W.A. Hussain, I. Garvey, K.N. Plunkett

ORGN 403. Synthesis of new dopant-free hole transport materials for perovskite solar cells. **W. Li**, Y.S. Tingare, S. Akula, W. Lin, C. Su

ORGN 404. Systematic investigation of photinduced electron transfer in coumarins: Applications in triazine detection. **J. Dorsheimer**, **W.R. Luksic**, R.R. Walvoord

ORGN 405. New organic hole transporting materials with various acceptors for efficient inverted (p-i-n) perovskite solar cells. **S. Akula**, C. Su, Y. Zheng, W. Li

ORGN 406. New phosphonate lipid tubules and their use as a delivery device. **X. Xie**, P. Persichini

ORGN 407. Carbon nanodots doped with fluorescent naphthalene and perylene derivatives. **L. Huang**, **G. Aryal**, K.W. Hunter

ORGN 408. Hydrogel polymers as sensors for the quantitation of metal ions in aqueous solutions. **T.G. Fenske**, S. Oehm, T. Hagemann, P. Henning, J. Labeots, J. Aldstadt, P. Geissinger, A.W. Schwabacher

ORGN 409. Photothermal electrode from conjugated polymers for emission color control. **J. Hwang**, Y. Kim, E. Kim

Section A



TECHNICAL PROGRAM

Orange County Convention Center
West Hall C

Molecular Recognition & Self-Assembly

E. C. McLaughlin, *Organizer*

5:30 - 7:30

ORGN 410. Halogen bonds strength in complexes of diiodine with heteroaromatic N-oxides. **B. Watson, W. Borley, Y. Nizhnik, M. Zeller, S.V. Rosokha**

ORGN 411. Photochemical assisted synthesis of interlocked organic molecules. **V. Ramalingam, M. Pattabiraman**

ORGN 412. Supramolecular catalysis. **S. Teng, X. Shi**

ORGN 413. Synthesis and characterization of a quinoxaline ethylene resorcin[4]arene capsule. **C. Sarabia, L.M. Tunstad**

ORGN 414. Quantification of halogen-bonding ability for neutral and charged electrophilic iodine reagents. **N. Hirbawi, J.R. Jagannathan, A.K. Franz**

ORGN 415. Heteroditopic and multitopic supramolecular hosts. **d. Liu, F.X. Han, Y. Zhao**

ORGN 416. Design, synthesis, and self-assembling properties of hybrid glycoclusters and glycolipids. **J.M. Bietsch, A. Chen, G. Wang**

ORGN 417. Design and synthesis of molecular gelators derived from 4,6-O-(p-chlorobenzylidene)-acetal protected D-glucosamine. **M. Olson, J.M. Bietsch, G. Wang**

ORGN 418. Spectra, structures, and thermodynamics of anion- π complexes of p-benzoquinones with halide anions. **S. Kepler, M. Zeller, S.V. Rosokha**

ORGN 419. Synthesis and exploration of 7,7'-azaindigo and its derivatives. **J.A. Shriver, J. De Young**

ORGN 420. Coordination chemistry of molecular topologies. **L. Zhang, D.A. Leigh**

ORGN 421. Optical chirality sensing with a stereodynamic, aluminum biphenolate probe. **Z. De los Santos, L.A. Joyce, E.C. Sherer, C.J. Welch, C. Wolf**

ORGN 422. Self-organization of highly emissive porphyrin lantern nanoarrays using a single component short G-rich sequence. **P. Pathak, R. Vik, J. Jayawickramarajah**

ORGN 423. Investigating the specificity of thiourea host molecules for inorganic phosphate. **T.A. Davis, A. Cullen, B. Bagnall, T.S. Goebel, R. Lascano**

ORGN 424. Self-assembly of supramolecular prisms using tetraterpyridine-porphyrin ligand. **A.A. Filosa, H. Wang, J. Piccolo, X. Li**



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- ORGN 425.** Self-assembly of tetraphenylethylene-based dimer with tunable fluorescence. **Y. Yan**, G. Yin, X. Li
- ORGN 426.** Self-assembly of ring-in-ring metallacycle with alkynylplatinum(ii) bzimpy and the study of its aggregation behavior. **Y. Li**, G. Huo, W. Sun, H. Yang, X. Li
- ORGN 427.** Spontaneous resolution of an octahedral supramolecular cage. **R. Ni**, C. Xu, X. Li
- ORGN 428.** Effects of small molecules that selectively bind to phosphatidylglycerol(PG). **B. Seelam**, D. Burns
- ORGN 429.** Synthesis of small bis-phenolic ether scaffold cationic molecule that binds to phosphatidylglycerol at the membrane interface. **K. Donavalli**, D. Burns
- ORGN 430.** Developing a basket-shaped host molecule based on calix[4]arene featuring urea groups for volatile guest molecules. **V. Lokugama Widanelage**
- ORGN 431.** Synthesis and characterization of N-acetyl-glucosamine-based macrocycles by S_N2 reactions. **S. Adhikari**, A. Chen, G. Wang
- ORGN 432.** Tightly-knit dual hydrogen bonding for fluorescence turn-on detection of cyanide: Evolving design principles and synthetic implementations. **H. Park**, D. Lee
- ORGN 433.** Supramolecular hexagonal prism with antimicrobial activity. **H. Wang**, K. Wang, M. Wang, R. Brzozowski, B. Xu, J. Cai, P. Eswara, X. Li
- ORGN 434.** Self-assembly of supramolecular pentagonal prisms. **B. Song**, H. Wang, M. Wang, X. Li
- ORGN 435.** Self-assembly salen complexes utilizing π -related interactions for efficient cooperative catalysis. **T. Imahori**, K. Tsunogaya, K. Suzuki
- ORGN 436.** Effect of electron demand on sensing behavior of carbazolopyridinophanes. **G. Abban**, A.B. Brown
- ORGN 437.** Effect of bridge length on sensing behavior of carbazolopyridinophanes. M. Ramadan, D.C. Schultz, E.M. El-Sheref, G.S. Blaustein, **A.B. Brown**
- ORGN 438.** Cage with intrinsic microporosity based on pillar[5]arene organic cage. **L.E. Khalil Cruz**, V. Carboni, C. Maaliki, N.M. Khashab
- ORGN 439.** Cucurbit[8]uril and perylene-based red-NIR host-guest complexes for detection of drugs in urine sample. **G. Aryal**, L. Huang, K.W. Hunter
- ORGN 440.** Structural effect of perylene dyes on the binding and optical properties of their complexes with Cucurbit[8]uril. **G. Aryal**, L. Huang, K.W. Hunter
- ORGN 441.** Functional thin films on plastic surfaces for applications in bacterial biosensor. **E. Hjelvik**, A. Anderson, H. Mukundan
- ORGN 442.** Design and synthesis of an enlarged M_8L_6 -metallocubes for encapsulation of nanocrystals. E. Tiernan, **J.D. Thoburn**
- ORGN 443.** Construction of nano-tube via terephthalic acid linked G-octamer. **M. Liu**, X. Shi



TECHNICAL PROGRAM

ORGN 444. Synthesis of diazaperopyrenium dication as a guest in a switchable molecular cage. **Z.M. Preyer**, H. Jacquot de Rouville, R. Djemili, S. Durot, V. Heitz

Section A

Orange County Convention Center
West Hall C

Physical Organic Chemistry: Calculations, Mechanisms, Photochemistry & High-Energy Species

E. C. McLaughlin, *Organizer*

5:30 - 7:30

ORGN 445. Structure-signal relationship investigations of an efficient chemosensor for fluoride anions: 2-, 3- and 4-amino analogues of a hydroxyaromatic 1,2,3-triazolyl scaffold. **U.T. Ofulue**, R. Govan, V. Hernandez, A. Ugboya, D. Ghosh, S.M. Landge, K.S. Aiken

ORGN 446. Computational study of substituent effects on the intramolecular cyclization of benzaldehyde oxime ethers containing a thiophene or furan group. **A.M. Abiad**, A.S. Petit, J. Gillette, D. Torres

ORGN 447. How does varying levels of DMSO change the -OH peak in ethanol containing chemicals? **P. Tamilselvan**, R.E. Rosenberg

ORGN 448. Heavy-atom tunneling in planar bond shifting of [16]annulene. **P.P. Lampkin, j. shezaf**, C. Michel, C. Castro, W.L. Karney

ORGN 449. Pyrolysis of biodiesel: Density functional theory investigations into thermal decomposition of methyl linoleate. **M. Bakker**, M.R. Siebert

ORGN 450. Structural effects on the temperature dependence of primary kinetic isotope effects in hydride transfer reactions in solution. **S. Wilhelm**, L. Ma, Y. Lu

ORGN 451. Comparison of the tunneling-ready-state electronic structures in hydride versus deuteride transfer reaction. **M. Bai**, Y. Lu

ORGN 452. Mechanistic study of photocatalytic [2+2] cycloaddition of α,β -unsaturated ketones. **K. Kuan**, D.A. Singleton

ORGN 453. Advances in the development of organic active materials for grid-scale energy storage. **M.E. Cook**, M.S. Sanford

ORGN 454. Oxidation kinetics of porphyrin-manganese(IV)-oxo intermediates generated by chemical and photochemical methods. **S.E. Klaine**, M. Winchester, R. Zhang

ORGN 455. Efficient chemoselective oxidations of sulfides catalyzed by manganese corrole with iodobenzene diacetate. D. Ranburger, B. Willis, B. Kash, **C. Alcantar**, R. Zhang

ORGN 456. Synthesis and spectroscopy of 2,5-diphenyl-3,4-diarylcyclopentadienones. **A.J. Orozco**, **H. Ruiz**, **R.A. Isovitsch**



TECHNICAL PROGRAM

ORGN 457. Computational investigation of the cyclization of benzaldehyde oxime ether radical cation intermediates containing a thiophene or furan group. **J.K. Gillette**, C. Taylor, A.M. Abiad, D. Torres, P. De Lijser, A.S. Petit

ORGN 458. Iptycenyly effect: Primary vs. secondary stereoelectronic bias of bridged bicyclic molecular skeleton. **H. Kim**, T. Kang, D. Lee

ORGN 459. Continuing puzzle of the mechanism of phenylchlorocarbene addition to dibenzocyclooctyne. **K.K. Glaser**, **S.K. Rana**, **S. Simpson**, A. Nadeem, Y. Saperstein, A. Urquilla, D.C. Merrer

ORGN 460. Aqueous kinetics of α -hydroxyhippuric acid derivatives as a function of pH, buffer and metal-ion concentration. **M.I. Rafie**, K.A. Feken, R.W. Nagorski

ORGN 461. *Para*-sulfonamide analogue of green fluorescent protein chromophore: Excited-state proton transfer. Y. Chen, R. Sung, **K. Sung**

ORGN 462. Stabilizing effects in the photochlorination and photobromination of haloalkanes. **N. Mielke**, **M. LaPorte**

ORGN 463. Evaluation of the alkylating potential of glyoxal and ethyl carbamate: A kinetic study. **E. Monge-Fernandez**, I.F. Cespedes-Camacho

ORGN 464. Mechanistic study of oxime ligation via *in situ* oxidation of *N*-phenylglycinylyl peptides. **J.B. Lumpan**, C. Proulx

ORGN 465. Generation of solid-state, efficient emitters based on 6-membered ring Excited State Intramolecular Proton Transfer (ESPIIT) systems. **E. Hermosillo Guzman**, T. Pariat, A. De Nicola, G. Ulrich

WEDNESDAY MORNING

Section A

Orange County Convention Center
Room W230A

New Reactions & Methodology

S. M. Silverman, *Organizer*
Z. Liu, *Presiding*

8:20 ORGN 466. Heterocyclic phosphonium salts as new reagents for medicinal chemistry. **D. Ryan**

8:40 ORGN 467. Diversification of allenyl esters: α -Selective reactions leading to products containing all-carbon quaternary centers. S. Maki, S. Jana, **S.D. Lepore**

9:00 ORGN 468. Synthesis of biodiesel fuel from waste cooking oil using nano-reactors. **A. Azieva**, N.N. Shaw

9:20 ORGN 469. Esterification of carboxylic acids for analysis via gas chromatography. **E.B. Vaughan**, N.N. Shaw



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

9:40 ORGN 470. Transition metal-free direct dehydrogenative arylation of activated C(sp³)-H bonds: Synthetic ambit and DFT reactivity predictions. **K.A. Lovato**, L. Guo, Q. Xu, F. Liu, M. Yousufuddin, D.H. Ess, L. Kürti, H. Gao

10:00 ORGN 471. Hypervalency aided route to 3,3,3-trifluoropropenylated heterocycles, 1,2-diamines and *N*-aryl-2-(trifluoromethyl)aziridines. **Á. Mészáros**, A. Székely, F. Béke, Á. Tóth, J. Csenki, A. Stirling, Z. Novák

10:20 ORGN 472. Nickel-catalyzed intermolecular alkene carboacylation via activation of amide C-N bonds. **A.A. Kadam**, T. Metz, L.M. Stanley

10:40 ORGN 473. Cesium base promoted alkylations: Mild & efficient synthesis of carbon-heteroatom bonds and synthetic applications. **R.N. Salvatore**

11:00 ORGN 474. Stereoselective synthesis of *O*-vinyl oximes using dialkyl acetylenic ester as efficient Michael acceptor through microwave irradiation. **V. Srivastava**, A. Mishra

11:20 ORGN 475. [4+3] Cycloaddition reactions of 3-alkenyl indoles. **F. Taenzler**, J. Xu, V.H. Rawal

11:40 ORGN 476. Synthesis of bioactive heterocycles by tandem Pd(II) catalysis: A platform for diversity oriented synthesis. **A.J. Ansari**, D. Sawant

Section B

Orange County Convention Center
Room W230B

Total Synthesis of Complex Molecules

S. M. Silverman, *Organizer*
N. Choy, *Presiding*

8:20 ORGN 477. Synthesis-enabled stereochemical assignment of the C1-C28 region of hemicalide: A potent cytotoxic polyketide of marine sponge origin. **N.Y. Lam**, B. Han, C. MacGregor, J.M. Goodman, I. Paterson

8:40 ORGN 478. Designed analogues of the aplyronines for next-generation antibody-drug conjugates. **R. Porter**, T. Pettigrew, I. Paterson, D.R. Spring, **J. Parker**

9:00 ORGN 479. Early process route to fungicide DAS-087. **N. Choy**, F. Li, G.T. Whiteker

9:20 ORGN 480. Synthesis of derhodinosylurdamycin A analogues bearing diverse 2-deoxy sugar subunits. **P. Acharya**, H. Khatri, S. Janda, J. Zhu

9:40 ORGN 481. Copper-mediated conjugate addition approach to aconitine analogues. **N.A. Doering**, K.G. Kou, K. Norseeda, J.C. Lee, C. Marth, G.M. Gallego, R. Sarpong

10:00 ORGN 482. Efficient strategies for the synthesis of complex antibody-drug conjugate payloads. **J. Parker**

10:20 ORGN 483. Towards the total synthesis of rishirilide A. **R. Ragbirsingh**



TECHNICAL PROGRAM

10:40 ORGN 484. Submonomer-based approach towards Piperazic acid (Piz) natural products: The total synthesis of L-156,373. **Y.M. Elbatrawi**, C. Kang, J.R. Del Valle

11:00 ORGN 485. Total synthesis of the baulamycins. **J. Thielman**, R.M. Williams

Section C

Orange County Convention Center
Room W230C

Heterocycles & Aromatics

S. M. Silverman, *Organizer*
J. Cole, *Presiding*

8:00 ORGN 486. Synthesis of novel, pharmaceutically relevant fluorinated amines. **P. Mykhailiuk**, O.O. Stepaniuk

8:20 ORGN 487. Behind the worm therapy. **Y. Zhang**, M. Manohar, F.J. Tenjo, F. Schroeder

8:40 ORGN 488. Anion-pool-driven selective functionalization of indazole. **M.M. Dissanayake**, A.K. Vannucci

9:00 ORGN 489. Developing green synthesis of quinazoline, quinazolin-4-one, and benzoxazole derivatives by microwave and electrochemical reactions. **Y. Huang**

9:20 ORGN 490. Pseudo five-component reaction towards densely functionalized spiro[indole-3,2'-pyrrole] by an efficient *syn* diastereoselective catalyst - picric acid: An insight to the diastereoselection on C(sp³)-C(sp³) axial conformation. A. Sengupta, A. Mondal, S. Maity, P. Ghosh, **S. Rudra**, C. Mukhopadhyay

9:40 ORGN 491. Zeolite-catalyzed synthesis of novel imidazolone: Coumarin Schiff bases and their characterization, antiinflammatory, analgesic, anticancer, antioxidant, and antimicrobial studies. **N. Prameela Subhashini**

10:00 ORGN 492. Applications of multi-component reaction chemistry in heterocyclic synthesis. **M. Konstantinidou**, S. Kurhade, F. Sutanto, K. Kurpiewska, J. Kalinowska-Tluscik, A. Doemling

10:20 ORGN 493. Isomerically pure indophenines: Teaching an old dog new tricks. **T.M. Pappenfus**, A.J. Helmin, W.D. Wilcox, D.E. Janzen

10:40 ORGN 494. Angled isomers of linear aromatic diimides. **D.D. Cao**

11:00 ORGN 495. Synthesis and SAR investigation of insecticidal *N*-(2-(pyridinyl-3-yl) thiazole-5-yl) amides. **N.V. Garizi**, A. Buysse, T.K. Trullinger, J.D. Eckelbarger, M.C. Yap

11:20 ORGN 496. Photochemistry of pyridazine *N*-oxides: A versatile tool for heterocycle synthesis. **M. Borger**, J. Frederich

11:40 ORGN 497. Heterocycles for switching GPCR ligand conformation and activity. **D. Fairlie**, **R. Reid**, J. Rowley, K. Wu, M. Yau, J. Lim, A. Iyer

Section D



TECHNICAL PROGRAM

Orange County Convention Center
West Hall F3

Biologically Related Molecules & Processes

S. M. Silverman, *Organizer*
R. Rafferty, *Presiding*

8:20 ORGN 498. Origin of high cyclopropanation stereoselectivity by myoglobin-based carbene transfer biocatalyst. Y. Wei, Y. Zhang

8:40 ORGN 499. Scalable synthesis of enantiomerically pure 5-substituted-piperazine-2-acetic acid esters as building blocks for library production. I.O. Raji, P. Jain, B. Ebright, S. Chamakuri, K.R. MacKenzie, C. Santini, D.W. Young

9:00 ORGN 500. Studies toward total synthesis of enantiopure hydnocarpin D. P.S. Rajaram, A.S. Rivera, Q. Chen

9:20 ORGN 501. Insights into rigidity-activity relationships in bisQAC amphiphilic antiseptics. R. Kontos, K.P. Minbiole

9:40 ORGN 502. 4-*N*-alkyl gemcitabine analogues with NOTA chelators for 68-gallium labelling. M. de Cabrera, J.E. Pulido, A. Amor-Coarasa, A. McGoron, S.F. Wnuk

10:00 ORGN 503. Novel metal-chelating and stimuli-responsive peptoid oligomers. Y. Minko, J.G. Schmidt, C.E. Strauss, R.F. Williams

10:20 ORGN 504. Exploiting synthesis inherent in total synthesis campaigns: New avenues for bioactive agent discovery. R. Rafferty

10:40 ORGN 505. Exploring the spatial effects of charge upon porin-mediated gram-negative bacteria transport. R. Rafferty

Section E

Orange County Convention Center
West Hall F4

Earle B. Barnes Award for Leadership in Chemical Research Management

J. Aube, *Organizer, Presiding*

8:00 ORGN 506. Increasing global access to health care through process intensification. F. Gupton

8:45 ORGN 507. Novel approaches in the design of CNS drug candidates and PET ligands. A. Villalobos, X.J. Hou, P.R. Verhoest, T. Wagner, L. Zhang

9:30 ORGN 508. Flow chemistry for greener and more efficient API synthesis. J. Hawkins

10:15 ORGN 509. Peering into the microbial world with chemistry. L.L. Kiessling



TECHNICAL PROGRAM

11:00 ORGN 510. Award Address (Earle B. Barnes Award for Leadership in Chemical Research Management sponsored by The Dow Chemical Company Foundation). Reflections on 31 years of collaboration and innovation in the pharmaceutical industry. **S.E. Kelly**

WEDNESDAY AFTERNOON

Section A

Orange County Convention Center
Room W230A

New Reactions & Methodology

S. M. Silverman, *Organizer*
D. Weingarten, *Presiding*

1:00 ORGN 511. Metal-free C-C bond cleavage of cholestane model aldehydes in water. **M.A. Fernandez-Herrera, J. Hilario-Martínez, W. Delit-García, R. Zeferino-Díaz, J. Sandoval-Ramírez, G. Merino, Z. Jin**

1:20 ORGN 512. Room temperature cross-coupling of unactivated arenes and nitriles via photoactivation of π -conjugated triazenes. **A. Bugarin**

1:40 ORGN 513. Exploitation of carbamoyl radicals to create a shortcut for the synthesis of pyrroloindolines and spirooxindoles. **L. Helgueira de Andrade, V.G. Correia, M. Sanabria, M.M. Hornink, C. Guedes**

2:00 ORGN 514. Development of strategies for the application of eliminative cross-coupling to polyfunctional alkene targets. **S. Tanpure, P.R. Blakemore**

2:20 ORGN 515. Toward a general route to nanographenes *via* a [2+2+2] / cyclodehydrogenation sequence. **H. Nguyen, G.R. Kiel, T. Tilley**

2:40 ORGN 516. Purine nucleosides with reactive β -halovinyl, β -aminovinyl and β -keto sulfones at C8 and C2 positions. **A. Howlader, S.H. Suzol, K. Blanco, M. Pasteris, S.F. Wnuk**

3:00 ORGN 517. Base-catalyzed stereospecific isomerization of electron-deficient allylic halides. **S. Martinez Erro, V. García-Vázquez, A. Sanz-Marco, B. Martín-Matute**

3:20 ORGN 518. Aryne-based multi-component coupling reactions enabled by silver-catalyzed addition of isonitriles. **S. Ghorai, D. Lee**

3:40 ORGN 519. Exploration of amide bond coupling in nano-reactors. **K. Machen, N.N. Shaw**

4:00 ORGN 520. Future of computer-aided synthesis design technology for organic synthetic chemistry. **J. Taylor, O. Ravitz**

4:20 ORGN 521. Titrimetric study of used cooking oil and biodiesel fuel. **C. McCall, N.N. Shaw**

Section B



TECHNICAL PROGRAM

Orange County Convention Center
Room W230B

Asymmetric Reactions & Syntheses

S. M. Silverman, *Organizer*
Z. Chen, *Presiding*

1:00 ORGN 522. Interlocked catalysts for asymmetric organocatalysis. **J. Niemeyer**

1:20 ORGN 523. Organocatalytic enantioselective synthesis of functionalized decalins *via* desymmetrization of substituted dihydropyrans and 1,3-diketones. **R. Aher**, P. Chouthaiwale, F. Tanaka

1:40 ORGN 524. Chiral building blocks *via* Lewis base-silicon complexes. **C. Reep**, n. takenaka

2:00 ORGN 525. Asymmetric alkylation reaction of glycine derivatives catalyzed by core-corona polymer microsphere-supported cinchonidium salt. **M. Ullah**, N.T. Thao, T. Sugimoto, N. Haraguchi, S. Itsuno

2:20 ORGN 526. Synthesis of phthalans *via* copper-catalyzed enantioselective cyclization/carboetherification of 2-vinylbenzyl alcohols. **D. Chen**, S.R. Chemler

2:40 ORGN 527. Iodo-arene peptides for asymmetric hypervalent iodine chemistry. **D.C. Whitehead**

3:00 ORGN 528. Enantiopurity determination of alkyl *P*-chiral compounds with $\text{Eu}(\text{hfc})_3$: The terminal methyl group signal is most enantiotopically affected. **P. Ly**, T. Tran, C. Pace, K. Nakayama

3:20 ORGN 529. Medium-sized heterocycles: Stereoselective synthesis and functionalizations. **Y. Zhao**

3:40 ORGN 530. Design principles in catalysis: Cobalt-catalyzed cycloisomerizations and *in-silico* catalyst design. **J. Riedel**

4:00 ORGN 531. Catalytic enantio- and regioselective alkynylation of pyridines. **K. Olsen**, M. Pappoppula, A. Aponick

4:20 ORGN 532. Manufacturing process development for GPR40 MK-8666: Small molecules, big challenges. **Z. Liu**

4:40 ORGN 533. Stereoselective hydrofunctionalizations and cycloisomerizations *via* Rh-catalysis. **Z. Chen**, V.M. Dong

Section C

Orange County Convention Center
Room W230C

Photoredox Chemistry

S. M. Silverman, *Organizer*
M. Ashley, *Presiding*



TECHNICAL PROGRAM

- 1:00 ORGN 534.** Multicomponent synthesis of tertiary alkylamines by photocatalytic olefin-hydroaminoalkylation. **D. Reich**, A. Trowbridge, M. Gaunt
- 1:20 ORGN 535.** Visible-light-induced radical silylation to dibenzosiloles via dehydrogenative cyclization. **C. Jiang**, C. Yang
- 1:40 ORGN 536.** Pyrenedione as a metal-free visible-light photocatalyst for aerobic alkylation and epoxidation. **Y. Zhang**, J. Wu, D. Huang
- 2:00 ORGN 537.** Mild ketyl radical generation via atom transfer catalysis. **J. Rutherford**, S. Rafferty, D. Nagib
- 2:20 ORGN 538.** Translating organic photoredox catalyst design from polymer synthesis to new reactivity. **J. Cole**
- 2:40 ORGN 539.** Decarboxylative elimination of carboxylic acids via photoredox/ cobalt dual catalysis. **K. Cartwright**, J.A. Tunge
- 3:00 ORGN 540.** Speciation and photoexcitation of Ni-amine complexes in light-driven C-N cross coupling reactions. **M. Kudisch**, C. Lim, B. Liu, G. Miyake
- 3:20 ORGN 541.** *N*-aryl phenoxazines as strongly reducing organic photoredox catalysts. **B. McCarthy**
- 3:40 ORGN 542.** Decarboxylative sp^3 C–N coupling via dual copper/photoredox catalysis. **Y. Liang**, X. Zhang, D.W. MacMillan
- 4:00 ORGN 543.** C-N cross-coupling via photoexcitation of nickel-amine complexes. **C. Lim**, M. Kudisch, B. Liu, G. Miyake
- 4:20 ORGN 544.** Photoredox-catalyzed, site-selective α -C(sp^3)-H alkylation of primary amine derivatives. **M. Ashley**, C. Yamauchi, J.C. Chu, S. Otsuka, H. Yorimitsu, T. Rovis
- 4:40 ORGN 545.** Solar-driven photoredox catalysis: The development of the LSC photomicroreactor. **T. Noel**

Section D

Orange County Convention Center
West Hall F3

Flow Chemistry & Continuous Processes

S. M. Silverman, *Organizer*
K. K. Laali, *Presiding*

- 1:00 ORGN 546.** Machine learning meets continuous flow chemistry: Multi-objective self-optimisation. **A.D. Clayton**, A. Schweidtmann, N. Holmes, E. Bradford, A. Lapkin, R. Bourne
- 1:20 ORGN 547.** Development of increased spontaneous nucleation rates for continuous crystallization processes of organic molecules in solution. **B. Rimez**, R. Debuysschère, B. Scheid



TECHNICAL PROGRAM

- 1:40 ORGN 548.** Organocatalytic continuous flow strategies for the upgrading of biobased molecules. **R. Gérardy**, Z. Wang, J.M. Monbaliu
- 2:00 ORGN 549.** Boosting electrochemical transformations by using continuous flow. **T. Noel**
- 2:20 ORGN 550.** Continuous plug flow antisolvent crystallization using surface-energy modified substrates. **A.H. Bond**, K.A. Nordquist, K.M. Schaab
- 2:40 ORGN 551.** On-demand rapid synthesis of lomustine under continuous flow conditions. **Z. Jaman**
- 3:00 ORGN 552.** Application of continuous and semi-continuous flow methods in synthesis of active pharmaceutical intermediates in fluconazole and hydroxychloroquine. **N.S. Telang**, F. Gupton, S. Amir, H. Mangunuru, P. Tosso, B. Desai
- 3:20 ORGN 553.** Organocatalyzed atom transfer radical polymerization in continuous photo-flow reactors. **B. Buss**, G. Miyake
- 3:40 ORGN 554.** Renaissance of the Heumann indigo process. **C. Crifar**, F. Dücker, s. Nguyen, v. kairouz, W. Lubell

WEDNESDAY EVENING

Section A

Orange County Convention Center
West Hall C

Asymmetric Reactions & Syntheses

Cosponsored by MEDI⁺
E. C. McLaughlin, *Organizer*

7:00 - 9:00

- ORGN 555.** Developing atroposelective syntheses to access diverse pharmaceutically relevant scaffolds. **M.M. Cardenas**, A.N. Sanchez, C.J. Robinson, M.A. Saputra, J.L. Gustafson
- ORGN 556.** Asymmetric synthesis of a potent CXCR7 modulator featuring a hindered tertiary β -amino amide stereocenter. D. Canterbury, F. Godin, **S. Desjardins**, M. Bayrakdarian, J. Albert, D.A. Perry, K. Hesp
- ORGN 557.** Asymmetric organocatalyzed double Michael reaction of γ , δ -unsaturated β -ketoesters with nitroalkenes generates functionalized 4-nitrocyclohexanone derivatives. **N. Fuentes**, **L. Truong**, B. Ni
- ORGN 558.** Functional peptides for enantioselective hypervalent iodine(III)-mediated chemistry. **M.L. Spritzky**, M.I. Swasy, T.R. Lex, D.C. Whitehead
- ORGN 559.** Multifunctional, MAP-based catalytic systems for cascade reactions and hybrid catalysis. **S.S. Eliseenko**, F. Liu
- ORGN 560.** Catalytic bis(imino)pyridine iron complexes for carbene reactions of diazo compounds. **B. Wang**, **I. Howard**, Y. Deng



TECHNICAL PROGRAM

- ORGN 561.** Co-catalyzed hydroacylation of cyclic aldehydes to afford bicyclic ring systems. **J. PARK**, J. Riedel, V.M. Dong
- ORGN 562.** Planar chiral palladacycle precatalysts for asymmetric catalysis. C.J. Richards, **R.A. Arthurs**
- ORGN 563.** Highly enantioselective chiral copper(I)-catalyzed [3 + 3]-cycloaddition reactions of enoldiazosulfones with nitrones. F.G. Gouany, **K. Marichev**, M. Doyle
- ORGN 564.** Diversity-oriented synthesis of substituted 5-oxo-5H-chromeno[3,4-c]pyridine-1-carbonitriles. **S. Ahmed**
- ORGN 565.** Catalytic, asymmetric synthesis of chiral aryl esters from ketenes and allyl aryl ethers. **N. Kerrigan**, A. Ibrahim
- ORGN 566.** Studies toward a general and enantioselective synthesis of 2-substituted and 2,3-disubstituted azetidines using organocatalysis. **K.J. Ruud**, **M.C. O'Reilly**
- ORGN 567.** Asymmetric synthesis of enolizable alpha-azido aldehydes from sulfonyl epoxides: Challenges and opportunities. **A. Anderson**, S.K. Allen, T.C. Coombs
- ORGN 568.** Total synthesis of (+)-DMDP and (+)-hyacinthacine A2. **Y. Jung**, S. Park, J. Jung, Y. Kim
- ORGN 569.** Installation of contiguous chiral centers in Mukaiyama-Michael reactions. **Q.T. Waulters**, H. Subramanian, S. Adachi, M.P. Sibi
- ORGN 570.** Stereoselective multicomponent couplings of conjugated aldehydes. **H. Bauer**, S. Luesse
- ORGN 571.** Asymmetric synthesis of ROCK inhibitor, netarsudil: A new therapeutic for open-angle glaucoma. **J.M. Sturdivant**, M.A. DeLong
- ORGN 572.** Synthesis, characterization, and biological activity of novel carvacrol derivatives as possible agrochemicals. **K. Reyes Colon**, C. Otero-Vélez, P. Ortiz, T. Díaz, C. Fontánez, G. Galarza, Y. Delgado-Reyes, A. Ríos-Ramos, C. Báez-Félix

Section A

Orange County Convention Center
West Hall C

CH Activation

Cosponsored by MEDI[†]
E. C. McLaughlin, *Organizer*

7:00 - 9:00

ORGN 573. Understanding the site-selectivity and enantioselectivity of dirhodium-catalyzed C-H functionalization. **Z. Ren**, W. Liu, J. Fu, J. Musaev, H.M. Davies

ORGN 574. Site- and stereoselective functionalization of piperidine derivatives. **W. Liu**, T. Babl, O. Reiser, H.M. Davies



TECHNICAL PROGRAM

ORGN 575. *In situ* kinetic studies to develop rhodium-catalyzed cyclopropanation with extremely high catalyst turnover number. **B. Wei, P. Lin**, S. Wilkerson-Hill, D. Hill, D. Blackmond, H.M. Davies

ORGN 576. Single-operation, palladium-catalysed C(sp³)-H functionalisation of tertiary aldehydes: Investigations into transient imine directing groups. **S. St John-Campbell**, A.J. White, J.A. Bull

ORGN 577. Formation of aminocyclopentadienes from silyldihydropyridines: Ring contractions driven by anion stabilization. **M. Walker**, S. Chen, B.Q. Mercado, K.N. Houk, J.A. Ellman

ORGN 578. Electrochemically enabled copper-catalyzed C-H amination using electricity as an oxidant. **K. Suppan**

ORGN 579. New ligand design for C (SP³) H activation and boron-templated, acid-catalyzed cyclization of allylic alcohols to form 1, 3 diols. **K. Forson**

ORGN 580. Process development of febuxostat using palladium- and copper-catalyzed C-H arylation. **M. Komiyama**, H. Tsuchiya, M. Teramoto, N. Yajima, M. Kurokawa, K. Minamizono, N. Tsuchiya, Y. Kato, Y. Sato, M. Dohi

ORGN 581. One-step approach to generate annulated indoles through a palladium-catalyzed norbornene-mediated cascade reaction. **Y. Gao**, J. Li, X. Qi, C. Jiang

ORGN 582. Aromatization reaction from nitrones with MBH adducts via two different pathways. **S. Han**

ORGN 583. Chelation-assisted decarboxylative C-N bond formation. **K. Das**, P. Kilaru, S. Acharya, P. Zhao

ORGN 584. Catalytic 3,3'-bis-functionalization of BINOLs and biphenols. **H.H. Nguyen**, Y. Hua, P. Asgari, J. Jeon

ORGN 585. Functionalization of allylamines via carbon dioxide directed C-H activation. **J. Maxwell**, M. Kapoor, M.C. Young

ORGN 586. Oxidative Mannich reactions using Cu(II) 2-quinoxalinol salen catalyst and tert-butyl hydroperoxide. **C. Black**, A.E. Gorden

ORGN 587. Cp*Co^{III}-catalyzed C-C and C-N bond forming reactions through directed hydroarylation and amidation protocol: A route towards direct access of important heterocycles. **S.S. BERA**

ORGN 588. Development of radical decarboxylative nitration and oximation of carboxylic acids via redox activating NHPI esters. **S. Lee, M. Fellows**, N. Boaz

ORGN 589. General solution to amine and heterocycle poisoning during C-H alkenylation, arylation, and carbonylation using thioether-palladium catalysis. **L. Wang**, B.P. Carrow

ORGN 590. Role of solvent, ligand, and oxidant in reactivity and selectivity in platinum-catalyzed C-H functionalization. **N. Laloo**, M.S. Sanford

Section A

Orange County Convention Center
West Hall C

Heterocycles & Aromatics



TECHNICAL PROGRAM

Cosponsored by MEDI⁺
E. C. McLaughlin, *Organizer*

7:00 - 9:00

ORGN 591. Facile approach to polycyclic 3-unsubstituted tetrahydroisoquinolonic acid. **M. Alturki**, R. Clark, J. Deruiter, F. Smith

ORGN 592. Novel arrangement of a 3-(oxiran-2-yl)prop-2-enamide to a 2-amino furan rifamycin derivative. **K.D. Combrink**

ORGN 593. AgTFA-catalyzed ketonization and intramolecular aldol condensation of ortho-alkynylarylketones for the synthesis of β -naphthols and naphtho[2,3-*B*]furan-2(3*H*)-one: Toward the synthesis of negundin A. **P. Nimnual**, K. Norseeda, B. Akkachairin, J. Tummatorn, P. Laohapaisan, N. Supantanapong, P. Chuangsoongnern, C. Thongsornkleeb, S. Ruchirawat, S. Sittihan, W. Rodphon

ORGN 594. Strategies toward the synthesis of Juliet blue. **B. Dawson**, N. Cross, B. Thomas, G.D. Smith, V.J. Chen, A.M. Wilson

ORGN 595. Cycloaddition reactions of vinyl-dihydroisoquinolines for the synthesis of complex alkaloids. **A.N. Specht**, G. Moura-Letts

ORGN 596. Synthesis of photoswitchable azobenzene-based derivative with potential biological activity. **N.A. Al-Sulaiti**

ORGN 597. Intramolecular hydroalkylation of *in situ*-generated *bis*-homoallylic chiral piperazinonates. **A. Moreno**, T.K. Beng, B. Mankser, C. Gordner

ORGN 598. Solvatochromic behavior of a sterically hindered 4-aminonaphthalimide dye. **A.A. Pollock**, **H.A. Huther**, D.E. Lewis

ORGN 599. Development of carbon-carbon bond formation reactions: Multicomponent coupling reactions in heterocycles synthesis. **F. Guo**, D. Parker, S. Bass, B. Tania

ORGN 600. Synthesis of dibromoindigo isomers via a biosynthetic pathway. **S. Nahhas**, A.M. Wilson, G.D. Smith, V.J. Chen

ORGN 601. Enantioselective synthesis of *gem*-disubstituted *N*-Boc diazaheterocycles via decarboxylative asymmetric allylic alkylation. **A. Sun**, B.M. Stoltz

ORGN 602. Preparation of isomeric 3-bromopropanol capped oligoviologens. **M.E. Molina**, E.B. Smith, M. Chapman, B. Tase, S. Dane, O. Morgan, R.J. Morgan

ORGN 603. Development of an asymmetric zinc phthalocyanine as a NIR fluorescent probe for EGFR. **G. Ducharme**, E.E. Nesterov

ORGN 604. Synthesis of indole derivatives from 2-alkenylanilines utilizing an oxidation-transannulation-elimination sequence. **R. Chapman**, J.R. King, C.J. Monceaux

ORGN 605. Microwave-promoted synthesis of 2,4-diamido-5-aminooxazoles. **J.S. Benner**, A. Purohit, A. Cottingham, S.A. Habay



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- ORGN 606.** Development of a rapid synthesis of highly substituted oxazoles. **A. Purohit**, J.S. Benner, A. Cottingham, J. Miller, G. Falcone, S.A. Habay
- ORGN 607.** Effects of an amide group on a multicomponent synthesis of highly substituted oxazoles. **A.L. Cottingham**, A. Purohit, J.S. Benner, J. Miller, G. Falcone, S.A. Habay
- ORGN 608.** Sulfur-monoxide transfer from a 4,5-disubstituted fluorene trisulfide-2-oxide. **C. Prior**, R. Grainger
- ORGN 609.** Orthogonal biolabeling using modified SNO- OCTs with tunable alkyne polarizability. **A.S. Mat Lani**, J.M. Schomaker
- ORGN 610.** Synthesis of alkyl-chain linked carbohydrate-porphyrin conjugates. **C.F. Dixon**, D.V. Shchirov, N.L. Snyder, J.V. Ruppel
- ORGN 611.** Synthesis of porphyrin- and bacteriochlorin-based glycoconjugates using an azide-alkyne 1,3 dipolar cycloaddition reaction. **M. Parris**, M.C. Bennion, D.G. Dennis, M.B. Burch, A. Henderson, M.E. Lech, J.E. Cuadra, N. Fendler, A. Strasser, N.L. Snyder, J.V. Ruppel
- ORGN 612.** Synthesis of anti-MRSA marine natural products. **S.K. Bruffy**, C.E. Parks, T.L. Suyama
- ORGN 613.** Reactions of homophthalic anhydride with Michael acceptors. **G. Wodarczyk**, **M. Epley**, L.M. Bradley, D.A. Hunt
- ORGN 614.** Synthesis of quinazoline and quinazolin-4-one derivatives in green pathway: Utilizing microwave and electrochemical reactions. **K. Mo**, **Y. Huang**
- ORGN 615.** Pentacene-fused porphyrin dimer exhibiting high stability and solubility. **Y. Hu**, W. Webre, F. D'Souza, H. Wang
- ORGN 616.** Dicationic cyclic ionic liquids for energy applications. **C. Do-Thanh**, B. Prasad Thapaliya, I. Popovs, S. Dai
- ORGN 617.** Synthesis of functionalized polypyridyl ligands using Suzuki coupling. **J. Stash**, J.J. Paul
- ORGN 618.** Synthesis of 5-oxa-2-aza-spiro[3.4]octane: Duality novelty/nightmare. **S. Mayer**
- ORGN 619.** Synthesis and metalation of internally alkylated porphyrinoids. **T.D. Lash**, A.N. Latham
- ORGN 620.** Synthesis of alkoxybenzporphyrins and related benzporphyrin dimers. **R.A. Tomlovich**, T.D. Lash
- ORGN 621.** Efficient aza-Michael additions to tricarbonyl(tropone)iron enabling the synthesis of an unprecedented bridged azapolycycle. **D. Griffith**, Z. Huang, Z. Phelan
- ORGN 622.** Synthesis and functionalization of BODIPY dyes using TMS-nucleophiles. **A. Merriweather**, M. Wang, G. Zhang, G. Vicente
- ORGN 623.** Oxone as an effective reagent for 2-(alkylthio)pyrimidine oxidation. **A.S. Bunev**
- ORGN 624.** Progress towards the synthesis and chemistry of 2-sulfobenzoyldiaziridines. **C. Mitzel**, S.M. Bonser



TECHNICAL PROGRAM

ORGN 625. Mild and efficient synthesis of phosphanecarbodithioates via a three-component coupling reaction of a phosphine, carbon disulfide, and an alkyl halide. **M.O. Ikhane**, H.J. Danboyi, L.E. Victorio, M.E. Steury, R.N. Salvatore

ORGN 626. Rapid and efficient method for the reduction of quinoxalines using LiBH_4 and CH_3I : Synthesis of 1, 2, 3, 4-tetrahydroquinoxalines. **R.W. Roberts**, T.E. Gavin, R.N. Salvatore

ORGN 627. Efforts toward the synthesis of 3,4-dihydroxyphenylacetaldehyde (DOPAL): A potential endogenous neurotoxin that may play a role in the development of Parkinson's disease. **D. Huber**, T. Scheffler, N. Schofield, J. Deslauriers, J.R. Hobby, T.E. Gavin, **R.N. Salvatore**

ORGN 628. Purification of flavone derivatives: 3-hydroxy-2-phenylchrom-4-one via Algar-Flynn-Oyamada reaction. C. Kelley, **Z. Poulos**, E. Chong Ng

ORGN 629. Straightforward general-purpose synthesis of regioisomerically pure type I porphyrin isomers. **M. Kielmann**, M. Roucan, S. Connon, M.O. Senge

ORGN 630. First stable α -lactam with a secondary alkyl substituent in position three. **M. Fitzsimmons**, M. Benitez, Y. Wang, I. Lengyel, V.O. Cesare

ORGN 631. DAST-mediated preparation of *N*-substituted 3-alkoxyisoindolinones. **F.A. Luzzio**, J.M. Ronnebaum

ORGN 632. Novel design and preparation of an triazole-based axial chiral P,N-ligand. **J. Wang**, X. Shi

ORGN 633. Synthesis and functionalization of novel heterocyclic compounds from [3+3]-cycloadditions for biological activity screening. **E.S. Garza-Herrera**, K. Marichev, M. Doyle

ORGN 634. Synthesis of functionalized γ -thiolactones via xanthate-mediation for potential polymerization and gold nanoparticles stabilization. **X. Xhani**

Section A

Orange County Convention Center
West Hall C

Peptides, Proteins & Amino Acids

Cosponsored by MEDI⁺
E. C. McLaughlin, *Organizer*

7:00 - 9:00

ORGN 635. Synthesis of computationally derived ERK2 substrates to probe kinase activity during oxidative stress. **W.A. LeFever**, A.J. Wommack, O.P. Tornow

ORGN 636. Synthesis of carbetocin using photochemical cyclization conditions. **J. O'Brien**, H.L. Dixon, O.P. Tornow, E.J. Barksdale, L. Werner, M.C. Srougi, A.J. Wommack

ORGN 637. Site-selective chemical protein modification *via* Umpolung catalysis. **L.M. Gooch**, M. Fascione



TECHNICAL PROGRAM

- ORGN 638.** New evidence for the mechanism of Strecker synthesis with ketones as substrates. W. Li, **X. Song**, I.J. Posey, A. Mondie
- ORGN 639.** Synthesis of enantiopure ϵ -oxapipecolic acid. **E. Howard**, C. Kang, J.R. Del Valle
- ORGN 640.** Zwitterionic methacrylate cross-linkers from peptide coupling of serine derivatives. **M. Chakraborty**, J.M. Scott, K.V. Waynant
- ORGN 641.** Novel resin for chemical protein synthesis. **T. Siegford**, J. Weidmann, P. Dawson, K.V. Waynant, D.A. Thompson
- ORGN 642.** Synthetic enzyme design by computational studies. **J. Parkman**, M. Kinghorn, G. Valdivia, J. Tretbar, M. Campbell, D.J. Michaelis
- ORGN 643.** Disulfide rich peptides: Automating optimized syntheses and regioselective formation of disulfide bonds. **E. Denton**, J.R. Bickler
- ORGN 644.** Screening and characterization of C-C bond forming reactions catalyzed by promiscuous biocatalysts in non-aqueous media. **M.P. Patel**, N.T. Green, J.K. Burch, K.A. Kew, **R.M. Hughes**
- ORGN 645.** Progress towards a peptoid siderophore analogue. **D.O. Baumann**, R.F. Williams, J.C. Gordon
- ORGN 646.** Exploring the impact of backbone N-heteroatom substitution. **M.P. Sarnowski**
- ORGN 647.** N-amino peptide macrocycles as constrained α -helices. **B.M. Rathman**, C. Solanilla, J.R. Del Valle
- ORGN 648.** Synthesis and computational studies of peptidomimetics as potential anticancer agents. R.N. Salvatore, **A.J. Todman**, **R.W. Roberts**, Q. Rossow, M.E. Steury, L.S. Kline, N. Jordan
- ORGN 649.** Design, synthesis, and evaluation peptide-based Fluorescence Resonance Energy Transfer (FRET) probes for the development of protease activity assays. **E.E. Rastede**, M.J. Lampon, E. Berthier, D.H. Appella

Section A

Orange County Convention Center
West Hall C

Total Synthesis of Complex Molecules

Cosponsored by MEDI[†]
E. C. McLaughlin, *Organizer*

7:00 - 9:00

- ORGN 650.** Total synthesis of cladosin B. **J. Kim**, K.P. Reber
- ORGN 651.** Total synthesis of a cyclopropanone-containing sesquiterpenoid. **I.W. Gilbert**, K.P. Reber
- ORGN 652.** Total synthesis of (*R*)-dihydroresorcylic acid via Pd enolate ring closure. **K. Haney**



TECHNICAL PROGRAM

ORGN 653. Total synthesis of unnatural enantiomers of bioactive C – 19 methyl substituted sarpagine/macrolin/ajmaline indole alkaloids. **K. Pandey**, M. Rahman, J.R. Deschamps, J.M. Cook

ORGN 654. Synthesis of novel ceramide analogs to target skin cancer. **A. Weather**

ORGN 655. Synthetic studies of luteoside B. **C.A. Starnbach**, J.L. Koviach-Cote

ORGN 656. General synthetic approach for the lauroxocane family of natural products. **Y. Zhang**, N. Yaw, S.A. Snyder

ORGN 657. Total synthesis of anti-MRSA calopins. **N. Thacker**, K.L. Yearty, R.W. Morrison

ORGN 658. Chemoenzymatic approaches to the total synthesis of epoxyquinol A. **M.S. Duncan**, W.B. Kline, **J.A. Collins**

ORGN 659. Protecting-group-free and unified total synthesis of nicotianasesterpenes A, B and a polygonum sesquiterpenoid. **M. Jeong**, G. Kim, H. Lee, J. Jo, S. Jeon, H. Yun

ORGN 660. Design and synthesis of new fluorescent thymidine analogues. **A. Shalamberidze**, K. Dinh, J. Ceja, G.N. Samaan, B.W. Purse

ORGN 661. Synthetic studies toward the 4-alkylideneproline natural products eleganine A and 17-nor-excelsinidine. **C.F. Cain**, J.A. Goodwin, E.H. Howard, J.R. Del Valle

ORGN 662. Asymmetric synthesis of (-)-naltrexone. **S. Dongbang**

ORGN 663. Ring contraction and formation of spironolactone during reaction of dihydrolevoglucosenone with 2-pyridyancarboxaldehyde. H. Arcure, **Z.J. Witczak**, R. Bielski, D.E. Mencer

ORGN 664. Total synthesis of tuberatulide B. **K. Maurent**, A. Corbu, S. Arseniyadis

ORGN 665. Progress towards the stereoselective total synthesis of scytophycin B. **H. Waldschmidt**, W.R. Roush

ORGN 666. Synthesis and development of a certified reference material of 18-hydroxycorticosterone. **M.L. Liu**, U. Sreenivas, I. Dilek

ORGN 667. Efforts toward the total synthesis of a cis-decalin inhibitor of Rad52: Inducing synthetic lethality in BRCA deficient cancers. **E. Hewlett**, M. Nieborowaska-Skorska, M. Abou-Gharbia, t. skorski, W. Childers

ORGN 668. Total synthesis of mansouramycins A and B. **A. Zepeda**, B. Gamez, S. Mito

ORGN 669. Strategy for sampling *cis*-pseudoguaianolide chemical space. **F. Emmetiere**, E. Bevan-Smith, A.J. Grenning

ORGN 670. Progress toward cryptomaldamide congeners. **N. Falcone**, R.B. Kinnel

ORGN 671. Toward a macrocyclic precursor of bielschowskysin. **N. Falcone**, A. Novak, D. Trauner

General Posters



TECHNICAL PROGRAM

Sponsored by MEDI, Cosponsored by ORGN[‡]

THURSDAY MORNING

Section A

Orange County Convention Center
Room W230A

New Reactions & Methodology

S. M. Silverman, *Organizer*
M. C. Young, *Presiding*

8:20 ORGN 672. Photoredox-catalyzed oxidative ortho-addition of pyridine N-oxides with alkynes. **J. Markham**, Y. Deng

8:40 ORGN 673. Efficient and complete synthesis of 3,4-dihydropyrimidin-2(1H)-ones/thiones for pharmaceutical applications using nano-reactors. **E. Finlay**, N.N. Shaw

9:00 ORGN 674. Development of the enyne Cope rearrangement for applications in complex molecule synthesis. **S. Scott**, K. White, A.J. Grenning

9:20 ORGN 675. Reagent-controlled, stereoselective aldol reaction of methyl phenylacetate. **P.B. Chanda**, P. Ramachandran

9:40 ORGN 676. Bis-heterobiaryl synthesis through phosphorus ligand-coupling. **M. Hilton**, B. Boyle, X. Zhang, J. Alegre Requena, R.S. Paton, A. McNally

10:00 ORGN 677. Cycloaddition of vinylcyclopropanes through energy transfer photocatalysis. **D. Chen**, G. Miyake

10:20 ORGN 678. Hydrofunctionalization of diene. **x. yang**

10:40 ORGN 679. Selective α -amination of ethers, alcohols, and carboxylic acids using *n*-haloimides. **S. Lulhe**, M. Gasonoo, C.D. Irving

11:00 ORGN 680. Selective functionalization of nitrogen heteroaromatics via heterocyclic phosphonium salts. **J.L. Koniarczyk**, D. Hesk, A. Overgard, I.W. Davies

11:20 ORGN 681. Synthesis of functionalized dicyclopenta[*a,d*]cyclooctene (5-8-5) ring systems via a photoinduced cycloisomerization reaction. **A.E. Salvati**, J. Frederich

11:40 ORGN 682. One-pot, multi-component assembly for synthesis of 1, 4-dihydropyridine scaffold and their bio-availability. **H.M. Patel**, M.G. Sharma

Section B



TECHNICAL PROGRAM

Orange County Convention Center
Room W230B

Total Synthesis of Complex Molecules

S. M. Silverman, *Organizer*
G. Cortez, *Presiding*

8:20 ORGN 683. Synthetic approach to the total synthesis of chimonanthine: Using a stereospecific photodecarbonylation reaction in the crystalline solid state. **J.J. Dotson**, M.A. Garcia-Garibay, N.K. Garg

8:40 ORGN 684. Total synthesis of akuammiline alkaloids. **R.B. Susick**, N.K. Garg

9:00 ORGN 685. Studies on total syntheses of tronocarpine and dippinine B. **S. Taylor**, S.M. Weinreb

9:20 ORGN 686. Synthesis and biological evaluation of spirastrellolide A analogues. **J. Manda**, B. Butler, A. Aponick

9:40 ORGN 687. Divergent approach for the rapid synthesis of picolinamide macrocycles inspired by the fungicidal natural product UK-2A. **W.H. Dent**, K. DeKorver, J. DeLorbe, R. Heemstra, C. Yao, K.G. Meyer

10:00 ORGN 688. New strategy toward icetexane natural products. **A. Amiri Naeini**, G.P. Yap, W.J. Chain

10:20 ORGN 689. Lagunamide C: Total synthesis efforts, final structural determination, and biological evaluation. **R. Rafferty**

10:40 ORGN 690. Synthetic studies for the elucidation of the paraherquamide, malbrancheamide, and brevianamide biological pathways in the *Aspergillus*, *Penicillium*, and *Malbranchea* genera. **K.R. Klas**, K. Ikeuchi, J. Sunderhaus, S. Newmister, D.H. Sherman, S. Tsukamoto, R.M. Williams

Section C

Orange County Convention Center
Room W230C

Materials, Devices & Switches

S. M. Silverman, *Organizer*
E. R. Draper, *Presiding*

8:00 ORGN 691. Reversible modulation of semiconducting performance of conjugated polymer entailing azobenzene groups in the side chains by light irradiations. **D. Zhang**

8:20 ORGN 692. Self-assembled naphthalene diimides for smart-window devices. L. Gonzalez, D. Honecker, **E.R. Draper**

8:40 ORGN 693. Design of strongly oxidizing organic photosensitizers for use in high voltage solar cell devices. **J.H. Delcamp**, R.R. Rodrigues, A. Peddapuram, H. Cheema

9:00 ORGN 694. Enhancing pyromellitic diimide electron acceptor ability through cationic core functionalization. **D.D. Cao**



TECHNICAL PROGRAM

- 9:20 ORGN 695.** Pore-forming self-assembled metal-organic complexes for thermally reversible permeabilization of cell membranes. **N.M. Khashab**
- 9:40 ORGN 696.** Suzuki approaches to quinone based diarylethene photochromes: Synthetic challenges and optical rewards. **D.G. Patel**, T.B. Mitchell, D. Carter, S.D. Myer, F.A. Novak
- 10:00 ORGN 697.** Synthesis and polymerization of diynes containing thiocyanate and thiophene end-groups en route towards polydiacetylenes. **R. DeCicco**
- 10:20 ORGN 698.** Development of a logic controlled trigger unit for self-immolative polymers. **M. Nichol**, K. Clark, J. Read de Alaniz
- 10:40 ORGN 699.** Expanding the scope of metastable photoacids into material applications. **M. Sanchez Zayas**, N. Dolinski, J.L. Self, A. Abdilla, C.J. Hawker, C.M. Bates, J. Read De Alaniz
- 11:00 ORGN 700.** Dimerization modes of graphene flakes. **M. Kertesz**, Z. Mou
- 11:20 ORGN 701.** Tuning the electronic properties of (porphinato)zinc(II)-derived supramolecular polymers by design. C. Liu, K. Liu, A. Ashcraft, J.T. Klutke, S. Steefel, **O. Jean-Hubert**
- 11:40 ORGN 702.** Gas transport through intrinsic defects of graphene sheets. **J. Roh**, H. Park

PHYS

Division of Physical Chemistry

A. McCoy, *Program Chair*

SUNDAY MORNING

Section A

Orange County Convention Center
Valencia Ballroom B-D - Theater 1

Advances in Data Collection & Analysis of Biomolecular Structures

Cosponsored by COMP
S. Lindert, S. Yang, *Organizers*
K. Sanbonmatsu, F. Tama, *Presiding*

8:00 PHYS 1. CryoFIT: User-friendly fitting of high-resolution cryo-EM reconstructions in PHENIX. D. Kim, **K. Sanbonmatsu**



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

8:35 PHYS 2. Structural characterization of an engineered adenovirus vector with cryoEM, *de novo* structure prediction, and molecular dynamics. **P. Stewart**, C. Emerson

9:10 PHYS 3. Interplay of domain dynamics and catalysis in *Escherichia coli* Prolyl-tRNA synthetase: Combined computational and experimental study. **S. Bhattacharyay**, H. Hu, M. Weinzetl, K. Weeks, S. Hati

9:30 PHYS 4. Hybrid approaches to reveal structure and dynamics of large biological complexes from single molecule experiments.. **F. Tama**

10:05 Intermission.

10:25 PHYS 5. Integrated structural biology for alpha-helical membrane protein structure determination. **J. Meiler**

11:00 PHYS 6. Refining conformational ensembles using vibrational probe group data and frequency simulations. **C.H. Londergan**, R.J. Xu, C. Fu

11:20 PHYS 7. Automated *de novo* model building in cryoEM with Pathwalking. **M.L. Baker**

Section B

Orange County Convention Center
Valencia Ballroom B-D - Theater 2

Materials & Techniques to Advance Redox Flow Batteries

Progress in Active Materials Development

F. Brushett, S. A. Odom, *Organizers*
S. Odom, *Presiding*

8:30 Introductory Remarks.

8:35 PHYS 8. Recent progress in organic-based aqueous flow batteries. **M.J. Aziz**

9:05 PHYS 9. High energy density anolyte for aqueous organic redox flow batteries. **W. Wang**

9:25 PHYS 10. Enhancing the physicochemical properties of multimetallic metal-oxide assemblies for electrochemical energy storage. L.E. VanGelder, M.A. Kosswattaarachchi, T.R. Cook, **E.M. Matson**

9:45 PHYS 11. Delivering robust, high-performance flow battery active materials using bioinspired design-principles. **P.J. Cappillino**, S. Pahari, T.C. Gokoglan, E. Agar

10:05 Intermission.

10:25 PHYS 12. Benzothiadiazole based anolyte materials for nonaqueous redox flow cells. **L. Zhang**, J. Zhang, F. Brushett, X. Wei, I.A. Shkrob



TECHNICAL PROGRAM

10:45 PHYS 13. Strategies in electrolyte design for organic redox flow batteries. G. Charlton, F. Alkhayri, S. Barbon, J.B. Gilroy, **C. Dyker**

11:05 PHYS 14. Comparative study on the chemical and cycling stabilities of redox active organic polysolutes with their voltages for non-aqueous redox flow battery applications. N.H. Attanayake, O. Harris, T. Suduwella, F. Qin, W. Eubanks, **A. Kaur**, S. Parkin, M. Tang, S. Odom

11:25 PHYS 15. Viologen redox flow batteries. **T. Liu**

Section C

Orange County Convention Center
Valencia Ballroom B-D - Theater 3

New Frontiers in the Confluence of Experimental Thermodynamics, Structural Investigations & Theory/Computation

Experimental Thermodynamics

Cosponsored by GEOC
N. Birkner, *Organizer*
K. Lilova, D. Wu, *Organizers, Presiding*
N. Birkner, *Presiding*

8:00 PHYS 16. Thermocon: An international triumvirate of experimental thermodynamics, theory/computation, and structural investigations. **K. Lilova**

8:15 PHYS 17. Are nanomaterials always metastable? **A. Navrotsky**

8:45 PHYS 18. Energetics of nanophase layer and tunnel structure manganese oxides. **N. Birkner**, M. Zhao, A. Navrotsky, K. Brinkman

9:15 PHYS 19. Structure and energy landscapes in biomineral formation. **P. Gilbert**

9:45 PHYS 20. Can thermodynamics help predicting the defect populations: Grain boundaries and oxygen vacancies, in electroceramics? **S. Guillemet-Fritsch**, P. Dufour

10:15 Intermission.

10:30 PHYS 21. Heat capacity and thermodynamic functions of loaded and unloaded zinc imidazole metal organic frameworks. J.J. Calvin, P. Rosen, Z. Akimbekov, G.S. Ayoub, A. Katsenis, A. Navrotsky, T. Friscic, **B. Woodfield**

11:00 PHYS 22. Thermodynamics - structure - performance relations of nickel - aluminum layered double hydroxide as supercapacitor electrode materials. **D. Wu**, G. Li, L. Fu, Z. Liu, B. Wang, X. Zhang, D. Qiu, J. Zhang, B. Sudduth, J. Sun, Y. Wang, X. Guo, H. Sun

11:30 PHYS 23. Thermodynamics and kinetics of heterogeneously nucleated calcium carbonate on quartz. **Y. Jun**, Q. Li

Section D



TECHNICAL PROGRAM

Orange County Convention Center
Valencia Ballroom B-D - Theater 4

Frontiers in Vibrational Spectroscopy: Experiments & Theory

Applications

E. Garand, R. Steele, *Organizers*
C. J. Johnson, *Presiding*

8:30 PHYS 24. Probe-dependent vibrational dynamics in heterogeneous mixtures. K. Oh, **C.R. Baiz**

9:05 PHYS 25. Ultra-high resolution single molecule vibrational spectroscopy in a nanoaperture optical trap. **J. Li**, C. Zhang, R. Gelfand

9:25 PHYS 26. Quantum state-resolved studies of gas/surface reaction dynamics by vibrational spectroscopies. **R.D. Beck**

9:45 Intermission.

10:05 PHYS 27. Investigation of biological electron transfer via isotopologues and resonance Raman spectroscopy. **J.E. Kim**, J. Rivera

10:40 PHYS 28. Linking molecular organization and orientation to chemical selectivity at complex liquid/liquid interfaces using vibrational sum frequency generation spectroscopy. **B. Doughty**, A.U. Chowdhury, Y. Ma

11:00 PHYS 29. Electrochemical tip enhanced Raman spectroscopy (EC-TERS): An asset for observation of molecular-scale manipulation. **V. Brasiliense**, X. Chen, R.P. Van Duyne

11:20 PHYS 30. Second-order spectral lineshapes from charged interfaces. **F. Geiger**

11:40 PHYS 31. Ultra-low frequency SERS spectroscopy for in-situ observation of electrified interfaces. **K. Ikeda**

Section E

Orange County Convention Center
Valencia Ballroom B-D - Theater 5

Quantum Embedding Electronic Structure Methods

Cosponsored by COMP
A. Wasserman, *Organizer*
M. Pavanello, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 PHYS 32. Frozen-Density Embedding Theory (FDET) based multi-level simulations for electronic structure of embedded species: approximations, procedures, and benchmarking.. **T.A. Wesolowski**



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

8:45 **PHYS 33.** What we can learn from exact embedding potentials of model systems. **Y. Oueis**, A. Wasserman

9:05 **PHYS 34.** Overlapped embedded fragment stochastic density functional theory. M. Chen, D. Neuhauser, R. Baer, **E. Rabani**

9:45 Intermission.

10:05 **PHYS 35.** Novel charge embedding scheme for Extended Symmetry-Adapted Perturbation Theory (XSAPT). **K. Liu**, K. Lao, J. Herbert

10:25 **PHYS 36.** Subsystem density-functional theory for molecular materials. A. Schulz, D. Schmitt-Monreal, **C. Jacob**

11:05 **PHYS 37.** Embedded correlated wavefunction methods based on DFT embedding with a unique embedding potential. **X. Zhang**, J.P. Martinez, E.A. Carter

Section F

Orange County Convention Center
Valencia Ballroom B-D - Theater 6

Structure & Dynamics of Electrolytes: From the Bulk to Interfaces

Electrolytes & Energy Storage

R. Jorn, R. Kumar, D. G. Kuroda, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 **PHYS 38.** Multivalent ions in aprotic solvents: “Ion solvation spectra” and their impact on thermodynamic characteristics of electrolytes. **A. Baskin**, D. Prendergast

8:55 **PHYS 39.** Electrolytes for superoxide batteries. **Y. Wu**

9:25 **PHYS 40.** Alkali metal / solid electrolyte interface. **P. Bruce**, J. Kasemchainan, S. Zekoll, D. Spencer Jolly, Z. Ning, C. Marriner-Edwards, F. Richter, G. Hartley, A. Hekselman, C. Kuss, D. Armstrong, D. Cai, R. Wallace

9:55 Intermission.

10:10 **PHYS 41.** Molecular dynamics of lithium ion transport in a model solid electrolyte interphase. A. Muraldiharan, M. Chaudhari, L.R. Pratt, **S.L. Rempe**

10:40 **PHYS 42.** Electrolytes and additives for lithium-ion batteries. **D. Abraham**

11:10 **PHYS 43.** Understanding the electrolyte concentration and the effect of solvation for Li-S batteries. **Y. Qi**, Y. Lin

11:40 **PHYS 44.** Structure and dynamics of high salt concentration electrolytes. **S. Galle Kankanamge**, D.G. Kuroda

Section G



TECHNICAL PROGRAM

Orange County Convention Center
Valencia Ballroom B-D - Theater 7

Sustainable Software for Computational Molecular Science

Interoperability & Reproducibility in the Computational Molecular Sciences

Cosponsored by COMP
E. Marin, J. A. Nash, D. G. Smith, *Organizers*
T. Crawford, *Organizer, Presiding*

8:30 Introductory remarks.

8:35 PHYS 45. Improving reproducibility of molecular simulations with reference data and open source software. **H.W. Hatch**, D.W. Siderius, V.K. Shen

9:05 PHYS 46. Detecting problems in molecular simulation outputs and preventing them to begin with. **M.R. Shirts**, P. Merz, D.L. Mobley, D.M. Zuckerman

9:35 PHYS 47. Modular and efficient interfacing of computational chemistry programs. **M.J. Frisch**

9:55 Intermission.

10:15 PHYS 48. Coupling first principle molecular dynamics and many body perturbation theory codes. **G.A. Galli**

10:45 PHYS 49. Multisite computations of electronic properties using many-body perturbation theory and interoperable software building blocks. **M. Govoni**, H. Ma, F. Gygi, G.A. Galli

11:05 PHYS 50. Challenges for software sustainability and Interoperability. **J.E. Rice**

Electron-Molecule & Molecule-Molecule Interactions

Sponsored by COMP, Cosponsored by PHYS[‡]

Interdisciplinary Chemistry for New Frontiers in Biology & Medicine

NanoBio

Sponsored by ANYL, Cosponsored by BIOL, COLL, MPPG, PHYS and PMSE[‡]

Symposium in Honor of Chuck Peden's Research Career: Catalysis for Energy & the Environment

Sponsored by CATL, Cosponsored by ENFL, ENVR, I&EC and PHYS



TECHNICAL PROGRAM

Elucidation of Mechanisms & Kinetics on Surfaces

Mechanisms on Surfaces: C-C Coupling, C-H & C-O Bond Manipulations

Sponsored by CATL, Cosponsored by ENFL, ENVR, INOR and PHYS

Advances in Methods for Comparing Molecular & Supramolecular Simulations to Experiments

Sponsored by CATL, Cosponsored by CINP, COMP and PHYS

SUNDAY AFTERNOON

Section A

Orange County Convention Center
Valencia Ballroom B-D - Theater 1

Advances in Data Collection & Analysis of Biomolecular Structures

Cosponsored by COMP
S. Lindert, S. Yang, *Organizers*
M. Buck, M. Pond, *Presiding*

1:30 PHYS 51. Advanced methods for rapid multidimensional NMR spectroscopy with applications to proteins and metabolomics. **R. Bruschweiler**

2:05 PHYS 52. Structural characterization of Hck-membrane association based on the analysis of neutron reflectometry and solution NMR data with restrained-ensemble molecular dynamics simulations. **M. Pond**, R. Eells, F. Heinrich, M. Lösche, B. Roux

2:40 PHYS 53. Effects of small amphiphilic molecules on the structure and stability of Sphingomyelin bilayer: A molecular dynamics study. **P. Kumari**, S. Kaur, S. Sharma, H.K. Kashyap

3:00 PHYS 54. Dynamic protein complexes: Perspective from NMR studies and from molecular dynamics simulations for structure determination. **M. Buck**

3:35 Intermission.

3:55 PHYS 55. Biomolecular solution scattering at the life science X-ray scattering beamline. **L. Yang**

4:30 PHYS 56. Independent component analysis of smFRET photon data for resolving conformational heterogeneity of biomolecules. **K. Ishii**, M. Sakaguchi, T. Tahara

4:50 PHYS 57. Models for liquid-liquid phase separation of disordered proteins. **W. Zheng**, G. Dignon, M. Brown, R.B. Best, Y. Kim, J. Mittal



TECHNICAL PROGRAM

Section B

Orange County Convention Center
Valencia Ballroom B-D - Theater 2

Materials & Techniques to Advance Redox Flow Batteries

Modeling & Design of Electrolyte Materials

S. A. Odom, *Organizer*
F. Brushett, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 **PHYS 58.** Continuum modeling of redox flow batteries to inform cell and material development. **K.C. Smith**, V.P. Nemani

1:55 **PHYS 59.** Rapid computational discovery of novel anolyte and catholytes with targeted redox properties. **G. Hutchison**

2:15 **PHYS 60.** Exploring chemical subtleties to foster improved materials design for redox flow batteries. **C. Risko**

2:35 Intermission.

2:55 **PHYS 61.** Property quantification for new flow-battery architectures using adaptive simulations. **C.W. Monroe**, K. Smith, P. Ascencio, D. Howey

3:15 **PHYS 62.** Bottom-up approach to superior battery materials: Refinement on the structure of redoxmers for redox flow batteries. **M.E. Cook**, M.S. Sanford

3:35 **PHYS 63.** Solving for solvation (and more!) in redox flow batteries: In situ spectroscopic methods for resolving complex, solvation-driven properties. **E.V. Carino**, J.G. Connell, N.M. Markovic, G. Crabtree

Section C

Orange County Convention Center
Valencia Ballroom B-D - Theater 3

New Frontiers in the Confluence of Experimental Thermodynamics, Structural Investigations & Theory/Computation

Experimental Thermodynamics

Cosponsored by GEOC
N. Birkner, *Organizer*
K. Lilova, D. Wu, *Organizers, Presiding*
N. Birkner, S. McCormack, *Presiding*

1:30 **PHYS 64.** Framework dopant effects in tunnel-structured hollandite waste forms for Cs-immobilization. **K. Brinkman**



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- 2:00 PHYS 65.** Energetics of formation and disordering in RE_3TaO_7 weberites. **T. Subramani**, A. Navrotsky
- 2:20 PHYS 66.** Experimental and computational thermodynamics for phase relationship. **W. Gong**
- 2:40 PHYS 67.** Thermodynamics of transition metal ion-exchanged mordenite. **X. Zhang**, Z. Huang, G. Li, X. Guo, D. Wu
- 3:00 PHYS 68.** Thermodynamic and kinetic analysis of oxyanions sorption on ferrihydrite using microcalorimetry and density functional theory. **N. Kabengi**, J.D. Kubicki, A. Namayandeh
- 3:30** Intermission.
- 3:45 PHYS 69.** Characterization and thermodynamics of a novel water filtration nanomaterial. **N. Johnson**, A. Sahu, R. Sheikh, K. Durkin, J.C. Poler
- 4:05 PHYS 70.** Novel insight into defect behavior of irradiated materials: Combined neutron total scattering and high temperature calorimetry investigation. **M. Lang**, E.C. O'Quinn, R.I. Palomares, C. Chung, A. Shelyug, J. Neufeind, A. Navrotsky
- 4:35 PHYS 71.** He irradiation-induced structural degradation, interfacial phenomena, and energetic evolution for defect-fluorite $\text{Gd}_2\text{Zr}_2\text{O}_7$ ceramics. **Z. Huang**, J. Qi, X. Guo, T. Lu, **D. Wu**
- 4:55 PHYS 72.** In-situ phase diagram determination of the HfO_2 - Ta_2O_5 binary up to 3000 C. **S. McCormack**, K. Tseng, R. Weber, S. Ushakov, D. Kapush, A. Navrotsky, W. Kriven

Section D

Orange County Convention Center
Valencia Ballroom B-D - Theater 4

Modeling Dynamics in Dense Manifolds of Electronic States

Electronic Structure

Cosponsored by COMP
B. G. Levine, P. Slavicek, *Organizers*
P. Narang, *Presiding*

- 1:30 PHYS 73.** Modeling spin-dynamics with relativistic two-component time-dependent electronic structure method. **X. Li**
- 2:10 PHYS 74.** Dynamical correlation models for variational two-electron reduced-density matrix methods. **A.E. DePrince**
- 2:50 PHYS 75.** Coherent electron dynamics in systems with a high density of states. A. Bruner, F. Mauger, A. Meyer, P. Abanador, M. Gaarde, K. Schafer, **K. Lopata**
- 3:30** Intermission.
- 3:50 PHYS 76.** Plane-wave pseudopotential formulation of real-time TDDFT: Recent progress, challenges, and application to excitation in dense manifolds. **Y. Kanai**



TECHNICAL PROGRAM

4:30 PHYS 77. Time-dependent complete active space embedded in polarizable force field. **H. Liu**, A. Jenkins, A. Wildman, M.J. Frisch, F. Lipparini, B. Mennucci, X. Li

4:50 PHYS 78. Density Functional Theory in real-time: Access to electron dynamics in light-harvesting systems. **S. Kümmel**, I. Schelter

Section E

Orange County Convention Center
Valencia Ballroom B-D - Theater 5

Quantum Embedding Electronic Structure Methods

Cosponsored by COMP
M. Pavanello, *Organizer*
A. Wasserman, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 PHYS 79. TDDFT with accurate density-based embedding. **J. Neugebauer**, M. Böckers, J. Tölle, D. Schnieders

2:15 PHYS 80. Quantum embedding for excited states in molecules and solid states: A state-averaged approach. **X. Wen**, D. Chulhai, J. Goodpaster

2:35 PHYS 81. Polarizable frozen density embedding method for molecules on metal clusters. **L. Jensen**

3:15 Intermission.

3:35 PHYS 82. Automatic partition of orbital spaces based on singular value decomposition in the context of embedding theories. **D. Chaves Claudino**, N. Mayhall

3:55 PHYS 83. Forefront dynamic methods for the condensed phase. **S. Luber**

Section F

Orange County Convention Center
Valencia Ballroom B-D - Theater 6

Structure & Dynamics of Electrolytes: From the Bulk to Interfaces

Electrolytes & Energy Storage

R. Jorn, R. Kumar, *Organizers*
D. G. Kuroda, *Organizer, Presiding*
A. L. Serrano, *Presiding*

1:30 PHYS 84. Transport in superconcentrated LiPF₆ propylene carbonate electrolytes. **K. Persson**, J. Self, K. Fong



TECHNICAL PROGRAM

2:00 PHYS 85. Molecular modeling insight into electrochemistry of battery electrolytes at bare and passivated electrodes. **T.P. Pollard**, O. Borodin, M. Schroeder, K. Xu

2:20 PHYS 86. Structural water in transition metal oxides: Effects of nanoconfinement on energy storage mechanisms and kinetics. **V. Augustyn**

2:50 PHYS 87. Nanochannel permeation by ionic solutions under electric control. **A. Luzar**

3:20 Intermission.

3:35 PHYS 88. Electrolytes at air-water and mineral-water interfaces: Structure and SFG spectroscopy by AIMD simulations. **M.P. Gaigeot**

3:55 PHYS 89. Computational vibrational spectroscopy of aqueous acid and base solutions. **S. Corcelli**

4:25 PHYS 90. Vibrational signatures of ion pairing in bulk and at interfaces with *ab initio* DFT. **M.D. Baer**

4:55 PHYS 91. Computational studies of solvation structure and dynamics of lithium salts in carbonate-based electrolytes. **X. Zhang**, D.G. Kuroda

Section G

Orange County Convention Center
Valencia Ballroom B-D - Theater 7

Sustainable Software for Computational Molecular Science

Workflows

Cosponsored by COMP
T. Crawford, E. Marin, J. A. Nash, D. G. Smith, *Organizers*
J. Nash, *Presiding*

1:30 PHYS 92. Building scalable workflows with Orion, a cloud-based platform for drug discovery. **J. LaFon**

2:00 PHYS 93. Integration via Python: Building blocks for simulation and analysis workflows for molecular dynamics. **O. Beckstein**

2:30 PHYS 94. Best in class computational drug discovery platform by integration. **A. Gobbi**, M. Lee, B.D. Sellers

3:00 PHYS 95. Is the Force with us? Automating generalizable torsions. **C.D. Stern**, D.G. Smith, C.I. Bayly, J. Chodera

3:30 Intermission.

3:50 PHYS 96. RADICAL approach to subverting RADICAL's second law of cyberinfrastructure. **S. Jha**, A. Merzky, M. Turilli

4:20 PHYS 97. Open Chemistry, JupyterLab and data: Reproducible quantum chemistry. **M.D. Hanwell**



TECHNICAL PROGRAM

4:50 PHYS 98. Building rocket propellant combustion models from scratch via automated procedures. **K.B. Moore, S.J. Klippenstein**

Electron-Molecule & Molecule-Molecule Interactions

Sponsored by COMP, Cosponsored by PHYS[‡]

Interdisciplinary Chemistry for New Frontiers in Biology & Medicine

Microbia

Sponsored by ANYL, Cosponsored by BIOL, COLL, MPPG, PHYS and PMSE[‡]

Symposium in Honor of Chuck Peden's Research Career: Catalysis for Energy & the Environment

Sponsored by CATL, Cosponsored by ENFL, ENVR, I&EC and PHYS

Elucidation of Mechanisms & Kinetics on Surfaces

Reductions & Hydrogenations

Sponsored by CATL, Cosponsored by ENFL, ENVR, INOR and PHYS

Advances in Methods for Comparing Molecular & Supramolecular Simulations to Experiments

Sponsored by CATL, Cosponsored by CINF, COMP and PHYS

MONDAY MORNING

Section A

Orange County Convention Center
Valencia Ballroom B-D - Theater 1

Advances in Data Collection & Analysis of Biomolecular Structures

Cosponsored by COMP
S. Lindert, S. Yang, *Organizers*
M. Levitus, J. Seffernick, *Presiding*



TECHNICAL PROGRAM

8:00 PHYS 99. Data processing approach to overcome insufficient signal strength in spectroscopy. M. Srivastava, **J.H. Freed**

8:35 PHYS 100. Photoinduced response of biological systems: An optimal mix of organization and disorder. **B. Mennucci**

9:10 PHYS 101. Translating data from surface-induced dissociation mass spectrometry (SID-MS) into high-resolution structures of protein complexes. **J. Seffernick**, S. Harvey, V.H. Wysocki, S. Lindert

9:30 PHYS 102. Self-assembled DNA nanostructures, biomineralization and SAXS characterization. **X. Liu**, C. Fan

10:05 Intermission.

10:25 PHYS 103. Protein oligomerization and self-assembly monitored by fluorescence correlation spectroscopy. **M. Levitus**

11:00 PHYS 104. Unveiling molecular mechanisms of Kinesin-5 function using multiscale computational techniques. **A. Davtyan**, Q. Wang, A. Kolomeisky

11:20 PHYS 105. Generalized method for designing phase masks for 3D super-resolution imaging. **C.F. Landes**

Section B

Orange County Convention Center
Valencia Ballroom B-D - Theater 2

Materials & Techniques to Advance Redox Flow Batteries

Expanding Techniques & Environments

F. Brushett, S. A. Odom, *Organizers*
J. R. McKone, *Presiding*

8:30 Introductory Remarks.

8:35 PHYS 106. Electrochemical versatility of flowable redox-active polyelectrolytes: Implications for uses beyond energy storage. E.C. Montoto, A. Rajput, M.J. Coughlan, **J. Rodriguez Lopez**

8:55 PHYS 107. Characterizing chemical redox of battery active materials. **G. Koenig**, D. Gupta

9:15 PHYS 108. What is the right way to measure flow battery kinetics? **J.R. McKone**, T.V. Sawant

9:35 PHYS 109. *Operando* Raman spectroscopy of quinone batteries. **C. Tseng**, J. Dawlaty, P. Goyal, Y. Yao

9:55 PHYS 110. In-situ technique to measure the membrane crossover rate of active ions in a redox flow battery. **T.V. Nguyen**

10:15 Intermission.



TECHNICAL PROGRAM

10:30 PHYS 111. Electrolytes to expand the range of options for flow batteries. **T. Zawodzinski**, K. Lou

10:50 PHYS 112. Nature-derived organic mesomeric electrolyte for low cost and high capacity aqueous flow battery. **A. Mukhopadhyay**, **H. Zhu**

11:10 PHYS 113. Eutectic electrolytes for high-energy-density redox flow batteries. **G. Yu**

11:30 PHYS 114. Towards the development of membrane-free redox flow batteries by using immiscible electrolytes. **R. Marcilla**, P. Navalpotro, I. Montes, J. Palma

Section C

Orange County Convention Center
Valencia Ballroom B-D - Theater 3

Frontiers in Vibrational Spectroscopy: Experiments & Theory

Thermodynamic Information from Vibrations

E. Garand, R. Steele, *Organizers*
C. R. Baiz, *Presiding*

8:00 PHYS 115. Sequential capture of O(³P) and alkenes by helium nanodroplets: Infrared spectroscopy and Ab initio computations of the triplet biradical intermediates. **G.E. Douberly**

8:35 PHYS 116. Are carbon dioxide phases III and VII actually the same phase? **G.J. Beran**

8:55 PHYS 117. Very strong Raman probe groups report on protein structural changes. **C.H. Londergan**, E.V. von Krusenstiern, N.R. John

9:15 PHYS 118. On-the-fly MCTDH: Accurate quantum dynamics for simulating electronic and vibrational spectra. G. Richings, C. Robertson, **S. Habershon**

9:50 Intermission.

10:05 PHYS 119. Vibrational manifestations of acid-base chemistry in atmospheric clusters. **C.J. Johnson**, Y. Yang, J. Kreinbihl

10:40 PHYS 120. Investigation of iron(II) phthalocyanine catalyzed oxygen reduction reaction using *operando* electrochemical tip-enhanced Raman spectroscopy. **Z. Chen**, S. Jiang, G. Kang, R.P. Van Duyne

11:00 PHYS 121. Confined molecules: Thermodynamic properties from simulations. **P. Roy**

Section D

Orange County Convention Center
Valencia Ballroom B-D - Theater 4



TECHNICAL PROGRAM

Modeling Dynamics in Dense Manifolds of Electronic States

Light-Matter Interaction

Cosponsored by COMP
B. G. Levine, P. Slavicek, *Organizers*
L. Greenman, *Presiding*

8:00 PHYS 122. Simulation of barrier suppression ionization in molecules interacting with intense laser fields. **H.B. Schlegel**

8:40 PHYS 123. Excited-state dynamics and correlated light-matter interactions from first principles. **P. Narang**

9:20 PHYS 124. Attosecond dynamics of electrons in liquids. **H.J. Woerner**

10:00 Intermission.

10:20 PHYS 125. Coherent ultrafast photoinduced coupled electronic-nuclear dynamics in dense manifolds of electronic states in molecules. **F. Remacle**

11:00 PHYS 126. Mixed quantum classical dynamics and surfaces for photons. **N.M. Hoffmann**, C. Schäfer, A. Kelly, H. Appel, N.T. Maitra, A. Rubio

11:20 PHYS 127. Attosecond coupled electron and nuclear dynamics in molecules. **F. Martin Garcia**

Section E

Orange County Convention Center
Valencia Ballroom B-D - Theater 5

Quantum Embedding Electronic Structure Methods

Cosponsored by COMP
M. Pavanello, A. Wasserman, *Organizers*
J. Goodpaster, *Presiding*

8:30 Introductory Remarks.

8:35 PHYS 128. Simplifying site occupation embedding theory further by learning from the one-particle density matrix or Green function. L. Mazouin, B. Senjean, M. Saubanère, **E. Fromager**

9:15 PHYS 129. Splitting a system into small fragments: Electron dynamics from real-time density matrix embedding theory. **J. Kretchmer**, G. Chan

9:35 Intermission.

9:55 PHYS 130. Regional DMET—Efficient and accurate single-fragment embedding of wave functions in Kohn-Sham DFT. **G. Knizia**, J.E. Klein



TECHNICAL PROGRAM

10:35 PHYS 131. Systematically improvable hierarchy of embedding approaches for the prediction of molecular properties. **D. Lambrecht**

Section F

Orange County Convention Center
Valencia Ballroom B-D - Theater 6

Structure & Dynamics of Electrolytes: From the Bulk to Interfaces

Polymer Electrolytes

D. G. Kuroda, *Organizer*
R. Jorn, R. Kumar, *Organizers, Presiding*

8:30 PHYS 132. Non-additive ion effects in mixed salt solutions. **E.E. Bruce**, P.T. Bui, B.A. Rogers, P.S. Cremer, N. van der Vegt

8:50 PHYS 133. Molecular simulations of the assembly and conformation of charged macromolecules. **S.W. Rick**

9:20 PHYS 134. Behavior of hydrated excess protons in heterogeneous electrolyte systems. **G.A. Voth**

9:50 Intermission.

10:05 PHYS 135. From single molecules to menras: molecular dynamic simulation insight into ionizable co-polymers. **D. Perahia**, D. Aryal, M. Senanayake, G.S. Grest

10:35 PHYS 136. Counterion condensation and ionic conductivity in microphase separated block copolymer electrolytes. **C.G. Arges**, Q. Lei, K. Li, R. Kumar

11:05 PHYS 137. Ohm's Law, polymer electrolytes, and lithium batteries. **N.P. Balsara**

Section G

Orange County Convention Center
Valencia Ballroom B-D - Theater 7

Sustainable Software for Computational Molecular Science

Experiences & Challenges Developing Open & Modular Software

Cosponsored by COMP
T. Crawford, J. A. Nash, D. G. Smith, *Organizers*
E. Marin, *Organizer, Presiding*

8:30 PHYS 138. MolSSI: Working together to build better software for tomorrow. **T.L. Windus**, C. Clementi, R. Harrison, T.L. Head-Gordon, S. Jha, A. Krylov, V. Panda, P. Saxe, D. Altarawy, T. Barnes, S. Ellis, E. Marin, L. Naden, J. Nash, J. Moussa, B. Pritchard, D.G. Smith, T. Crawford



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

9:00 PHYS 139. Experiences developing and maintaining Cassandra, an open source atomistic Monte Carlo simulation package. **E. Maginn**

9:30 PHYS 140. Reusable components for quantum chemistry software. **R. Di Remigio**

9:50 PHYS 141. CMakePackagingProject: Reliable, reproducible, and reusable build systems made easy. **R.M. Richard,** T.L. Windus

10:10 Intermission.

10:30 PHYS 142. How to professionally develop reusable scientific software — and when not to. C.S. Adorf, V. Ramasubramani, J. Anderson, **S.C. Glotzer**

11:00 PHYS 143. Lessons learned from developing LAMMPS. **S. Plimpton**

11:30 PHYS 144. Benevolent Dictator vs Eager Beaver: How expertise limits our perspective on user experience. **S. Dwaraknath**

ACS Award in Surface Chemistry: Symposium in Honor of Hajo Freund

Sponsored by COLL, Cosponsored by CATL[‡] and PHYS

Electron-Molecule & Molecule-Molecule Interactions

Sponsored by COMP, Cosponsored by PHYS[‡]

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Sponsored by PROF, Cosponsored by AGFD, ANYL, BIOL, BIOT, CARB, CELL, CHED, CMA, COLL, COMP, ENVR, GEOC, I&EC, MEDI, MPPG, NUCL, ORGN, PHYS, PMSE, POLY, PRES, WCC and YCC

Interdisciplinary Chemistry for New Frontiers in Biology & Medicine

Biomarker Discovery

Sponsored by ANYL, Cosponsored by BIOL, COLL, MPPG, PHYS and PMSE[‡]

Symposium in Honor of Chuck Peden's Research Career: Catalysis for Energy & the Environment



TECHNICAL PROGRAM

Sponsored by CATL, Cosponsored by ENFL, ENVR, I&EC and PHYS

ACS Award in Colloid Chemistry: Symposium in Honor of Naomi Halas

Sponsored by COLL, Cosponsored by PHYS

Recent Advances in Plasma-Enhanced Catalysis

Sponsored by CATL, Cosponsored by ENFL, ENVR and PHYS

MONDAY AFTERNOON

Section A

Orange County Convention Center
Valencia Ballroom B-D - Theater 1

Advances in Data Collection & Analysis of Biomolecular Structures

Cosponsored by COMP
S. Lindert, S. Yang, *Organizers*
M. R. Chance, T. R. Sosnick, *Presiding*

1:30 PHYS 145. Using SAXS to measure the solvent quality of water for disordered proteins as well as the collapse induced by FRET fluorophores. J.A. Riback, M.A. Bowman, A.M. Zmyslowski, K.W. Plaxco, P.L. Clark, **T.R. Sosnick**

2:05 PHYS 146. Integrative structural modeling of multidomain polo-like kinase 1. H. Ruan, J. Kiselar, W. Zhang, Y. Liu, S. Yang, **L. Lai**

2:40 PHYS 147. Direct experimental characterization of contributions from self-motion of hydrogen and from interatomic motion of heavy atoms to protein anharmonicity. **Z. Liu**, C. Yang, J. Huang, G. Ciampalini, J. Li, V.G. Sakai, M. Tyagi, H.M. O'Neill, Q. Zhang, S. Capaccioli, K. Ngai, L. Hong

3:00 PHYS 148. Access to atomic resolution structural information of homo-repeats by NMR: The Huntingtin case. **P. Bernadó**, A. Urbanek, M. Popovic, A. Morato, C. Elena-Real, A. Estaña, F. Allemand, A. Fournet, A.I. Jimenez, C. Cativiela, J. Cortes, S. Delbecq, N. Sibille

3:35 Intermission.

3:55 PHYS 149. Structure and dynamics of macromolecules using molecular footprinting. **M.R. Chance**

4:30 PHYS 150. Integrative modeling of biomolecular assembly structures and pathways. **A. Sali**



TECHNICAL PROGRAM

5:05 PHYS 151. Accurately modeling the heterogeneous ensemble of structures of intrinsically disordered proteins using enhanced sampling molecular dynamics simulations. **U.R. Shrestha**, P. Juneja, J.M. Borreguero, S. Pingali, Q. Zhang, V. Urban, H.M. O'Neill, J. Smith, L. Petridis

Section B

Orange County Convention Center
Valencia Ballroom B-D - Theater 2

Emerging Frontiers in Fluorescence Microscopy: From Single Molecules to Super Resolution

Cosponsored by ANYL
T. Lee, J. C. Vaughan, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 PHYS 152. Developments in cryogenic single-molecule super-resolution imaging and dynamics of photosynthetic antennas in solution. **P. Dahlberg**

2:05 PHYS 153. Holistic molecular imaging and rapid phenotyping of complex biological systems. **K. Chung**

2:35 PHYS 154. Three-dimensional imaging with high-spatiotemporal resolution. B. Chang, R. Fiolka, **K.M. Dean**

2:55 PHYS 155. Quantitative imaging of molecular complexes with high resolution. **M. Lakadamyali**

3:25 Intermission.

3:40 PHYS 156. Spontaneously blinking dyes for single molecule localization microscopy. **F. Jradi**, T. Vu, T.A. Brown, C. Galbraith, E. Jorgensen, L.D. Lavis

4:00 PHYS 157. Two-color long time-lapse super-resolution imaging with lipid probes. **L. Chu**, A. Schepartz

4:20 PHYS 158. Super-resolution imaging at 1 nm with single-step photoswitching polymer dots. **J.D. McNeill**

4:40 PHYS 159. Super-resolution microscopy made simple. **J.C. Vaughan**

Section C

Orange County Convention Center
Valencia Ballroom B-D - Theater 3

Frontiers in Vibrational Spectroscopy: Experiments & Theory

Coupled Electronic & Molecular Motion Effects

E. Garand, R. Steele, *Organizers*
M. Reber, *Presiding*



TECHNICAL PROGRAM

1:30 PHYS 160. Recent advances in THz/far-IR vibrational spectroscopy, synergy DFT-MD simulations and experiments. **M.P. Gaigeot**

2:05 PHYS 161. Photoelectron spectroscopy of cold vinylidene anions. **J. DeVine**, D.M. Neumark

2:25 PHYS 162. Molecular vibrational signatures of exciton trapping in self-assembled hybrid organic-inorganic quantum nanostructures. **A. Rury**, A. Sanni, S. Lavan

2:45 PHYS 163. Withdrawn

3:05 Intermission.

3:20 PHYS 164. Dynamic ab initio methods for vibrational spectroscopy. **S. Luber**

3:40 PHYS 165. Low-energy electron transport in water. **R. Signorell**

4:15 PHYS 166. Simulating vibrational action spectroscopy in hydrogen bonded systems and in anomalous carbocations using some new and some older developments in ab initio molecular dynamics. **S.S. Iyengar**

4:35 PHYS 167. Fourth-order vibrational perturbation theory: Equations, verification, results for bond states and transition states. **J. Stanton**

Section D

Orange County Convention Center
Valencia Ballroom B-D - Theater 4

Modeling Dynamics in Dense Manifolds of Electronic States

Dense Manifolds in Molecules

Cosponsored by COMP
B. G. Levine, P. Slavicek, *Organizers*
T. Nelson, *Presiding*

1:30 PHYS 168. Quantum effects in cold molecular collisions from spatial polarization of electronic wave function. **N. Moiseyev**

2:10 PHYS 169. Correlated electronic dynamics including ionization: Grid methods and continuum states. **L. Greenman**

2:50 PHYS 170. Ab initio finite temperature auxiliary field quantum Monte Carlo. **B.M. Rubenstein**, Y. Liu, M. Cho

3:30 Intermission.

3:50 PHYS 171. Status of nonlocal complex potential theory of dissociative electron attachment. **I. Fabrikant**

4:30 PHYS 172. Electronic states embedded in continuum probed by two-dimensional electron spectroscopy. **J. Fedor**

4:50 PHYS 173. Metastable states: electronic structure, dynamics, and chemistry. **K.B. Bravaya**



TECHNICAL PROGRAM

Section E

Orange County Convention Center
Valencia Ballroom B-D - Theater 5

New Frontiers in the Confluence of Experimental Thermodynamics, Structural Investigations & Theory/Computation

Experimental Thermodynamics & Theory/Computation

Cosponsored by GEOC

N. Birkner, *Organizer*

K. Lilova, D. Wu, *Organizers, Presiding*

N. Birkner, S. McCormack, *Presiding*

1:30 PHYS 174. Understanding the thermodynamics and energetic properties of synthetic and natural metal-organic frameworks. **T. Friscic**

2:00 PHYS 175. Thermodynamics of ethanol adsorption in metal-organic frameworks: Effects of material topology and design rules for adsorption cooling applications. **H. Chen**, Z. Chen, L. Zhang, O.K. Farha, R. Snurr

2:30 PHYS 176. Elucidating the function of each metal in a bimetallic single catalytic grain for hydrodeoxygenation reactions. B. Wong, A. Hensley, J. Bray, N. Chaudhary, J. Shangguan, G.B. Collinge, Y. Wang, Y. Chin, **J. McEwen**

3:00 Intermission.

3:15 PHYS 177. Epitaxial stabilization of polar phases in ABO_3 compounds: High throughput computational study. T. Angsten, L. Martin, **M. Asta**

3:45 PHYS 178. Thermodynamics in cosmology: the composition and expansion of the dark universe. **C.A. Melendres**

4:05 PHYS 179. First-principles thermochemistry and phase diagrams of polymorphic molecular crystals. **G.J. Beran**

4:25 PHYS 180. Using DFT and the hindered translator/rotor models to determine entropy of adsorbates in catalytic reactions.. **L. Arnadottir**, C.T. Campbell, L.H. Sprowl

4:55 PHYS 181. Improving reproducibility of experimental data for crystalline porous materials. **D. Sholl**, A. Chen, F. Gharagheizi, M. Agrawal, R. Han

Section F

Orange County Convention Center
Valencia Ballroom B-D - Theater 6

Structure & Dynamics of Electrolytes: From the Bulk to Interfaces

The Spectroscopy of Electrolytes



TECHNICAL PROGRAM

R. Kumar, *Organizer*
R. Jorn, D. G. Kuroda, *Organizers, Presiding*

1:30 PHYS 182. Experimental determination of the Debye screening length from nonlinear optics. **F. Geiger**

2:00 PHYS 183. Solvent reduction at Si electrode/electrolyte junctions: SEI evolution probed by vibrational spectroscopy. **C.W. Schlenker**

2:30 PHYS 184. Structure and dynamics of battery electrolyte solutions. **C. Tibbetts**, N.J. Gimble, B.M. Luther, A.L. Prieto, A.T. Krummel

2:50 PHYS 185. Insight into how ions influence structure and dynamics of interfacial water at silica surfaces. **A. Tuladhar**, S. Dewan, S. Pezzotti, F. Siro Brigiano, M.P. Gaigeot, E. Borguet

3:20 Intermission.

3:35 PHYS 186. Structural characterization of a solid electrolyte for 3D microbatteries by NMR spectroscopy. **M.N. Garaga**, D. Clarkson, S.G. Greenbaum, M. Lifshitz, E. Cohen, D. Golodnitsky

4:05 PHYS 187. Sum frequency generation of Li-ion battery solvents and electrolyte on amorphous silicon. **R.L. Sacci**, B. Doughy, A. Chowdhury, D.A. Lutterman

4:35 PHYS 188. Electrolyte effects on the infrared combination band of liquid water. **C.H. Londergan**, C. Dhoonmoon

4:55 PHYS 189. Combined 2DIR spectroscopic and computational study of the effects of Hofmeister cations on peptides. **A.L. Serrano**

Section G

Orange County Convention Center
Valencia Ballroom B-D - Theater 7

Sustainable Software for Computational Molecular Science

Best Practices in Software Development from CMS Communities & Beyond

Cosponsored by COMP
T. Crawford, E. Marin, J. A. Nash, *Organizers*
D. G. Smith, *Organizer, Presiding*

1:30 PHYS 190. Academic publication and evaluation practices deter high quality software development. **G. Knizia**

2:00 PHYS 191. Let's talk about your software: Best practices for developing and sustaining software. **D.E. Bernholdt**

2:30 PHYS 192. SGCI and the conceptualization of URSSI: Addressing challenges in software sustainability. **S. Gesing**

3:00 Intermission.



TECHNICAL PROGRAM

3:20 PHYS 193. Composing and decomposing quantum chemistry software: Adventures with the Psi4 ecosystem. **L.A. Burns**

3:50 PHYS 194. Best practices for engineering molecular science simulation, analysis, and visualization codes. **J. Anderson, S.C. Glotzer**

4:20 Panel Discussion.

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Sponsored by PROF, Cosponsored by AGFD, ANYL, BIOL, BIOT, CARB, CELL, CHED, CMA, COLL, COMP, ENVR, GEOC, I&EC, MEDI, MPPG, NUCL, ORGN, PHYS, PMSE, POLY, PRES, WCC and YCC

ACS Award in Surface Chemistry: Symposium in Honor of Hajo Freund

Sponsored by COLL, Cosponsored by CATL⁺ and PHYS

Electron-Molecule & Molecule-Molecule Interactions

Sponsored by COMP, Cosponsored by PHYS⁺

Interdisciplinary Chemistry for New Frontiers in Biology & Medicine

DNA/RNA & Disease Diagnosis

Sponsored by ANYL, Cosponsored by BIOL, COLL, PHYS and PMSE

Symposium in Honor of Chuck Peden's Research Career: Catalysis for Energy & the Environment

Sponsored by CATL, Cosponsored by ENFL, ENVR, I&EC and PHYS

Elucidation of Mechanisms & Kinetics on Surfaces

Experimental Surface Science

Sponsored by CATL, Cosponsored by ENFL, ENVR, INOR and PHYS



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

ACS Award in Colloid Chemistry: Symposium in Honor of Naomi Halas

Sponsored by COLL, Cosponsored by PHYS

Recent Advances in Plasma-Enhanced Catalysis

Sponsored by CATL, Cosponsored by ENFL, ENVR and PHYS

MONDAY EVENING

Section A

Orange County Convention Center
West Hall C

Sci-Mix

A. B. McCoy, *Organizer*

8:00 - 10:00

352, 358-359, 361, 366, 369, 371-374, 380, 384, 387, 394, 396, 399. See subsequent listings.

TUESDAY MORNING

Section A

Orange County Convention Center
Valencia Ballroom B-D - Theater 1

Advances in Data Collection & Analysis of Biomolecular Structures

Cosponsored by COMP
S. Lindert, S. Yang, *Organizers*
T. E. Cheatham, A. C. Pan, *Presiding*

8:00 PHYS 195. Developing models for chromatin folding and function. **J.N. Onuchic**

8:35 PHYS 196. Characterizing amyloid beta monomers and oligomers with long-timescale molecular dynamics simulations. **A.C. Pan**

9:10 PHYS 197. Investigating structural and mechanistic changes in metal-substituted human carbonic anhydrase II QM-cluster models. **T. Summers**, Q. Cheng, J. Emerson, N.J. Deyonker



TECHNICAL PROGRAM

9:30 PHYS 198. Multiscale simulations of amyloid formation and conversion. **U. Hansmann**

10:05 Intermission.

10:25 PHYS 199. Enhanced molecular dynamics simulations of G-protein-coupled receptor-G protein interactions. **Y. Miao**, J. Wang, A. Bhattarai

11:00 PHYS 200. Parallel analysis of large ensembles of molecular dynamics simulation derived trajectories with the open-source CPPTRAJ tools. **T.E. Cheatham**, R. Galindo, D.R. Roe

11:20 PHYS 201. Life in the fast lane: Binding to glutamate receptors. **A. Lau**

Section B

Orange County Convention Center
Valencia Ballroom B-D - Theater 2

Emerging Frontiers in Fluorescence Microscopy: From Single Molecules to Super Resolution

Cosponsored by ANYL[‡]

T. Lee, J. C. Vaughan, *Organizers, Presiding*

8:00 PHYS 202. Looking at chromosomes. **T. Wu**, G. Nir, I. Farabella, C. Perez Estrada, C. Ebeling, B. Beliveau, H. Sasaki, S. Lee, S. Nguyen, R. McCole, S. Chatteraj, J. Erceg, J. AlHaj Abed, N. Martins, H. Nguyen, M. Hannan, S. Russell, N. Durand, S. Rao, J. Kishi, P. Soler-Vila, M. Di Pierro, J. Onuchic, S. Callahan, J. Schreiner, J. Stuckey, P.L. Yin, E. Lieberman Aiden, M. Marti-Renom

8:30 PHYS 203. Super-resolution study of nuclear structure and dynamics. **Y. Sun**

9:00 PHYS 204. Spatial transcriptomics through single-molecule imaging. **R. Nicovich**, B. Long, M. Taormina, T. Nguyen, E. Garren, Z. Maltzer, M. Gorham, E. Thomsen, B. Levi, C. Baker, J. Close, B. Tasic, E. Lein, H. Zeng

9:20 PHYS 205. Spatial organization of cellular structures and activities in superresolution. **J. Xiao**, X. Yang, J. Lyu, X. Weng, K. Bettridge, C. Bohrer

9:50 Intermission.

10:05 PHYS 206. 4D characterization of spatiofunctional multi-enzyme droplets in living cells. **M. Kyoung**

10:35 PHYS 207. Super-resolution imaging in living bacteria: Biological understanding requires advances in single-molecule imaging. **J.S. Biteen**

11:05 PHYS 208. Super-resolution correlated optical and electric imaging microscopy analysis of the dynamic aggregations in the neuronal ion channel receptors in live cells. **H. Lu**, R. Yadav, D.K. Sasmal

11:25 PHYS 209. Active PSF shaping and adaptive optics enable volumetric single molecule super-resolution microscopy through brain sections. **F. Huang**

Section C



TECHNICAL PROGRAM

Orange County Convention Center
Valencia Ballroom B-D - Theater 3

Frontiers in Vibrational Spectroscopy: Experiments & Theory

Tracking Chemical Reactivity via Vibrations

E. Garand, R. Steele, *Organizers*
S. Lubner, *Presiding*

8:00 PHYS 210. Tracking ultrafast dynamics via two-dimensional optical spectroscopy. **J.M. Anna**, Y. Lee, R.M. Malamakal, D.M. Chenoweth, R. Gera, S. Meloni

8:35 PHYS 211. Uncovering the structure and dynamics of aqueous proton transfer with ultrafast infrared spectroscopy. **W. Carpenter**, J. Fournier, N. Lewis, A. Tokmakoff

8:55 PHYS 212. Expanding the scope of surface phonon polaritons to new materials. **V.M. Breslin**, A.B. Grafton, D.C. Ratchford, K.P. Fears, C.R. So, A.D. Dunkelberger, J. Owrutsky

9:15 PHYS 213. Stark shift spectroscopy for measurement of electric fields at interfaces. J. Patrow, S. Sarkar, M.J. Voegtle, A. Pennathur, **J. Dawlaty**

9:50 Intermission.

10:05 PHYS 214. 2DIR spectroscopy of molecular vibrational polariton. **W. Xiong**

10:40 PHYS 215. 2D-IR studies of NCN infrared reporter for biomolecules: Uncovering the origins of mysterious peaks. **M.J. Tucker**

11:00 PHYS 216. Direct determination of proton transfer rate by 2D IR chemical exchange spectroscopy and *ab initio* molecular dynamics simulation. **R. Yuan**, C. Yan, M.D. Fayer

11:20 PHYS 217. Ultrafast spectroscopy with frequency combs: Enabling new measurements in time-resolved vibrational spectroscopy. **M. Reber**, N.D. Cooper, P. Nyaupane, W.M. Jones, R. Basnet, K. Warren

Section D

Orange County Convention Center
Valencia Ballroom B-D - Theater 4

Modeling Dynamics in Dense Manifolds of Electronic States

Materials & Surfaces

Cosponsored by COMP
B. G. Levine, P. Slavicek, *Organizers*
B. M. Rubenstein, *Presiding*



TECHNICAL PROGRAM

8:00 PHYS 218. Nonadiabatic dynamics in noble metal nanoclusters. **C.M. Aikens**, R.D. Senanayake, P. Pandeya, O. Hull

8:40 PHYS 219. Coherent exciton-vibrational dynamics and energy transfer in conjugated organics. **T. Nelson**, D. Ondarse-Alvarez, N. Oldani, B. Rodriguez-Hernandez, L. Alfonso-Hernandez, J. Galindo, V.D. Kleiman, S. Fernandez-Alberti, A.E. Roitberg, S. Tretiak

9:00 PHYS 220. Modeling singlet-fission biexciton states as an ab initio spin model: Justifications and applications. V. Abraham, **N. Mayhall**

9:40 PHYS 221. Unravelling the roles of decoherence and dissipation on photoisomerization yields. **A. Schile**, D. Limmer

10:00 Intermission.

10:20 PHYS 222. Combined reduced density matrix: ab initio electronic treatment and applications to the photoinduced dissipative dynamics of atomic clusters adsorbed on semiconductor surfaces. **D.A. Micha**

11:00 PHYS 223. Simulating electron dynamics of complex molecules with time-dependent complete active space configuration interaction. **W. Peng**, B. Fales, B. Levine

11:20 PHYS 224. Molecules in cavities: Polariton chemistry. **J. Yuen-Zhou**

Section E

Orange County Convention Center
Valencia Ballroom B-D - Theater 5

New Frontiers in the Confluence of Experimental Thermodynamics, Structural Investigations & Theory/Computation

Experimental Thermodynamics

Cosponsored by GEOC
N. Birkner, *Organizer*
K. Lilova, D. Wu, *Organizers, Presiding*
N. Birkner, C. Chung, *Presiding*

8:00 PHYS 225. Structure and stability of uranium silicides for nuclear fuel applications. **H. Xu**, X. Guo, C. Chung, A. Migdisov, J. White, A. Nelson, R. Roback, A. Navrotsky

8:30 PHYS 226. Thermodynamics and structural evolution of $\text{Er}_2\text{Ti}_2\text{O}_7$ pyrochlores damaged by swift heavy ion irradiation and mechanical milling (*LA-UR-18-29804*). **C. Chung**, E.C. O'Quinn, A.F. Fuentes, H. Xu, M.K. Lang, A. Navrotsky

8:50 PHYS 227. High-temperature drop-solution calorimetry of PuO_2 : Preliminary studies. **X. Guo**, H. Xu, C. Armstrong, C. Parker, K. Kriegsman, K. Popa, H. Boukhalfa, J. Mitchell, M. Ramos, A. Gaunt, R. Roback

9:20 PHYS 228. Experimental thermochemistry of neptunium phosphates and neptunium peroxide monomer and nanoclusters. **L. Zhang**, S.N. Perry, S. Hickam, J. Szymanowski, P.C. Burns

9:50 Intermission.



TECHNICAL PROGRAM

10:00 PHYS 229. Probing ensemble effects on the selective conversion of CO₂ and CO to methanol over metal-promoted Chevrel-phase sulfides. **J. Perryman**, A. Lam, K. Lilova, A. Kulkarni, C.J. Patridge, A. Navrotsky, J. Velázquez

10:30 PHYS 230. Thermodynamics - Still the best tool in the shed for engineered-materials processing. **R.E. Riman**, A.M. Anderko, D. Kopp, P. Kim

11:00 PHYS 231. Thermochemistry of multi principal element alloys. **S. Hayun**, A. Navrotsky

11:30 PHYS 232. Molten salts: a unique medium for synthesis of lithium conducting garnets with control over formation temperature, ionic conductivity, particle size, and composition. **J.M. Weller**, C.K. Chan

Section F

Orange County Convention Center
Valencia Ballroom B-D - Theater 6

Quantum Embedding Electronic Structure Methods

Cosponsored by COMP
M. Pavanello, A. Wasserman, *Organizers*
D. Lambrecht, *Presiding*

8:30 Introductory Remarks.

8:35 PHYS 233. Electrostatically-embedded fragment method with simple (and correct!) analytic gradient. **J. Herbert**, J. Liu, K. Liu, B. Rana

9:15 PHYS 234. On the road to polarizable embedding for femtochemistry, catalysis & more. **A.O. Ougaard Dohn**, E.Ö. Jónsson, H. Jonsson

9:35 PHYS 235. Locally coupled open subsystems and their application to the computation of ground-state and time-dependent electronic properties. **M. Mosquera**

10:15 Intermission.

10:35 PHYS 236. Embedded cluster density approximation for exchange-correlation energy: a natural extension of the local density approximation. **C. Huang**

11:15 PHYS 237. Second-order dispersion and induction energies based on multireference description of monomers. **M. Hapka**, K. Pernal

Section G

Orange County Convention Center
Valencia Ballroom B-D - Theater 7

Sustainable Software for Computational Molecular Science

High-Performance & Massively-Parallel Chemistry



TECHNICAL PROGRAM

Cosponsored by COMP
T. Crawford, E. Marin, J. A. Nash, D. G. Smith, *Organizers*
B. Pritchard, *Presiding*

8:30 PHYS 238. Challenge or opportunity? Navigating change in the era of exascale and big-data. **R.J. Harrison**

9:00 PHYS 239. Further explorations of single-precision algorithms within coupled-cluster and equation-of-motion coupled-cluster framework. **P. Pokhilko**, A. Krylov

9:30 PHYS 240. Time stepping and exchange-correlation modules for massively-parallel real-time time-dependent density functional theory. Y. Kanai, D. Yost, Y. Yao, X. Andrade, A.A. Correa, E. Draeger, A. Kononov, E. Constantinescu, **A. Schleife**

9:50 PHYS 241. Evolving with the hardware: Porting Massively Parallel Quantum Chemistry (MPQC) program to modern heterogeneous architectures. **C. Peng**, E.F. Valeev

10:10 Intermission.

10:30 PHYS 242. Breaking performance portability bottlenecks in NWChem. **J.R. Hammond**

11:00 PHYS 243. Facing exascale and big data challenges with modular software, resilient workflows and productivity tools. **M. Keceli**, C. Bertoni, S.N. Elliott, G.D. Fletcher, Y. Georgievski, W.H. Green, S.J. Klippenstein, A.F. Wagner, P. Zapol, H. Zhang

11:20 PHYS 244. Lessons learned from improving portability and stability of two scientific software packages for current and towards exascale systems. **C. Bertoni**, S. Leang, L. Carrington, G.D. Fletcher, M.S. Gordon, M. Keceli, K. Keipert, A. Tiwari

11:40 PHYS 245. CLEAVE: Implementation of cluster expansion method in atomic simulation environment package. **J. Garcia Lastra**, J.H. Chang, T. Vegge

ACS Award in Surface Chemistry: Symposium in Honor of Hajo Freund

Sponsored by COLL, Cosponsored by CATL[‡] and PHYS

Exploring the Frontiers of Chemistry through NASA Research

Getting There: Advanced Materials for Space Travel

Sponsored by COMSCI, Cosponsored by ANYL, BIOL, BIOT, CELL, COLL, ENFL, I&EC, INOR, NUCL, PHYS, PMSE and POLY

Elucidation of Mechanisms & Kinetics on Surfaces



TECHNICAL PROGRAM

Kinetic Modeling

Sponsored by CATL, Cosponsored by ENFL, ENVR, INOR and PHYS

Interdisciplinary Chemistry for New Frontiers in Biology & Medicine

Structure, Imaging & Sensing

Sponsored by ANYL, Cosponsored by BIOL, COLL, PHYS and PMSE‡

Planetary & Meteoritic Chemistry

Sponsored by GEOC, Cosponsored by ANYL and PHYS

GSSPC: Artificial Molecular Machines & the Next Generation of Molecular Control

Sponsored by CHED, Cosponsored by COLL, I&EC, ORGN‡, PHYS, POLY and PRES

Light-Driven Chemistry: Photoelectrochemistry & Photocatalysis

Sponsored by CATL, Cosponsored by COLL, ENFL, I&EC, INOR and PHYS

ACS Award in Colloid Chemistry: Symposium in Honor of Naomi Halas

Sponsored by COLL, Cosponsored by PHYS

Elucidating the Roles of Electric Fields in Catalysis

Sponsored by CATL, Cosponsored by ENFL and PHYS

TUESDAY AFTERNOON

Section A

Orange County Convention Center
Room W414C



TECHNICAL PROGRAM

Division of Physical Chemistry Award Symposium

Cosponsored by COMP

A. B. McCoy, *Organizer, Presiding*

1:30 PHYS 246. Award Address (E. Bright Wilson Award in Spectroscopy sponsored by the ACS Division of Physical Chemistry). Raman origins of plasmonics. **M. Moskovits**

2:10 PHYS 247. Award Address (Ahmed Zewail Award in Ultrafast Science and Technology sponsored by the Ahmed Zewail Endowment Fund established by the Newport Corporation). Ultrafast spectroscopy and microscopy of plasmonic excitations in metals. **H. Petek**

2:50 Intermission.

3:10 PHYS 248. Award Address (Peter Debye Award in Physical Chemistry sponsored by DuPont). Adventures in spectroscopy and dynamics: From transition states to biomolecules. **D.M. Neumark**

3:50 PHYS 249. Award Address (Joel Henry Hildebrand Award in the Theoretical and Experimental Chemistry of Liquids sponsored by the ExxonMobil Research and Engineering Company). Computer Simulation Can Predict the Behavior of Complex Liquids. **G.A. Voth**

4:30 PHYS 250. Award Address (ACS Award in Theoretical Chemistry sponsored by the ACS Division of Physical Chemistry). Progress in electronic structure theory for ground and excited states. **D.G. Truhlar**

Elucidation of Mechanisms & Kinetics on Surfaces

Catalysis on Metal Interfaces with Metal Oxides

Sponsored by CATL, Cosponsored by ENFL, ENVR, INOR and PHYS

Exploring the Frontiers of Chemistry through NASA Research

Living There: Science for the Future of Manned Space Exploration

Sponsored by COMSCI, Cosponsored by ANYL, BIOL[‡], BIOT, CELL, COLL, ENFL[‡], I&EC[‡], INOR[‡], NUCL[‡], PHYS[‡], PMSE[‡] and POLY[‡]

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Sponsored by PROF, Cosponsored by ENVR, GEOC, I&EC, MEDI, MPPG, NUCL, ORGN, PHYS, PMSE, POLY, WCC and YCC



TECHNICAL PROGRAM

Planetary & Meteoritic Chemistry

Sponsored by GEOC, Cosponsored by ANYL and PHYS

GSSPC: Artificial Molecular Machines & the Next Generation of Molecular Control

Sponsored by CHED, Cosponsored by COLL, I&EC, ORGN‡, PHYS, POLY and PRES

Light-Driven Chemistry: Photoelectrochemistry & Photocatalysis

Sponsored by CATL, Cosponsored by COLL, ENFL, I&EC, INOR and PHYS

Elucidating the Roles of Electric Fields in Catalysis

Sponsored by CATL, Cosponsored by ENFL and PHYS

WEDNESDAY MORNING

Section A

Orange County Convention Center
Valencia Ballroom B-D - Theater 1

Producing Equilibrium Amorphous Packings

Vapor Deposited Glasses

Cosponsored by COLL and PMSE
Z. Fakhraai, D. Sussman, *Organizers*
C. B. Roth, *Presiding*

8:00 Introductory Remarks.

8:05 PHYS 251. Physical vapor deposition as a route to high density glasses with high chemical stability.. **M.D. Ediger**

8:45 PHYS 252. Stability dependence of vibrational modes and sound attenuation for simulated glasses: From poorly annealed to ultra-stable. **E. Flenner**

9:25 Intermission.

9:40 PHYS 253. Ideality and tunneling two level systems (TLS) in amorphous silicon films. **F. Hellman**, M. Molina-Ruiz, T. Dauer, K. Shukla, H. Jacks, D. Queen, X. Liu, M. Abernathy, T. Metcalf



TECHNICAL PROGRAM

10:20 PHYS 254. Effect of light on the packing and kinetic stability of vapor deposited amorphous selenium. **A. Zhang**, R.B. Stephens, Z. Fakhraai

10:40 PHYS 255. Morphology and thermal properties of polymer films by slow deposition. **R.D. Priestley**

Section B

Orange County Convention Center
Valencia Ballroom B-D - Theater 2

Emerging Frontiers in Fluorescence Microscopy: From Single Molecules to Super Resolution

Cosponsored by ANYL
T. Lee, J. C. Vaughan, *Organizers, Presiding*

8:00 PHYS 256. Deconstructing biology with simple single-molecule imaging: controlling conformation, confinement, and concentration. **S.R. Leslie**

8:30 PHYS 257. Extended field-of-view single-molecule imaging with a deep penetration depth. **K. Han**

8:50 PHYS 258. Dual-color and polarization super-resolution imaging: Investigation into energy transfer efficiency among donor-acceptor groups of quantum dots. **D. Ryan**, M. Dunlap, S. Majumder, C. Sheehan, M. Gelfand, J.A. Hollingsworth, P. Goodwin, A.K. Van Orden

9:10 PHYS 259. Orientation imaging of single molecules on plasmonic nanohole arrays by second harmonic generation microscopy. **S. Sahu**, A. Mahigir, B. Chidester, G. Veronis, M.R. Gartia

9:30 Intermission.

9:45 PHYS 260. Statistical learning for multi-resolution dynamics. **H. Yang**

10:15 PHYS 261. Sub-millisecond single-molecule fluorescence studies of electronically-coupled cyanine dimers in model DNA replication fork constructs. **A.H. Marcus**

10:45 PHYS 262. Fast three-color single-molecule FRET. **H. Chung**

Section C

Orange County Convention Center
Valencia Ballroom B-D - Theater 3

From Lab Book to Journal Article: Insights from Editors on the Publication Process

Cosponsored by COMP[‡]
A. B. McCoy, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 PHYS 263. Issues with publishing papers: Scope, impact, ethics. **G.C. Schatz**



TECHNICAL PROGRAM

8:30 **PHYS 264.** Publishing in the Journal of Chemical Theory and Computation. **H.B. Schlegel**

8:55 **PHYS 265.** Get your papers read! **T. Lian**, E.C. Brigham

9:20 Intermission.

9:40 **PHYS 266.** Communicating scientific advances to broader readership effectively. **P.V. Kamat**

10:05 **PHYS 267.** Publishing in JACS. **M. Coote**

10:30 **PHYS 268.** Emerging nexus of journals and data repositories in chemistry publishing. **J.S. Yeston**

10:55 Panel Discussion.

11:25 Concluding Remarks.

Section D

Orange County Convention Center
Valencia Ballroom B-D - Theater 4

Structure & Dynamics of Electrolytes: From the Bulk to Interfaces

Simulating Electrolytes & Theoretical Methods

R. Jorn, D. G. Kuroda, *Organizers*

R. Kumar, *Organizer, Presiding*

R. David, *Presiding*

8:30 **PHYS 269.** Using numerical simulation to study the screening dynamics of dilute electrolyte solutions. **A. Willard**

8:50 **PHYS 270.** Modeling solid-solid interfaces in batteries at atomic and coarse-grained length scales. **K. Leung**

9:20 **PHYS 271.** Charge density correlations in electrolyte solutions and their impact in electrochemical properties and dynamics. **D. Limmer**

9:50 Intermission.

10:05 **PHYS 272.** Modeling the effects of electrolyte properties using continuum approaches in first-principles simulations. **M. Truscott**, O. Andreussi

10:25 **PHYS 273.** Charge scaling as a "free lunch" approach to electronic polarization in modelling aqueous electrolytes. **P. Jungwirth**

10:55 **PHYS 274.** Fluctuating hydrodynamics of electrolytes at electroneutral scales. **C. Kim**

11:15 **PHYS 275.** Computational study of structure and dynamics of glyme based electrolytes for sodium rechargeable batteries. **K. Li**, R. Kumar



TECHNICAL PROGRAM

Section E

Orange County Convention Center
Valencia Ballroom B-D - Theater 5

New Frontiers in the Confluence of Experimental Thermodynamics, Structural Investigations & Theory/Computation

Theory/Computation & Structural Investigations

Cosponsored by GEOC

N. Birkner, *Organizer*

K. Lilova, D. Wu, *Organizers, Presiding*

N. Birkner, J. Perryman, *Presiding*

8:00 PHYS 276. DFT study of ZIF8 and its polymorph dia-Zn(Melm)₂. **W. Chen**, N. Ross, N. Greaves

8:20 PHYS 277. Estimating off-stoichiometry using density functional theory-based calculations and the sub-lattice formalism. **G. Sai Gautam**, E.A. Carter

8:40 PHYS 278. Predicting the surface phase diagram of Ag(111) using *ab initio* grand canonical Monte Carlo. **R. Wexler**, T. Qiu, A.M. Rappe

9:00 PHYS 279. Molecular thermodynamic model of viscosities for the solutions. W. Wang, Z. Wang, H. Chen, **W. Fu'An**

9:20 PHYS 280. Percolation behavior of anisotropic colloidal nanoparticles of different architectures in bulk and confinement system. **J. Yu**, W. Lee

9:40 PHYS 281. Generation and analysis of unique wurtzite quantum dot structures. N. Weeks, **K.C. Tvrdy**

10:00 Intermission.

10:10 PHYS 282. Effects of defects on electron polaron formation and transport in transition metal oxides. **Y. Ping**

10:40 PHYS 283. Identification of liquid-gas coexistence in supercritical fluid: The Widom delta. **M. Ha**, W. Lee

11:00 PHYS 284. Calculation of electric fields for better catalyst design. **V. Vaissier**

11:20 PHYS 285. Experimental determination of substitution effect on the intrinsic stability of isostructural ZIF-8 derivatives. **N. Novendra**, T. Friscic, A. Navrotsky

11:40 PHYS 286. Comparison of quantum simulation methods for computing equation of state of warm dense matter and plasmas. **H.D. Whitley**, S. Zhang, J. Gaffney, L. Yang, J. Pask, B. Militzer, K. Caspersen, M. Daene, M. Marshall, A. Lazicki, R. London, D. Swift, W. Johnson, J. Klepeis, P. Sterne, M. Martin, N. Kostinski, B. Maddox, A. Sharma, P. Suryanarayana, A. Kritcher, J. Castor, J. Nilsen

Section F

Orange County Convention Center
Valencia Ballroom B-D - Theater 6



TECHNICAL PROGRAM

Quantum Embedding Electronic Structure Methods

Cosponsored by COMP
M. Pavanello, A. Wasserman, *Organizers*
L. Visscher, *Presiding*

8:30 Introductory Remarks.

8:35 PHYS 287. DFT-based embedding theories: Wavefunction-embedding, dynamics, excited states, and applications. **T.F. Miller**

9:15 PHYS 288. Self-energy embedding theory (SEET) for molecules and solids. **D. Zgid**, T.N. Lan, S. Iskakov, A. Rusakov, A. Shee

9:35 PHYS 289. Predicting photoelectron spectra solvated species with WFT-in-DFT embedding. Y. Bouchafra, A. Shee, F. Real, V. Vallet, **A. Severo Pereira Gomes**

10:15 Intermission.

10:35 PHYS 290. Balancing the description of subsystems in wavefunction-in-DFT and DFT-in-lower embedding. **M. Welborn**, F.R. Manby, T.F. Miller

10:55 PHYS 291. Solvent embedding and molecular response properties. **T. Crawford**

11:35 PHYS 292. Analytical nuclear gradients for projection-based wavefunction-in-DFT embedding. **S.J. Lee**, F. Ding, T.F. Miller, F.R. Manby

Section G

Orange County Convention Center
Valencia Ballroom B-D - Theater 7

Sustainable Software for Computational Molecular Science

Data & Machine Learning

Cosponsored by COMP
T. Crawford, E. Marin, J. A. Nash, D. G. Smith, *Organizers*
D. Altarawy, *Presiding*

8:30 PHYS 293. Database driven research and the Novel Materials Discovery Laboratory. **P. Rinke**

9:00 PHYS 294. Platform approach to data, machine learning, and software in chemistry. **B. Meredig**

9:30 PHYS 295. Automated multiscale methods for benchmark-level lattice energies of molecular crystals with CrystaLattE. **C.H. Borca**, B.W. Bakr, L.A. Burns, D.D. Sherrill

9:50 Intermission.



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

10:10 PHYS 296. Neural networks learning quantum chemistry: The rise of the machines. **A.E. Roitberg**

10:40 PHYS 297. MolSSI quantum chemistry archive project. **L.N. Naden**, D.G. Smith, D. Altarawy

11:10 PHYS 298. Molecular machine learning with DeepChem. B. Ramsundar, **K. Leswing**

11:40 PHYS 299. Advancing molecular feature representation and machine learning design methodologies using the ChemML program suite. **M. Haghightlari**, J. Hachmann

Elucidating the Roles of Electric Fields in Catalysis

Sponsored by CATL, Cosponsored by ENFL and PHYS

Young Chemist: Earth & Space

Sponsored by YCC, Cosponsored by PHYS

Activation of Light (C1-C4) Hydrocarbons: Theory & Experiments

Sponsored by CATL, Cosponsored by ENFL, ENVR, INOR and PHYS

Light-Driven Chemistry: Photoelectrochemistry & Photocatalysis

Sponsored by CATL, Cosponsored by COLL, ENFL, I&EC, INOR and PHYS

Model Catalysis & Materials Complexity Frontiers

Sponsored by CATL, Cosponsored by PHYS

WEDNESDAY AFTERNOON

Section A

Orange County Convention Center
Valencia Ballroom B-D - Theater 1



TECHNICAL PROGRAM

Producing Equilibrium Amorphous Packings

Making & Transforming Stable Glasses

Cosponsored by COLL and PMSE
Z. Fakhraai, D. Sussman, *Organizers*
K. K. Mandadapu, *Presiding*

1:30 PHYS 300. Insights into the transformation mechanisms of vapor-deposited glasses. **J. Rodriguez-Viejo**, M. Gonzalez-Silveira, C. Rodriguez-Tinoco, A. Lopeandia, A. Vila, J. Ràfols-Ribé

2:10 PHYS 301. Bypassing glassy sluggishness by particle swap Monte Carlo in high dimensions. **J. Kundu**, P. Charbonneau, L. Berthier

2:30 PHYS 302. Dynamical constraints, trajectory methods and inactive states. **J. Garrahan**, **S. Katira**, **K.K. Mandadapu**

3:10 Intermission.

3:30 PHYS 303. Limits of marginally stable and ultrastable glasses. **P.G. Wolynes**

4:10 PHYS 304. Varying molecular shape and chemical interactions in simulated vapor deposited glass films. **A. Moore**, P.J. Walsh, Z. Fakhraai, R. Riggleman

Section B

Orange County Convention Center
Valencia Ballroom B-D - Theater 2

Modeling Dynamics in Dense Manifolds of Electronic States

Materials & Surfaces

Cosponsored by COMP
B. G. Levine, P. Slavicek, *Organizers*
M. Schuurman, *Presiding*

1:30 PHYS 305. Simulation of photoexcited dynamics in large molecules. **S. Tretiak**

2:10 PHYS 306. Hot carrier generation from single plasmons in metallic nanoparticles. **L. Roman Castellanos**, J. Lischner

2:30 PHYS 307. Ultrafast electron dynamics due to electronic stopping in bulk semiconductors. **A. Schleife**

3:10 PHYS 308. Variational relativistic two-component CASSCF for spectroscopy of transition metal complexes. **A.J. Jenkins**, H. Liu, J.M. Kasper, M.J. Frisch, X. Li

3:30 Intermission.

3:50 PHYS 309. Breakdown of the Born-Oppenheimer approximation in surface chemistry. **A.M. Wodtke**



TECHNICAL PROGRAM

4:30 PHYS 310. H-atom product channel in the ultraviolet photodissociation of the thiomethoxy radical (CH_3S) via the B^2A_2 state. G. Sun, X. Zheng, Y. Song, **J. Zhang**

4:50 PHYS 311. Singlet fission in perylene diimide dimers and crystals. **M. Farag**, A. Krylov

Section C

Orange County Convention Center
Valencia Ballroom B-D - Theater 3

Frontiers in Vibrational Spectroscopy: Experiments & Theory

Clusters & Ions

E. Garand, R. Steele, *Organizers*
M. J. Tucker, *Presiding*

1:30 PHYS 312. Infrared spectroscopy of metal ion-acetylene complexes: Coordination, solvation and reactions. **M.A. Duncan**

2:05 PHYS 313. On the nature of the strong hydrogen-bond: Fluoride and water. **J.T. Kelly**

2:25 PHYS 314. Diffusion Monte Carlo approaches for exploring neutral and protonated water clusters. **A.B. McCoy**, V.G. Lee, R.J. DiRisio

3:00 Intermission.

3:15 PHYS 315. Electronic and vibrational information on “solution species” from cryogenic ion spectroscopy. **J. Weber**

3:50 PHYS 316. Geometries and properties of neutral gold clusters in the gas phase: Transition from 2D To 3D structures? B.R. Goldsmith, J. Florian, J. Liu, P. Gruene, **J.T. Lyon**, D. Rayner, A. Fielicke, M. Scheffler, L.M. Ghiringhelli

4:10 PHYS 317. Full characterization of small discrete protonated water clusters in acetonitrile $n=1,2,3$ using the CN stretch as a spectator mode. E. Kozari, D. Pines, **E. Pines**

4:30 PHYS 318. Effects of temperature on long range ion-water interactions in aqueous nanodrops. **E.R. Williams**, M.J. DiTucci, C. Stachl

Section D

Orange County Convention Center
Valencia Ballroom B-D - Theater 4

Structure & Dynamics of Electrolytes: From the Bulk to Interfaces

Ionic liquids



TECHNICAL PROGRAM

R. Jorn, R. Kumar, D. G. Kuroda, *Organizers*
M. D. Baer, R. David, *Presiding*

1:30 PHYS 319. Dependence of interfacial electric fields on anion size of ionic liquids. **A. Pennathur**, J. Patrow, S. Sarkar, J. Dawlaty

1:50 PHYS 320. Simulating ionic liquids: Force field development and applications. **O. Acevedo**, B. Doherty, X. Zhong

2:20 PHYS 321. Structure and dynamics of salts from molecular simulations. **C.J. Margulis**

2:50 PHYS 322. Modeling, virtual high-throughput screening, and machine learning of deep eutectic solvents. **J. Hachmann**

3:10 Intermission.

3:25 PHYS 323. Characterization of the structure and dynamics of an unusual ionic solid. C. Uitvlugt, M. Saladin, J.F. Wishart, G.A. Baker, **M. Maroncelli**

3:55 PHYS 324. Solvation structure and Li ion transport in molten Li salt solvate electrolytes. **K. Ueno**, K. Dokko, M. Watanabe

4:25 PHYS 325. Development of low-temperature ionic liquid-organic solvents-salt electrolyte systems for MET seismometer. **W. Lin**, Y. Xu, S. MacDonald, M. Gliege, Z. Zhao, L. Dai

Section E

Orange County Convention Center
Valencia Ballroom B-D - Theater 5

New Frontiers in the Confluence of Experimental Thermodynamics, Structural Investigations & Theory/Computation

Thermodynamics of Material Synthesis & Structural Investigations

Cosponsored by GEOC
N. Birkner, *Organizer*
K. Lilova, D. Wu, *Organizers, Presiding*
N. Birkner, N. Novendra, *Presiding*

1:30 PHYS 326. High-throughput prediction of the structures and properties of atomic cluster. **P. Lile**, T. Mueller

1:50 PHYS 327. Fast, reliable computation of small-angle structure factors in Kirkwood-Buff theory. **D. Rogers**

2:10 PHYS 328. Binding free energy of protein complexes calculated from a framework based on the string method. **D. Suh**, S. Jo, C. Boughter, C. Chipot, B. Roux

2:30 PHYS 329. Inelastic neutron scattering study of zeolitic imidazolate frameworks. **N. Ross**, A.I. Kolesnikov, T. Friscic, A. Katsenis, M. Arhangelskis



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

3:00 PHYS 330. Green synthesis of zeolite and reconsideration on zeolite crystallization. **F. Xiao**

3:30 Intermission.

3:40 PHYS 331. Toward roll-to-roll production of nanomaterials by microwave approach. **X. Zhang**, D. Wu, S. Sarwar, J. Cook

4:10 PHYS 332. Relating structure to spectroscopic signatures: Experimental analysis and theoretical interpretation of different aluminum coordination environments. **C. Pearce**, M. Dembowski, T.R. Graham, C. Delegard, E. Martinez Baez, A. Wildman, M. Pouvreau, M. Prange, A. Krzysko, X. Zhang, D. Semrouni, H. Wang, X. Li, G.K. Schenter, A.E. Clark, K. Rosso, S.B. Clark

4:40 PHYS 333. Examining the effect of surface substructure on behavior of Self-Assembled Monolayers (SAMs). **A. Kadoma**, C. Du, M.M. Thuo

5:00 PHYS 334. Atomically-resolved spontaneous transformation of ferrihydrite to goethite. **K. Rosso**, M. Sassi, O. Qafoku, M. Bowden, A.T. N'Diaye, C. Pearce

Section F

Orange County Convention Center
Valencia Ballroom B-D - Theater 6

Quantum Embedding Electronic Structure Methods

Cosponsored by COMP
M. Pavanello, A. Wasserman, *Organizers*
O. Andreussi, *Presiding*

1:30 Introductory Remarks.

1:35 PHYS 335. Multi-projective variational approach to the quantum lattice problem. **C. Marianetti**, Z. Cheng

2:15 PHYS 336. Density-functional self-energy approach to site-occupation embedding theory. **L. Mazouin**, M. Saubanère, E. Fromager

2:35 PHYS 337. Correlation energy for embedded orbital groups. **K. Pernal**

3:15 Intermission.

3:35 PHYS 338. Direct embedding of excited electronic states using density matrix embedding theory. **H.K. Tran**, T.A. Van Voorhis, A. Thom

3:55 PHYS 339. Quantum embedding for molecular systems. **H. Ye**, N. Ricke, H.K. Tran, T.A. Van Voorhis

4:35 PHYS 340. Polarized many-body expansion: A perfect marriage between embedded mean-field theory and variational many-body expansion. **S. Veccham Krishna Prasad**, J. Lee, M.P. Head-Gordon

Section G



TECHNICAL PROGRAM

Orange County Convention Center
Valencia Ballroom B-D - Theater 7

Sustainable Software for Computational Molecular Science

Software Tools: Molecular Mechanics

Cosponsored by COMP
T. Crawford, E. Marin, J. A. Nash, D. G. Smith, *Organizers*
L. Naden, *Presiding*

1:30 PHYS 341. Molecular Simulation and Design Framework (MoSDeF): Framework for efficient, automated, reproducible simulations and computational screening of soft matter. **P.T. Cummings**, C. McCabe, C. Iacovella

2:00 PHYS 342. QM/MM in Amber: The past, the present, the future. **A.W. Goetz**

2:20 PHYS 343. Tools for computational design of artificial molecular machines. **K.B. Sezginel**, C. Wilmer

2:40 Intermission.

3:00 PHYS 344. Efficient and sustainable software for many-body molecular dynamics. **M. Riera Rimbau**, D.G. Smith, F. Paesani

3:30 PHYS 345. Standalone library for particle mesh Ewald theory. **A.C. Simmonett**, B. Brooks

3:50 PHYS 346. Development and implementation of classical and QM/MM methods with advanced polarizable potentials: LICHEM and pmemd.gem. H. Gokcan, R.E. Duke, **G.A. Cisneros**

Young Chemist: Earth & Space

Sponsored by YCC, Cosponsored by PHYS

Young Chemist: Earth & Space

Sponsored by YCC, Cosponsored by PHYS

Activation of Light (C1-C4) Hydrocarbons: Theory & Experiments

Sponsored by CATL, Cosponsored by ENFL, ENVR, INOR and PHYS

Light-Driven Chemistry: Photoelectrochemistry & Photocatalysis



TECHNICAL PROGRAM

Sponsored by CATL, Cosponsored by COLL, ENFL, I&EC, INOR and PHYS

Model Catalysis & Materials Complexity Frontiers

Sponsored by CATL, Cosponsored by PHYS

WEDNESDAY EVENING

Section A

Orange County Convention Center
West Hall C

PHYS Poster Session

A. B. McCoy, *Organizer*

6:00 - 8:00

PHYS 347. *Ab initio* study of the ground and excited states of N-hydroxyisocyanuric acid and its decomposition products. **Z. Drake**, D. Sirianni, N. Kraut, N. Kebede, G.J. Hoffman

PHYS 348. Quantum control of dynamical system depending on time scale. **Q. Wang**

PHYS 349. Optically triggered planarization of boryl substituted phenoxazine: Another horizon of TADF molecules and high performance OLEDs. **D. Chen**, P.P. Chou

PHYS 350. Correlation among hydrogen bond, excited-state intramolecular proton-transfer kinetics and thermodynamics for –OH type proton-donor molecules. **Z. Liu**, P.P. Chou

PHYS 351. New insight into mechanochromism induced by excited-state intramolecular proton transfer coupled excimer reaction. **Y. Wei**, P.P. Chou

PHYS 352. Binding free energy calculations on host-guest systems. **L. Song**, N. Bansal, Z. Zheng, K.M. Merz

PHYS 353. Incorporation of explicit water molecules to calculate standard redox potentials of organic molecules in aqueous solutions. J.C. Ortiz-Rodríguez, J.A. Santana, **D.D. Mendez**

PHYS 354. Competing proton and hydrogen atom transfer in excited states of indigo. **R. Rodriguez**

PHYS 355. Diffusion Monte Carlo simulation of a permanent guided wave-function with high entropic barriers to improve isotropic impurity sampling in large clusters. **A.D. Stringer**, E. Curotto

PHYS 356. Spectroscopic characterization of the tubulin E-hook: Implications of protein affinity for microtubules. A. Williams, J. Davis, J. Reynolds, N. Hammer, **D.N. Reinemann**



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- PHYS 357.** Synthesis of iron nanoparticles by thermal decomposition of diironnonacarbonyl in ionic liquid and potential use of ferromagnetic dispersions for mixer studies in liquids feeds. **N. Barashkov**, T. Sakhno, I. Irgibayeva, A. Mantel, S. Mendigaliyeva, I. Barashkova
- PHYS 358.** Chalcogenide doping in hybrid perovskites for enhanced stability of solar cells. **J. Gong**, M. Yang, D. Rebollar, P. Guo, J. Rucinski, Z. Liveris, K. Zhu, R. Schaller, T. Xu
- PHYS 359.** Multiple bonds between boron and metal atom: Matrix isolation infrared spectrometry and theoretical calculations of FBMF₂ (M = Re, Os and Ir) complexes. W. Li, **B. Xu**, W. Yu, X. Wang
- PHYS 360.** Physical astrochemistry quantum space and the evolution of the universe. **C.A. Melendres**
- PHYS 361.** Designing isotope-labeling schemes for protein 2D IR spectroscopy. **K.R. Webb**, K. Segner, L. Buchanan
- PHYS 362.** Band alignment, interlayer excitons, and enhanced valleytronics in hetero-stacks of transition-metal dichalcogenides. **R.N. Gunasinghe**, **J. Viera**, **B. Persaud**, D. Samarakoon, X. Wang
- PHYS 363.** Using the linearized semiclassical approximation to simulate nonadiabatic dynamics of complex molecular systems via the modified Redfield equation. **Y. Lai**, E. Geva
- PHYS 364.** Fitting a hydrogen-water dimer potential energy surface. **E.R. Knab**, E. Curotto
- PHYS 365.** Fluorescence-based contrast enhancement for macroscale damage characterization of S-2 glass/epoxy composite laminates. **J. Guy**, E. Bonyi, B. Kioko, O. Adesina, T. Obafemi-Babatunde, C. Meyer, D.J. O'Brien, B.z. Haque, J.W. Gillespie, **K. Aslan**
- PHYS 366.** Using surface enhanced Raman spectroscopy to monitoring photo-induced degradation of organic pollutants. **R. Lamb**, M.J. Nee
- PHYS 367.** Emission color tunability of upconversion film by modulating phonon relaxation. **S. Lim**, Y. Cho, C. Park, J. Kim, H. Kim
- PHYS 368.** Competition between energy transfer and stimulated emission in organic nanowire heterostructures for dual-wavelength switchable lasing. **K. Wang**, W. Zhang, Y. Yan, Y. Zhao
- PHYS 369.** Description of intermolecular charge transfer with subsystem density-functional theory. **A. Schulz**, C. Jacob
- PHYS 370.** Low-temperature-processed inorganic perovskite solar cells via solvent engineering with enhanced mass transport. **H. Zai**
- PHYS 371.** Ground and excited potential energy curves for diatoms and triatoms. **E.J. Hedrick**, J.B. Maddox
- PHYS 372.** Utilizing 2-D microwave techniques to simplify the spectra of allyl chloride, isoamyl acetate, and ethoxyethanol. **E. Riffe**, S.T. Shipman
- PHYS 373.** Study the *N,N*-Di(4-bromo)nitrenium ions in different solutions by time-resolved spectroscopic methods. **L. Du**, X. Lan, Z. Yan, D. Phillips
- PHYS 374.** Probing macromolecular protein interactions *in situ* via sum frequency generation (SFG) vibrational spectroscopy. **A.N. Marcano Delgado**, T. Lu, Z. Chen



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- PHYS 375.** Photophysics of exciplex based OLED materials revealed by optical microscopy. **M. Bauer**, J. Kim, T. Basché
- PHYS 376.** On Adam-Gibbs model of cooperative relaxation properties in glass-forming liquids: fluctuation effects. **A. Bhattarai**
- PHYS 377.** Thermodynamic and kinetics studies of DNA i-motif formation. L.R. Robinson, B. Sparks, R. Varkey, **R.D. Sheardy**
- PHYS 378.** Polyphenyleneoxide dielectric for flexible semitransparent organic transistors and circuits with good mechanical bending stability. **L. Guo**, X. Zhu, C. Cong, Q. Zhou, X. Sun
- PHYS 379.** Self-stratified poly(3-hexylthiophene)/ polystyrene (P3HT/PS) blends based organic thin-film transistor nitrogen dioxide gas sensors. **S. Hou**, J. Yu
- PHYS 380.** Analytical Hessians of ground state and excited states within a multiscale polarizable QM/MM method: applications to surface-enhanced molecular spectroscopies. **Z. Pei**, Y. Shao, W. Liang
- PHYS 381.** Degradation pathways of aminonaphthols. **K. Nelson**, K. Takematsu
- PHYS 382.** Unusual reactivity of metal oxides with aqueous vanadyl ions: Promising method for the synthesis of ternary metal vanadium oxides. **A. Alayyafi**, A.W. Apblett
- PHYS 383.** Far from equilibrium nonlinear chemical dynamics. **J.C. Webb**
- PHYS 384.** Characterization and synthesis of glassy materials. **M. Felix**, M.D. Sonntag
- PHYS 385.** Can spectroscopic techniques such as surface-enhanced raman scattering, circular dichroism, and UV-Vis spectroscopy reveal how carboplatin modifies DNA? **S.M. Williams**, C.R. Fraire, R.D. Sheardy, N. Mirsaleh-Kohan
- PHYS 386.** Discrete variable representation of the reduced density matrix for molecular relaxation dynamics. J.B. Maddox, **L.C. Curtis**
- PHYS 387.** Broadband light emission in hybrid perovskites: Assessing the role of molecular disorder. **A. Sanni**, S. Lavan, A. Rury
- PHYS 388.** Studying the effect of underdamped vibration on excitation energy transfer dynamics by a mixed quantum-classical dynamics method. **C. Kim**, Y.M. Rhee
- PHYS 389.** Withdrawn
- PHYS 390.** Monitoring GG-DNA and platinum-based chemotherapeutic drug complexes through sensitive chromatographic and spectroscopic techniques. **S. Wappes**, T. Nguyen, S. Khan, N. Mirsaleh-Kohan
- PHYS 391.** Quantifying chemical hardness by computational methods. **N. Henderson**
- PHYS 392.** Electronically excited states of closed-shell, functionalized benzene (-CN, -OH, -C₂H) anions. **T. Santaloci**, R.C. Fortenberry
- PHYS 393.** Rotational and vibrational fingerprints of the oxywater cation, a possible precursor to abiotic O₂. **W. Del Rio**, R.C. Fortenberry



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- PHYS 394.** Electronic couplings for the intermolecular energy transfer. **Z. Qu**, J. Gao
- PHYS 395.** Potential energy surface characterization of hydrazone complexes for use in solar thermal fuels (STFs). **K. Yokuda**, T. Kowalczyk
- PHYS 396.** Binding of the atomic cations hydrogen through argon to water and hydrogen sulfide. **B. Westbrook**, G.S. Tschumper, J.S. Francisco, R.C. Fortenberry
- PHYS 397.** Improved electronic structure methods for molecular junction transport. **E.P. Hoy**
- PHYS 398.** Effect of salt on the amide I vibrations of model peptides. **O. Cracchiolo**, A.L. Serrano, S. Corcelli
- PHYS 399.** Studying atmospherically relevant photochemical processes involving NO using multireference computational methods. **M. Marracci**, B. Ortega, R.T. Korb, K.J. Blackshaw, N. Quartey, A.K. Ajmani, D. Hood, C.J. Abelt, A.S. Petit, N.M. Kidwell
- PHYS 400.** Effect of strain on graphene functionalization dynamics. **R.M. Brinn**, K.Z. Rinaldi, A. Crowther
- PHYS 401.** Raman spectroscopic studies of the structure of CdSe/S alloyed quantum dots. **A. Oza**, N. Saenz, L. Hamachi, J.S. Owen, A. Crowther
- PHYS 402.** Comparison of quantum dot blinking behavior with different thiol-based ligands. **A.M. Keller**, D. Strong, H. Hart, A. Regier
- PHYS 403.** Rotational, fine and hyperfine structures of the doublet states of AuS. **T.D. Varberg**, B. Pearlman, I.A. Wyse
- PHYS 404.** Investigation of 2,5-dimethylfuran oxidation reaction initiated by O(³P) atoms *via* synchrotron photoionization. **H. Park**, G. Meloni
- PHYS 405.** Correlating plasmon dynamics with nuclear vibration. **G. Kuda Singappulige**, C.M. Aikens
- PHYS 406.** *Ab initio* study of CH₃I Rydberg states with spin-orbit coupling. **C. Huang**, H. Hao, B.M. Rubenstein
- PHYS 407.** Mass Spectrometry of ultra-small gold nanoparticles. **M.A. Hewitt**, G.E. Johnson, H. Hernandez
- PHYS 408.** Raman spectroscopic studies of two classes of two-dimensional materials: metal oxide halide sheets and linked Re₆Se₈Cl₂ clusters. **A. Hartnett**, A. Dismukes, J. Russell, X. Roy, A. Crowther
- PHYS 409.** Mass-selected soft-landing of Au₆(PPh₃)₆²⁺ nanocluster. **S. Paek**, G.E. Johnson, H. Hernandez
- PHYS 410.** Fundamental aspects of magnetic hyperthermia: Comparison of rotating vs alternating magnetic fields. **L. Bodnar**, V. Chikan
- PHYS 411.** Electronic structure and normal frequencies investigations of hydrogen bonding interactions between mono VS di cation of ionic liquids. **N.R. Dhumal**, D. Isaev, M. Helminen, B. Williams, S. Latortue
- PHYS 412.** Withdrawn



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- PHYS 413.** Automatic active space selection for multiconfiguration pair-density functional theory. **J. Bao**, S. Dong, L. Gagliardi, D.G. Truhlar
- PHYS 414.** Nonstatistical dissociation dynamics of nitrobenzene and *ortho*-nitrophenol. **N. Quartey**, K.J. Blackshaw, M. Marracci, W. Fritzeen, R.T. Korb, A.K. Ajmani, L. Montgomery, G.G. Vanegas, B. Ortega, Z. Sarvas, J. Galvan, A.S. Petit, N.M. Kidwell
- PHYS 415.** Raman characterization and theoretical study of semi-dative B-O bonds in organoborane molecules. **A. Dorris**, T. Vaughan, D.L. Mattern, R.C. Fortenberry, N. Hammer
- PHYS 416.** Probing the rotational spectra of methyl-substituted piperidines. **E. Johnson**, S.T. Shipman
- PHYS 417.** Rotational spectrum of eugenol as analyzed with double resonance and grid-based Autofit. E. Riffe, **S.T. Shipman**, S. Gaster, C.M. Funderburk, G.G. Brown
- PHYS 418.** Spectroscopic and computational comparison of the dipole-bound anions of nitrogen-containing molecules in space involved in potential proliferation of life. **A.E. Williams**, N. Hammer
- PHYS 419.** Applications of time-dependent configuration interaction for attosecond dynamics. **Z. Stewart**, I. Ulusoy, A.K. Wilson
- PHYS 420.** Implicit polarization and co-solvent preference: Modeling EC and PC solvation in lithium electrolytes. **K. Abo**, A. Leitgeb, R. Jorn
- PHYS 421.** Accurate representation of potential energy curves for alkali dimers. **L. Biolsi**
- PHYS 422.** Role of the electrode surface in Co-solvent preference: Lithium solvation in EC/PC mixtures. **A. Leitgeb**, K. Abo, R. Jorn
- PHYS 423.** Withdrawn
- PHYS 424.** Determining the pH of frozen and annealed solutions using infrared spectroscopy. **C. English**, R.R. Michelsen
- PHYS 425.** Chirped-pulse Fourier transform microwave spectroscopy at room temperature via direct digital synthesis. **A. Rodriguez**, S.T. Shipman
- PHYS 426.** Continued investigation of SCCCOS at 5 μm using high-resolution infrared spectroscopy. **J.B. Dudek**, S. Bentley, T. Salomon, S. Schlemmer, S. Thorwirth
- PHYS 427.** Microhydration studied with the cluster genetic algorithm program. **A.S. Frischmann**, **K. Lee**, S.A. Abrash
- PHYS 428.** Spectroscopic and gravimetric evaluation of water adsorption isotherms on combustion particles. **E. Richmond**, J.G. Navea
- PHYS 429.** Solvent induced structural dynamics of iron pentacarbonyl in ether and thioether solutions. **K. McDermott**, C. Laperle, S. DiRoma
- PHYS 430.** Molar composition and temperature effects on proton transfer from excited state pyranine to water in ethylene glycol-water solutions. **S.J. Bintrim**, B.H. Milosavljevic



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- PHYS 431.** Vibrational spectroscopy study of O(³P) reactions with adsorbed organic compounds. **C. Bennett-Caso**, A. Leonardi, C. Cang, J. Spagnoletti, J.G. Navea
- PHYS 432.** Computational study of fluoxetine's absorption and emission spectra. **D. Odhiambo**, P.M. Hare
- PHYS 433.** UV photodissociation dynamics of brown carbon chromophores: *ortho*-Nitrophenol and nitroresorcinol. **K.J. Blackshaw**, N. Quartey, D. Hood, S. Chen, M. Marracci, B. Ortega, A.S. Petit, N.M. Kidwell
- PHYS 434.** Conical intersections facilitate Auger Recombination in semiconductor nanoparticles. **A.C. Hartley**, M. Esch, S. Fales, B. Levine
- PHYS 435.** Double-feedback experimental and computational characterization of the interaction between metal-protoporphyrin photosensitizers and Human Serum Albumin. **E. Hernandez-Soraiz**, L. Brancaleon, J. Hu
- PHYS 436.** Chiral discrimination in sugar-based deep eutectic solvents. **L. VandenElzen**
- PHYS 437.** Effect of uracil in different sequence contexts on 2D NMR properties in DNA. **J. Becker**, G.A. Meints
- PHYS 438.** Modeling the quantum dynamics behind charge transport in photosynthetic reaction centers beyond the Spin-Boson model. **K. Lenn**, E. Geva, E. Mulvihill
- PHYS 439.** Catching water in the act of oxidation: Stepwise activation by reactive radicals. **E. Christensen**, R. Steele
- PHYS 440.** Strain-induced transformation and thermoelectric engineering of monolayer indium selenide. **L. Sprague**, C. Huang, J. Song, B.M. Rubenstein
- PHYS 441.** Photochemical mechanisms of light-activated drug molecules for potential cancer therapy. **S.J. Leger**, **C.J. Pasqua**, T. Karsili
- PHYS 442.** Spectroscopic and computational analysis of benzothiadiazole (BTD) building blocks and their copolymers. **A.E. Steen**, R.G. Rajapakse, N.H. Attanayake, D. Karunathilaka, D.R. Strongin, D.L. Watkins, N. Hammer
- PHYS 443.** Time-resolved photoelectron spectroscopy of *cis*-stilbene: Theory and experiment. **R.J. MacDonell**, K. Veyrinas, R. Forbes, M.A. Larsen, V. Makhija, M. Schuurman, A. Stolow
- PHYS 444.** Study of the effects of dihydrouracil lesion in DNA on non-exchangeable chemical shifts and NOE intensities using two dimensional NMR spectroscopy. **B.M. Boyd**, G.A. Meints
- PHYS 445.** Temperature dependence and medium effects on methylantracene fluorescence quenching by dimethylaniline. **Y. Yan**, **S. Marshall**, B.H. Milosavljevic
- PHYS 446.** New approaches to analysis of complex mixtures using chirped-pulse Fourier-transform microwave spectroscopy: Microsolvation of fluoroethylenes by CO₂. **R.A. Peebles**, S.A. Peebles, P.B. Kannangara, T. Ariyaratne, C.T. West, B.H. Pate
- PHYS 447.** Competing fragmentation pathways of nitrosothiophenol from UV photodissociation. **R. Korb**, K.J. Blackshaw, N. Quartey, A.K. Ajmani, D. Hood, M. Marracci, B. Ortega, C.J. Abelt, A.S. Petit, N.M. Kidwell
- PHYS 448.** Linear infrared and NMR spectroscopies for the determination of ϕ , ψ angles in peptides and proteins. **M.A. Kubasik**, M.C. Rotondaro, C. Foster-Spence, J. Dickovick



TECHNICAL PROGRAM

PHYS 449. Computational electronic structure investigations of the photophysics of Cr and group 13 bis(4'-arylterpyridyl) complexes. **P.K. Walhout**, B.M. Lovaasen

PHYS 450. Diffusion of water in nanoslit. **J. Li**, D. Lu

PHYS 451. Excitonic response of bulk GaAs to light carrying orbital angular momentum. **P. Navotnaya**, G.S. Engel

PHYS 452. Combined *ab initio* and experimental approaches for the quantification of IR spectra for alcohol clusters in solution. **J. Plascencia**, W.G. Killian, C. McAllister, A.B. Ahmed, J.A. Storer, C.T. Lira, J.E. Jackson

PHYS 453. Small molecules binding to Mn(II) in the active site of *Bacillus subtilis* oxalate decarboxylase studied by high-field EPR spectroscopy. **A. Montoya**, Z. Raad, A. Ozarowski, A. Angerhofer

PHYS 454. Pyrillium derivatives as anolytes for non-aqueous redox flow batteries. **G.C. Kulkarni**, N.H. Attanayake, A.G. Waltner, S. Odom, K.N. Plunkett

PHYS 455. Solvation energy of imidazole using explicit and implicit solvation models. **J.C. Fan**, H. Hernandez

PHYS 456. Molecular dynamics simulation studies for surface properties of aliphatic polyketone membranes for highly efficient emulsified oil–water separation. **A. Shaikh**

PHYS 457. Optimized collagen-like triple helix by density functional theory. **M. Tsai**

PHYS 458. Modeling the reactivity of the catalytic cage of triosephosphate isomerase. **Y. Kulkarni**, Q. Liao, D. Petrovic, F. Byléhn, J.P. Richard, S.C. Kamerlin

PHYS 459. NMR analysis of the effect of G-T mismatches in different sequence contexts on ¹H chemical shifts and NOE intensities. **K. Ljunggren**, G.A. Meints

PHYS 460. Solvation properties of supercritical carbon dioxide (sc-CO₂) using chirped-pulse Fourier-transform microwave spectra of CO₂/1,1-difluoroethene (DFE) mixtures. **T. Ariyaratne**, R.A. Peebles, S.A. Peebles, B.H. Pate, C.T. West

PHYS 461. Quantifying environmental influence on interfacial charge transfer kinetics involving near-infrared organic dyes using excited state lifetimes and transient absorption spectroscopy. **L. Hunt**, J.H. Delcamp, N. Hammer

PHYS 462. Thermo-optical characterization of organic verdazyl biradicals. **C.R. Clark**, E. Ingram, O. Gunaydin-Sen, D.J. Brook

PHYS 463. Effects of natural polymorphisms of non-B HIV-1 protease on protein conformations: A DEER and MD investigation. **T. Tran**, Z. Liu, G.E. Fanucci

PHYS 464. Using 2D spectroscopy to understand excited state dynamics. **M.A. Hermosilla**, S.E. Dominguez, L. Baraldo, V.D. Kleiman

PHYS 465. Effect of adding potassium or lithium chloride on the tetra-n-butylammonium chloride/water semi-clathrate system using differential scanning calorimetry. **D.C. Henriques**

PHYS 466. Vibrational frequency shifts of phosphoenolpyruvate upon binding to allosterically regulated pyruvate kinase. **R.E. Brenner**, C.J. Wurrey, A. Fenton



TECHNICAL PROGRAM

- PHYS 467.** Catalyst effect on dehydrogenation of bulk ammonia borane-polymer composites. **E.N. Ingram**, C. Clark, K. Kharel, W. Taylor, R. Seemaladinne, O. Gunaydin-Sen
- PHYS 468.** Radiation-induced reduction of (TPQ-2)³⁺. **M. Cover**, B.H. Milosavljevic
- PHYS 469.** Kinetics of substituted Wagner-Jauregg reactions studied by ¹H-NMR with an adaptive Python program for integration of poorly resolved spectra. **A. Enders**, A. Hill, S.S. Tartakoff
- PHYS 470.** Computational studies of the pathways for the reaction of hydroxyl (OH) with ketene. **C. Leung**, P. Marshall
- PHYS 471.** Withdrawn
- PHYS 472.** Macro- and micro-rheological behavior of supercooled ethylene glycol monohydrate. **E. Zimmerer**, **Y. Al Awadhi**, B.H. Milosavljevic
- PHYS 473.** New model in the determination of thermodynamic properties of mixed electrolyte solutions with a common ion. **M.A. Siddiq**, R. Wigent
- PHYS 474.** Computational approach to glucose detection with SERS. **S. Afroosheh**
- PHYS 475.** Withdrawn
- PHYS 476.** Employing fluorescence microscopy to interrogate single molecular catalysts and self-assembled nanocellulose structures. **Q. Easter**
- PHYS 477.** Partial molar volumes and isentropic compressions of sugar alcohols in aqueous solutions from 15°C to 40°C at atmospheric pressure. **Y. Bouchibti**, M. Mera, S. Brown, P. Bernal
- PHYS 478.** Twisting of a mechanosensitive molecular probe detects lipid order in membranes. **G. Licari**, E. Tajkhorshid
- PHYS 479.** Electron donor-donor-acceptor triad: Dual charge-transfer emission showing anti-kasha behavior. **J. Lin**, P.P. Chou
- PHYS 480.** Using vibrational sum frequency generation to investigate the adsorption of N3 dye in different pH conditions. **Y. Farah**, C. Rich, A.T. Krummel
- PHYS 481.** Self-assembly of nearly isotropic conjugated polymer aggregates with high quenching efficiency. **Y. Kwon**, J. Yang, L. Kaufman
- PHYS 482.** Plasmonic microneedles for continuous pH monitoring using surface-enhanced Raman spectroscopy. **J. Park**, R.P. Van Duyne, N. Tanyeri, M. Mrksich
- PHYS 483.** On a new path to computing the vibrational spectra of PAHs. **R.C. Fortenberry**, J.P. Layfield, T.J. Lee
- PHYS 484.** IR, Raman and SFG spectra from DFT-based molecular dynamics simulations: Simplifying the calculations and graph theory analysis of the vibrational modes. **D. Galimberti**, S. Bougueroua, S. Pezzotti, M.P. Gaigeot
- PHYS 485.** Investigation of cobalt phthalocyanine at the solid/liquid interface by electrochemical tip-enhanced Raman spectroscopy. **S. Jiang**, Z. Chen, X. Chen, D. Nguyen, R.P. Van Duyne



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- PHYS 486.** Waveguiding in single zinc oxide nanorods. **B. Chon**, Y. Lee, J. Hahm, J. Truong, M. Hansen
- PHYS 487.** Far-red photoactivatable BODIPYs for the super-resolution imaging of live cells. **Y. Zhang**, K. Song, C. Sun, H. Zhang, F.M. Raymo
- PHYS 488.** Withdrawn
- PHYS 489.** Adsorption and diffusion on a phosphorene monolayer: DFT study. **A. Sibari**, Z. Kerrami, A. Kara, M. Hamedoun, A. Benyoussef, O. Mounkachi, M. Benaissa
- PHYS 490.** Active tuning of phonons and surface-phonon polariton resonances. **A.D. Dunkelberger**, C. Ellis, D.C. Ratchford, A.J. Giles, S. Katzer, R.B. Davidson, A.B. Grafton, M. Kim, C. Kim, I. Vurgaftman, J. Tischler, J. Caldwell, J. Owrutsky
- PHYS 491.** Segmental ¹³C-labeling and Raman microspectroscopy of α -synuclein amyloid formation. **J.D. Flynn**, Z. Jiang, J.C. Lee
- PHYS 492.** Energy transfer among CdSe/CdS nanoparticles studied with time resolved super-resolution microscopy. **M. Dunlap**, D. Ryan, P. Goodwin, J. Werner, S. Majumder, J.A. Hollingsworth, M. Gelfand, A.K. Van Orden
- PHYS 493.** Tip-enhanced Raman excitation spectroscopy (TERES) for understanding localized plasmon in the tip-sample junction. **M. Yang**, M. Mattei, X. Chen, G.C. Schatz, R.P. Van Duyne
- PHYS 494.** Covert photonic barcodes based on light controlled acidochromism. **Y. Yan**, Z. Gao, Y. Zhao
- PHYS 495.** BODIPY-based photoactivatable probes for single molecule localization-based super-resolution microscopy. **C. Wijesooriya**, J. Peterson, A. Winter, E.A. Smith
- PHYS 496.** Conformational preference for triplet production in multichromophoric molecules via single molecule spectroscopy. **D.J. Walwark**, B. Datko, J.K. Grey
- PHYS 497.** Characterizing photophysics and solvent dependence of BODIPY dye derivatives through ultrafast two-dimensional electronic spectroscopy and pump-probe spectroscopy. **Y. Lee**, R.M. Malamakal, D.M. Chenoweth, J.M. Anna
- PHYS 498.** Molecular orientation at an organic light emitting diode material/substrate interface using Vibrational Sum Frequency Generation Spectroscopy. **D. Bhattacharyya**, A.V. Benderskii
- PHYS 499.** Nonadiabatic chemical transformations of nitric oxide radicals with combustion partners. K.J. Blackshaw, N. Quartey, M. Marracci, A.S. Petit, **N.M. Kidwell**
- PHYS 500.** Studies of molecular interactions by vibronically resolved solid-state fluorescence spectroscopy: From small molecules to MOFs. C. Grinnell, J. Dai, M.L. McKee, **A. Samokhvalov**
- PHYS 501.** Using density functional based tight binding methods in vibrational circular dichroism. T. Teodoro, M. Koenis, S. Galembeck, P. Nicu, W. Buma, **L. Visscher**
- PHYS 502.** Projected site-occupation embedding theory (P-SOET). **B. Senjean**, E. Fromager



TECHNICAL PROGRAM

PHYS 503. Linear infrared and ultrafast nonlinear infrared spectroscopies reveal detailed solute-solvent dynamics of NO-releasing molecules. **J. Wang**

PHYS 504. Thermal and mechanical stability of metal-organic frameworks. **M.R. Ryder**

PHYS 505. Three-dimensional spectroscopic single-molecule localization microscopy using bi-plane detection. **K. Song**, Y. Zhang, C. Sun, H. Zhang

PHYS 506. Using fluorescence anisotropy to monitor catalytic polymerization reactions confined in droplets. **A. Cavell**, V. Krasecki, R.H. Goldsmith

PHYS 507. Probing a strongly coupled system via surface enhanced Raman excitation spectroscopy. **Y. Wu**, T. Ueltschi, C. Cherqui, M. Bourgeois, G.C. Schatz, R.P. Van Duyne

PHYS 508. Ratio of the number of states in asymmetric and symmetric ozone molecules deviates from the symmetry driven value of 2. I. Gayday, A. Teplukhin, **D. Babikov**

PHYS 509. Structural analysis of amyloid beta oligomers responsible of Alzheimer's Disease using electronic structure methods. **E. Romero**, F. Hernandez

PHYS 510. Supramolecular triangular tiling of electron active macrocycles for the design of organic conductors and photoconductors. **Y. Beldjoudi**, M. Cetin, A. Narayanan, J.F. Stoddart

THURSDAY MORNING

Section A

Orange County Convention Center
Room W331A

Producing Equilibrium Amorphous Packings

Hard Spheres & Jammed Systems

Cosponsored by COLL and PMSE
Z. Fakhraai, D. Sussman, *Organizers*
D. Sussman, *Presiding*

8:00 PHYS 511. Machine-learned softness as a tool for understanding glass formation and properties. **A.J. Liu**, D. Sussman, F. Landes, G. Biroli, O. Dauchot, D.R. Reichman

8:40 PHYS 512. Equilibrium dynamics of thermal glasses derived from athermal hard spheres configurations. **F. Arceri**, E. Corwin

9:00 PHYS 513. Ultrastable amorphous packings of spheres. **C. Brito**

9:40 Intermission.



TECHNICAL PROGRAM

10:00 PHYS 514. Densest vs. jammed packings of 2D bent-core trimers. **R. Hoy**, A. Griffith

10:20 PHYS 515. Making glasses from crystals or vapors. **Y. Han**

11:00 PHYS 516. Crystallization vs. vitrification. **K.K. Mandadapu**

Section B

Orange County Convention Center
Room W330C

Modeling Dynamics in Dense Manifolds of Electronic States

Nonadiabatic Molecular Dynamics

Cosponsored by COMP
B. G. Levine, P. Slavicek, *Organizers*
D. Fedorov, *Presiding*

8:00 PHYS 517. Is an efficient intermolecular energy transfer from vibrations to electronic motion possible? **L.S. Cederbaum**

8:40 PHYS 518. Non-adiabatic dynamics with TDDFT. **L. Lacombe**, N.T. Maitra

9:00 PHYS 519. Dynamics in highly excited electronic states: Quantum dynamics and time-resolved spectroscopy. **M. Schuurman**

9:40 PHYS 520. Non-adiabatic molecular dynamics for (ultra-)strong light-matter interaction. **Y. Zhang**, T. Nelson, S. Tretiak

10:00 Intermission.

10:20 PHYS 521. From a dense manifold to a single surface: The exact factorization approach to coupled electron-ion dynamics. **N.T. Maitra**

11:00 PHYS 522. Excited state dynamics involved in the double photodetachment of $F^{\bullet}H_2O$ in an intense laser field. **L. McCaslin**, R. Gerber

11:20 PHYS 523. Using quasi-diabatic propagation scheme to simulate non-adiabatic dynamics in dense manifolds of states. **P. Huo**

Section C

Orange County Convention Center
Room W330B

Frontiers in Vibrational Spectroscopy: Experiments & Theory

New Theoretical Approaches to Vibrations



TECHNICAL PROGRAM

E. Garand, R. Steele, *Organizers*
S. Dasgupta, *Presiding*

8:00 PHYS 524. Domain localized vibrational method for studying hydrogen-bond network in biomolecules. **K. Yagi**

8:30 PHYS 525. OH-stretch Raman multivariate curve resolution spectroscopy of HOD/H₂O mixtures. **A.A. Kananenka,**
J.L. Skinner

8:50 PHYS 526. Novel coordinate based approaches for calculating vibrational spectra. **M.W. Hanson-Heine**

9:20 PHYS 527. Vibrations as seen through a neural network potential. **A.E. Roitberg**

9:50 Intermission.

10:05 PHYS 528. Computing vibrational spectra: Exploiting locality in adaptive potential energy surface construction and vibrational coupled cluster theory. **O. Christiansen**

10:35 PHYS 529. Simulation of Raman optical activity spectra using advanced quantum chemical methods. **A.M. James,**
T. Crawford

10:55 PHYS 530. Efficient calculation of overtones and combination bands in theoretical vibrational spectroscopy with localized modes. A. Hoeske, P. Panek, **C. Jacob**

11:15 PHYS 531. Quantum calculations of vibrational dynamics of the proton and H₂ molecule embedded in water clusters using many-body ab initio potentials.. **J.M. Bowman,** C. Qu, Q. Yu

Section D

Orange County Convention Center
Room W313

Structure & Dynamics of Electrolytes: From the Bulk to Interfaces

Electrolytes at Interfaces

R. Jorn, D. G. Kuroda, *Organizers*
R. Kumar, *Organizer, Presiding*
C. G. Arges, *Presiding*

8:30 PHYS 532. Computational studies of an acidic proton at the graphene-oxide – water interface. **R. David,** V. Subasingheghe Don, P. Du, A. Milet, R. Kumar

9:00 PHYS 533. Molecular simulation results on charged carbon-nanotube forest supercapacitors. **L.R. Pratt,** A. Muraldiharan, M. Chaudhari, S. Rempe, G.G. Hoffman

9:30 PHYS 534. Electron transfer in the solid-electrolyte interphase. **T.F. Miller**



TECHNICAL PROGRAM

10:00 PHYS 535. When bulk isn't: The Role of surface films and the electrode interface on ion solvation in lithium-ion electrolytes. **R. Jorn**

10:20 Intermission.

10:35 PHYS 536. Interfacial reactions at the surface of Li metal anodes of Li-S batteries: Effects of high salt concentration. **P.B. Balbuena**

11:05 PHYS 537. First-principles molecular dynamics study for SEI film formation mechanism of lithium ion batteries. **K. Sodeyama**

11:35 PHYS 538. Electrodes as polarizing functional groups: Correlation between Hammett parameters and electrochemical polarization. **S. Sarkar**, J. Patrow, M.J. Voegtle, A. Pennathur, J. Dawlaty

Section E

Orange County Convention Center
Room W312C

New Frontiers in the Confluence of Experimental Thermodynamics, Structural Investigations & Theory/Computation

Experimental Thermodynamics of Interfacial Phenomena

Cosponsored by GEOC
N. Birkner, *Organizer*
K. Lilova, D. Wu, *Organizers, Presiding*
N. Birkner, H. Sun, *Presiding*

8:00 PHYS 539. Modified Cu-BTC for highly-enhanced adsorption of organosulfur species. D. Wang, X. Han, B. Shen, **H. Sun**, D. Wu

8:20 PHYS 540. Energetics, structural and electrochemical studies on MXenes etched by cobalt fluoride. **C.B. Cockreham**, X. Guo, H. Xu, D. Wu

8:40 PHYS 541. Hydromagnesite: Case study of solid-state NMR tensors and the development of the Local Spectroscopy Data Infrastructure (LSDI) NMR database. H. Sun, J. Cui, D. Olmsted, S. Dwaraknath, M.D. Asta, K. Persson, **S.E. Hayes**

9:00 PHYS 542. Confinement of water in ion-exchanged chalcogenide UCR-20. **C. Yang**, X. Chen, G. Li, P. Feng, X. Bu, X. Guo, D. Wu

9:20 PHYS 543. Modification of carbon support for Pd-based catalysts to electro-oxidize formic acid. **S. Hu**, J. Hui, G. Luo, L. Scudiero, S. Ha, X. Zhang

9:40 PHYS 544. Effect of solvent polarity on the roughness-dependent wetting behavior of SAMs. **C. Du**, J. Chen, M.M. Thuo, Z. Wang

10:00 Intermission.



TECHNICAL PROGRAM

10:15 PHYS 545. Pore chemistry and size control in anion-pillared hybrid porous materials for highly efficient gas separation. **H. Xing**

10:45 PHYS 546. Thermodynamics of CO₂ capture using organoamine-functionalized halloysite. **M. Hawkins**, X. Zhang, H. Li, J. Sun, Y. Wang, X. Guo, D. Wu

11:05 PHYS 547. Microporous core-shell catalysts for the selective oxidation of benzyl alcohol. **S.R. Saunders**, E. Hammond-Pereira

11:35 PHYS 548. Ice nucleation far from equilibrium. **J. Belof**

Section F

Orange County Convention Center
Room W311H

Quantum Embedding Electronic Structure Methods

Cosponsored by COMP
M. Pavanello, A. Wasserman, *Organizers*
E. Fromager, *Presiding*

8:30 Introductory Remarks.

8:35 PHYS 549. Multi-state QM/QM extrapolation with electronic embedding for excitation energies. **M. Caricato**, S. Ren, K. Zhang

9:15 PHYS 550. Eliminating spin-contamination of spin-flip time-dependent density-functional theory within linear-response formalism by the use of zeroth-order mixed-reference reduced density matrix. **S. Lee**, M. Filatov, S. Lee, C.H. Choi

9:35 PHYS 551. Self-Attractive Hartree partitioning for density-based embedding. **P. de Silva**, T.A. Van Voorhis, T. Zhu

10:15 Intermission.

10:35 PHYS 552. Projection-based quantum embedding for molecular and periodic systems. **J. Goodpaster**

11:15 PHYS 553. Continuum embedding methods for electrolytes solutions in condensed-matter simulations. **O. Andreussi**

Section G

Orange County Convention Center
Room W311G

Sustainable Software for Computational Molecular Science

Software Tools: Quantum Mechanics



TECHNICAL PROGRAM

Cosponsored by COMP
T. Crawford, E. Marin, J. A. Nash, D. G. Smith, *Organizers*
J. Moussa, *Presiding*

8:30 PHYS 554. Efficient discovery of novel molecules: How to uncover gems in the haystack using open chemistry. **G. Hutchison**

9:00 PHYS 555. Chronus quantum: Next-generation modular quantum chemistry codes. **X. Li**, D. Williams-Young, E.F. Valeev

9:30 PHYS 556. New and efficient Python/C++ modular library for real and complex response functions at the level of Kohn-Sham density functional theory. **Z. Rinkevicius**, L. Xin, O. Vahtras, M. Brand, K. Ahmadzadeh, M. Ringholm, N. List, P. Norman

9:50 PHYS 557. Exploring convergence of thermodynamic and kinetic properties of QM-cluster enzyme models. **N.J. Deyonker**, Q. Cheng, T.J. Summers, M.A. Palma

10:10 Intermission.

10:30 PHYS 558. Thinking inside boxes: Modularizing electronic structure and ab initio molecular dynamics. S. Seritan, K. Thompson, S. Fales, C. Song, R. Parrish, E. Hohenstein, **T.J. Martinez**

11:00 PHYS 559. Using the highly accurate N-determinant quantum Monte Carlo (HANDE-QMC) package for electronic structure calculations in a new research group. H. Petras, T. Mihm, **J.J. Shepherd**

11:20 PHYS 560. Automating high-accuracy thermochemistry and kinetics for combustion. **S.N. Elliott**, M. Keçeli, A.V. Copan, C. Cavallotti, Y. Georgievski, H.F. Schaefer, S.J. Klippenstein

Section H

Orange County Convention Center
Room W340A

Emerging Frontiers in Fluorescence Microscopy: From Single Molecules to Super Resolution

Cosponsored by ANYL
T. Lee, J. C. Vaughan, *Organizers, Presiding*

8:00 PHYS 561. Real-time observation of flexible domain movements in CRISPR-Cas9. **S. Uemura**

8:30 PHYS 562. Brain region specific single molecule imaging of protein assembly. X. Fu, F. Moonschi, A.M. Loe, J. Pauly, **C.I. Richards**

9:00 PHYS 563. Single-molecule correlation spectroscopy reveals rapid conformational dynamics in photosynthetic proteins. T. Kondo, J. Gordon, **G. Schlau-Cohen**

9:30 Intermission.

9:45 PHYS 564. Measuring protein dynamics at nanoscale interfaces. **C.F. Landes**



TECHNICAL PROGRAM

10:15 PHYS 565. Active motility of enzyme-powered vesicle upon catalysis. **S. Ghosh**, F. Mohajerani, A. Somasundar, P.J. Butler, A. Sen

10:35 PHYS 566. (Bio)molecular machines, Markov walks, and single molecule tracking: Ion channels, enzymes, and synthetic polymers. **J.A. Brozik**, E.L. Taylor, M.J. Martinez, B. Lam, C. Barnaba

10:55 PHYS 567. Active feedback tracking of single viruses and fluorophores in solution. S. Hou, J. Exell, X. Lang, **K. Welscher**

11:15 PHYS 568. “Waltz” of Janus particles in cells: Tracking single-particle rotation to unravel cell functions. **Y. Yu**

Elucidation of Mechanisms & Kinetics on Surfaces

Sponsored by CATL, Cosponsored by ENFL, ENVR, INOR and PHYS

THURSDAY AFTERNOON

Section A

Orange County Convention Center
Room W331A

Producing Equilibrium Amorphous Packings

Glass Transition in Bulk & in Thin Films

Cosponsored by COLL and PMSE
D. Sussman, *Organizer*
Z. Fakhraai, *Organizer, Presiding*

1:30 PHYS 569. Glass Transition: Can new data shed light on which Interpretation we should believe? **P. Royall**

2:10 PHYS 570. Insights into the underlying physics of glass formation from long-time and high-throughput equilibrium simulations of glass-formers in thin films and the bulk. **D.S. Simmons**, D. Diaz Vela, J. Hung, T. Patra

2:50 Intermission.

3:10 PHYS 571. Dynamical phase transitions in amorphous thin films. **R. Ivancic**, R. Riggleman

3:30 PHYS 572. Uncovering factors causing dynamic coupling across dissimilar polymer domains. **C.B. Roth**

4:10 PHYS 573. Deformation mechanisms in ultra-thin polymer glasses. **A. Crosby**

Section B

Orange County Convention Center
Room W330C



TECHNICAL PROGRAM

Modeling Dynamics in Dense Manifolds of Electronic States

Nonadiabatic Molecular Dynamics

Cosponsored by COMP
B. G. Levine, P. Slavicek, *Organizers*
B. Levine, *Presiding*

1:30 PHYS 574. Unraveling open-system quantum dynamics of non-interacting Fermions. **R. Baer**, Z. Ruan

2:10 PHYS 575. *Ab initio* Ehrenfest dynamics including nuclear quantum effects. **J. Zheng**

2:30 PHYS 576. Excited-state dynamics with trajectories. **F. Agostini**

3:10 PHYS 577. On the rates of nonadiabatic reactions: Model study and comparison between statistical and dynamics approaches. **S. Mukherjee**, S.A. Varganov

3:30 Intermission.

3:50 PHYS 578. Avoiding trivial states in adiabatic dynamics can lead to unphysical changes in wave function symmetry. E.M. Lee, **A. Willard**

4:30 PHYS 579. *Ab initio* multiple cloning in dense manifolds of electronic states. **D. Fedorov**, B. Levine

4:50 PHYS 580. Exact approach for quantum statistics of multi-electronic-state systems. **J. Liu**

Section C

Orange County Convention Center
Room W330B

Frontiers in Vibrational Spectroscopy: Experiments & Theory

Clusters & Ions

E. Garand, R. Steele, *Organizers*
A. A. Kananenka, *Presiding*

1:30 PHYS 581. Combining ultra-high resolution ion mobility with cryogenic ion vibrational spectroscopy for the analysis of glycans. S. Warnke, A. Ben Faleh, **T.R. Rizzo**

2:05 PHYS 582. *Ab Initio* calculations of the resonance Raman spectrum of the hydrated electron. **S. Dasgupta**, M. Coons, J. Herbert

2:25 PHYS 583. Monitoring ion hydration through computational vibrational spectroscopy. **F. Paesani**

3:00 Intermission.



TECHNICAL PROGRAM

3:20 PHYS 584. Infrared spectroscopy hemibonded clusters of H₂S. **A. Fujii**

3:55 PHYS 585. Deciphering the vibrational signatures of the water-iodide binary complex through quantum computations.. **J. Talbot**, R. Steele

4:15 PHYS 586. Deconstructing the molecular level mechanics driving spectral diffusion in water with temperature-controlled cluster spectroscopy. **M.A. Johnson**

Section D

Orange County Convention Center
Room W313

Structure & Dynamics of Electrolytes: From the Bulk to Interfaces

Structure & Transport in Electrolytes

R. Jorn, D. G. Kuroda, *Organizers*
R. Kumar, *Organizer, Presiding*
R. David, A. Tuladhar, *Presiding*

1:30 PHYS 587. Scaling theory for access resistance: Golden aspect ratio for ion transport simulation in nanopores. **S. Sahu**, M. Zwolak

1:50 PHYS 588. Cross-influence of electromotive force and chemical potential in confined environment. **Y. Qiao**, M. Wang

2:10 PHYS 589. Interfacial water at graphene oxide surface: Ordered or disordered? **V. Subasinghe Don**, R. David, P. Du, A. Milet, R. Kumar

2:30 Intermission.

2:45 PHYS 590. Do electrons in water and electrolytes care of each other? **P. Slavicek**

3:05 PHYS 591. Effect of hydration and dehydration kinetics of the carbonic acid-carbon dioxide interconversion on ionizable solute dissolution in bicarbonate buffer: Hydrodynamics-dependent effective buffer pKa. **N. Salehi, J. Al-Gousous**, G. Amidon, R. Ziff, P. Langguth, G.L. Amidon

3:25 PHYS 592. Ultrafast dynamics of hot electrons in plasmon-excited metal gratings. **Y. Wang**, L. Shen, B. Hou, Y. Wang, S. Cronin, J. Dawlaty

3:45 PHYS 593. Electric fields break Lewis adducts: Relation to frustrated Lewis pairs. **M.J. Voegtle**, J. Patrow, J. Dawlaty

Section E

Orange County Convention Center
Room W312C



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

New Frontiers in the Confluence of Experimental Thermodynamics, Structural Investigations & Theory/Computation

Thermodynamics of Organic, Bioorganic & Physiological Systems

Cosponsored by GEOC

N. Birkner, *Organizer*

K. Lilova, D. Wu, *Organizers, Presiding*

N. Birkner, T. Subramani, *Presiding*

1:30 PHYS 594. New strategy to prepare highly porous polymer ultrafiltration membranes. R. Thankamony, X. Li, **Z. Lai**

1:50 PHYS 595. New catalysis and sensing on the Ionic liquid/ electric interface. **Z. Wang**

2:10 PHYS 596. Improved chemical kinetic model for combustion of sarin simulant based on shock tube experiments and computational investigations. **S. Neupane**, A. Masunov, S. Vasu

2:30 PHYS 597. Modeling peptides under simultaneous application of high pressure and plastic shear. **B.A. Steele**, S.M. Clarke, J.M. Zaug, V. Prakapenka, E. Greenberg, E. Stavrou, I.W. Kuo

2:50 PHYS 598. On the origin of the anomalous long-time tail in the solvation dynamics of DNA. S. Mukherjee, S. Mondal, S. Acharya, **B. Bagchi**

3:10 PHYS 599. Mitochondrial energetics with electrostatically localized protons: Do we have a thermotrophic feature? **J.W. Lee**

3:30 PHYS 600. Experimental determination of RMS & molecular velocity of all chemical elements. **S.N. Olatunji**

3:50 Intermission.

4:05 PHYS 601. Centrosymmetric versus non-centrosymmetric crystals for terahertz generation: Just one carbon away. **E.S. Weir**, G. Valdivia, J. Johnson, D.J. Michaelis, K. Kenney, A. Wayment, S.J. Smith

4:25 PHYS 602. Solubilities of tetrakis(2,2,6,6-tetramethyl-4-piperidiny)-N,N'-hexamethylenediaspartate in the N,N'-dimethylformamide and acetone. **W. Wang**, Z. Wang, J. Niu, W. Fu'An

4:45 PHYS 603. Insights into the role of counterions on polyelectrolyte-modified nanopore accessibility. **E. Gonzalez Solveyra**, L. Silies, A. Andrieu-Brunsen, I. Szleifer

5:05 PHYS 604. Hydration and ion-pairing properties of citrate in the presence of sodium ions. **B. Kutus**, C. Dudás, S. Friesen, A. Lupan, A.A. Attia, I. Palinko, G. Peintler, P. Sipos, R. Buchner

Section F

Orange County Convention Center
Room W311H

Quantum Embedding Electronic Structure Methods



TECHNICAL PROGRAM

Cosponsored by COMP
M. Pavanello, A. Wasserman, *Organizers*
M. Mosquera, *Presiding*

1:30 Introductory Remarks.

1:35 **PHYS 605.** Optimization of kinetic energy functionals for subsystem TD-DFT. S. Grimmel, T. Teodoro, **L. Visscher**

2:15 **PHYS 606.** Nonlocal kinetic energy density functionals appropriate for finite systems and embedding simulations. **W. Mi**, M. Pavanello

2:35 **PHYS 607.** Withdrawn

3:15 Intermission.

3:35 **PHYS 608.** Quasi diabatic representation for nonadiabatic quantum dynamics propagation. **S. Yamijala**, A. Mandal, P. Huo

3:55 **PHYS 609.** Fragment based ab initio molecular dynamics from symplectic decomposition of molecular structure: post-Hartree-Fock accuracy at DFT cost for both Born-Oppenheimer and Car-Parrinello-like implementations. **S.S. Iyengar**

Section G

Orange County Convention Center
Room W311G

Sustainable Software for Computational Molecular Science

Methods

Cosponsored by COMP
T. Crawford, E. Marin, J. A. Nash, D. G. Smith, *Organizers*
J. Moussa, *Presiding*

1:30 **PHYS 610.** Efficient rotation of multipole expansions in the Fast Multipole Method. **V. Anisimov**

1:50 **PHYS 611.** Exploiting symmetry to speed up symmetric nudge elastic band calculations. **J. Garcia Lastra**, N.R. Mathiesen, T. Vegge

2:10 **PHYS 612.** Improvements to the treecode-accelerated boundary integral Poisson--Boltzmann solver. **L. Wilson**, R. Krasny, W. Geng, J. Chen

2:30 Intermission.

2:50 **PHYS 613.** Unified efficient thermostat scheme for molecular dynamics and path integral molecular dynamics. **J. Liu**

3:10 **PHYS 614.** Nonadiabatic statistical theory with the Zhu-Nakamura transition probability for predicting the intersystem crossing rates. **A.O. Lykhin**, S.A. Varganov



TECHNICAL PROGRAM

3:30 PHYS 615. Exact solutions of a fully-correlated 3D few-electron gas. **J. Jerke**, E.R. Bittner, B. Poirier

3:50 PHYS 616. Large-scale benchmark of electronic structure solvers with the ELSI infrastructure. **V. Yu**, W. Dawson, A. García, V. Havu, B. Hourahine, W.P. Huhn, M. Jacquelin, W. Jia, M. Keçeli, R. Laasner, Y. Li, L. Lin, J. Lu, J. Roman, A. Vazquez-Mayagoitia, C. Yang, V. Blum

Section H

Orange County Convention Center
Room W340A

Emerging Frontiers in Fluorescence Microscopy: From Single Molecules to Super Resolution

Cosponsored by ANYL
T. Lee, J. C. Vaughan, *Organizers, Presiding*

1:30 PHYS 617. Optically modulated fluorescent proteins for improved fluorescence microscopy 1. **R. Dickson**

2:00 PHYS 618. Novel strategies to enhance the photostability of fluorescent dyes for single molecule imaging. **G. Cosa**

2:30 PHYS 619. Towards multiplexed detection of biomarkers with single-molecule FRET. A. Kaur, K. Sapkota, **S. Dhakal**

2:50 PHYS 620. Directed nanoparticle assembly based on super-resolution fluorescence microscopy. **S. Kim**, T. Lee

3:10 Intermission.

3:25 PHYS 621. Single molecule probes and single particles probed. **L. Kaufman**

3:55 PHYS 622. Single-molecule localization, orientation, and dynamics for super-resolution microscopy in polymer science. **M. Wang**, Z. Qiang, K. Shebek, J. Marr, M. Irie, J. Gilman, J.A. Liddle

4:15 PHYS 623. Counting multiple triplets on a single multi-chromophoric molecule using fluorescence quenching dynamics. **J.K. Grey**

4:35 PHYS 624. Super-resolution catalysis Imaging. **P. Chen**

Activation of Light (C1-C4) Hydrocarbons: Theory & Experiments

Sponsored by CATL, Cosponsored by ENFL, ENVR, INOR and PHYS

Elucidation of Mechanisms & Kinetics on Surfaces

Sponsored by CATL, Cosponsored by ENFL, ENVR, INOR and PHYS



TECHNICAL PROGRAM

POLY

Division of Polymer Chemistry

B. Helms, T. Epps and H. Brown, *Program Chairs*

SUNDAY MORNING

Section A

Rosen Centre Hotel
Signature 2

ACS Award in Polymer Chemistry in Honor of Tim Swager

M. Jeffries-El, S. A. Sydlik, *Organizers, Presiding*

8:10 Introductory Remarks.

8:15 **POLY 1.** Using light to grow materials. J.R. Lamb, K. Qin, **J.A. Johnson**

8:45 **POLY 2.** Programming macromolecules to encode functions. **V. Percec**

9:15 **POLY 3.** Photocontrolling dynamic covalent chemistry in polymer networks. **J.A. Kalow**

9:45 Intermission.

10:00 **POLY 4.** Instructed-assembly to form supramolecular polymers for controlling cell fates. H. Wang, Z. Feng, H. He, J. Wang, **B. Xu**

10:30 **POLY 5.** Amplifying fluorescent sensors based on molecular systems with extended electronic delocalization. **E.E. Nesterov**

11:00 **POLY 6.** Polymer films created by reactive vapor deposition and their application in wearable electronics. **T.L. Andrew**

11:30 **POLY 7.** Metal-free purely organic phosphors: Molecular design and applications. **J. Kim**

Section B

Rosen Centre Hotel
Salon 12

Synthesis & Properties of Densely Grafted Polymers



TECHNICAL PROGRAM

J. B. Matson, G. Stein, R. Verduzco, *Organizers*
J. G. Kennemur, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 POLY 8. Densely grafted polymers by ATRP. **K. Matyjaszewski**

8:50 POLY 9. Chain growth polycondensation via substituent effects for the synthesis of functional rigid rod polymer brushes. **S.G. Boyes**, F.C. Prehn, C. Reese, S. Vyas, A. Kennedy

9:10 POLY 10. Macromolecules with programmable shape, size, and chemistry. **D. Guironnet**, D. Walsh, C.E. Sing, S. Rogers, M. Wade, S. Dutta

9:30 POLY 11. Simple grafting-to, radical coupling strategy yields post-synthesis tuning of grafting density in bottlebrush polymers: Synthesis and characterization of bulk and confined properties. L. Li, K. Jin, X. Chen, **J.M. Torkelson**

9:50 Intermission.

10:20 POLY 12. Molecular polymer brush templating for compartmentalized hybrid materials and soft matter. **M. Muellner**

10:50 POLY 13. Thermodynamics of bottlebrush systems from low-strain cycloolefins. W.J. Neary, T. Isais, B.A. Fultz, **J.G. Kennemur**

11:10 POLY 14. Amphiphilic double-brushes as stabilizers of hydrophobic solutes. **M. Herrera-Alonso**

11:30 POLY 15. Ultrasound-induced chain scission of the dendronized polymers: The effect of side chains on the mechanochemical degradation. **K. Bang**, G.I. Peterson, T. Choi

Section C

Rosen Centre Hotel
Salon 19

The Fate of Plastics in Water

R. T. Mathers, S. A. Miller, *Organizers, Presiding*
A. P. Dove, U. Natarajan, M. A. Pasquinelli, *Presiding*

8:20 POLY 16. Quantification of polypropylene degradation as a function of depth in recovered ocean plastics. **S.V. Orski**, K. Beers, V. Rodriguez C.

9:00 POLY 17. Degradable materials by the radical polymerization of cyclic ketene acetals. **Y. Guillaneuf**

9:20 POLY 18. Weak link strategies for polymer degradation. **S.A. Miller**, S. Shen, G. Short, J. Smith, J. Torgunrud

10:00 POLY 19. Low density expanded poly(lactide) with star polymers via subcritical CO₂ processing for biodegradable floral foams. **P.T. Dirlam**, M.A. Hillmyer



TECHNICAL PROGRAM

10:20 Intermission.

10:35 **POLY 20.** Extraction, synthesis, and characterization of biopolymers from plant waste. **S. Shen**, J.A. Thomas, S.A. Miller

10:55 **POLY 21.** Natural biomass-based sustainable polymers: lignin as a crosslinker in shape memory polymers. **H. Chung**, H. Liu

11:25 **POLY 22.** Degradable epoxy resins containing multifunctional biobased components. **M. Shen**, G. Yang, R. Almallahi, Z. Rizvi, E. Gonzalez, T. Hendrix- Doucette, M.L. Robertson

Section D

Rosen Centre Hotel
Salon 23

General Topics: New Synthesis & Characterization of Polymers

D. Garcia, *Organizer*
A. Bristol, M. R. Elshaer, *Presiding*

8:00 **POLY 23.** Characterizing the molecular weight of conjugated polymers using gel permeation chromatography and static light scattering. **R. Fair**, R. Xie, R.H. Colby, E. Gomez

8:20 **POLY 24.** nano-FTIR based identification & characterization of polymers at 10nm resolution. **A. Huber**, T. Gokus, S. Mastel

8:40 **POLY 25.** BODIPY based ultra-low band gap D-A polymer with NIR absorption and emission. **G. Tarafdar**, U. Pandey, P. Ramamurthy

9:00 **POLY 26.** Characterization of PEEK filaments for extrusion-based additive manufacturing processes. **M. Garcia**, C. Basgül, B. Streifel, R.L. Middleton, S. Kurtz

9:20 **POLY 27.** Spectroscopic characterization of modified polyethyleneimine. **J.D. Mizvesky**, R. Wodzinski, **M.R. Elshaer**

9:40 **POLY 28.** Amphidynamic behavior in covalent organic frameworks probed via powder X-ray diffraction and ¹³C CP-MAS T₁ relaxation experiments. **D.A. Vazquez-Molina**, F.J. Uribe-Romo

10:00 **POLY 29.** Structure and dopant engineering in PEDOT thin films: Dramatic conductivity enhancement and application to 100% polymeric transparent film heaters. **J. Simonato**, A. Carella, M. Gueye, R. Demadrille, J. Faure-Vincent

10:20 **POLY 30.** High lithium-ion transference number electrolytes based on poly(lithium bis(alkenylmalonato)borate) solutions. **B.L. Dewing**, N.G. Bible, C.J. Ellison, M.K. Mahanthappa

10:40 **POLY 31.** Magneto-optics in semiconducting conjugated polymers. **P. Wang**, T.M. Swager



TECHNICAL PROGRAM

11:00 POLY 32. Advanced gas separation membranes from ionic-group-mediated polyimides of intrinsic microporosity: Ionic-PIM-PIs. **I. Kammakakam**, J.E. Bara

11:20 POLY 33. High dielectric constant semiconducting poly(3-alkylthiophene)s from side-chain modification with polar sulfinyl and sulfonyl groups. **C. Wang**, Z. Zhang, S. Pejic, R. Li, M. Fukuto, L. Zhu, G. Sauve

Section E

Rosen Centre Hotel
Salon 20

New Frontiers in Aerospace Polymers: Advances & Challenges in Experiments & Simulations

Advances in Thermoset Polymers & Composites

Cosponsored by PMSE

Financially supported by Air Force Research Laboratory; Bruker Instruments; Anasys Instruments; Boeing

M. A. Meador, D. Nepal, *Organizers*

J. S. Wiggins, *Organizer, Presiding*

C. Reynolds, *Presiding*

8:00 POLY 34. Multi-aromatic epoxy-amine thermosets with high performance properties. **R.J. Varley**, L.C. Henderson, L. Reyes

8:30 POLY 35. Novel furan-based thermosetting polymer systems. **G.R. Palmese**

9:00 POLY 36. Determining amine reactivities effect on epoxy network formation: Influence of chemical structure and processing conditions on local properties. **J. Bates**, J.S. Wiggins, D. Nepal, C. Estridge, H. Koerner, S.J. Tucker, V. Varshney

9:20 POLY 37. Development of a fundamental understanding of the curing kinetics of benzoxazine/epoxy blends *via in situ* Fourier transform infrared spectroscopy. **S. Hawkins**, A. Maffe, E. Barjasteh, D. Nepal

9:40 Intermission.

10:00 POLY 38. Directly spun, aligned carbon nanotubes and carbon fibre epoxy-based hybrid composites for the potential applications in aerospace engineering. **S. Rahatekar**, J. Chen, K. Hazra, A. Lekawa, K. Koziol

10:20 POLY 39. Phenylphosphine oxide functional benzoxazine as low earth orbit stable composite matrix polymers. **W.K. Fuchs**, J.S. Wiggins

10:40 POLY 40. Moisture adsorption of the benzoxazine-based thermoset matrix for advanced composite applications. **J. Bannuelos**, E. Barjasteh

11:00 POLY 41. Radical-anion complexes on plasma-treated thermoplastic composite surfaces. **T. Oldham**, D.R. Ferriell, M.A. Belcher, A. Rubin, E. Thimsen

Section F



TECHNICAL PROGRAM

Rosen Centre Hotel
Salon 21

Poly(2-oxazoline)s & Polypeptoids

R. Hoogenboom, H. Schlaad, R. N. Zuckermann, *Organizers*
M. Hruby, R. Luxenhofer, *Presiding*

8:00 Introductory Remarks.

8:05 POLY 42. Poly(2-oxazoline)s with 2,2'- imino diacetate end groups for conjugation with proteins. **J.C. Tiller**, M. Hijazi, P. Spiekermann, C. Krumm

8:35 POLY 43. Biomedical potentials for biomimetic peptoids. **K. Kirshenbaum**

9:05 POLY 44. Structure-property relationships and therapeutic efficacy of ultra-high drug loaded poly(2-oxazoline)/poly(2-oxazine) micelles. **R. Luxenhofer**, M. Lübtow, H. Malik, Z. He, X. Wan, R. Jordan, A. Kabanov

9:35 Intermission.

9:50 POLY 45. Amplification of protein detection signal using poly(2-methyl-2-oxazoline) based mixed brushes with switchable properties. **Y. Wang**

10:20 POLY 46. Polysaccharide-*graft*-poly(2-alkyl-2-oxazoline) hybrid copolymers: Versatile materials for bioapplications. **M. Hruby**, L. Loukotova, M. Rabyk

10:50 POLY 47. Functional bioinspired polypeptide-based polymers. **J. Sun**, Y. Ni, z. shi

11:20 POLY 48. POZ™ – poly(2-oxazoline) update on next generation in polymer therapeutics. **R. Moreadith**

Section G

Rosen Centre Hotel
Salon 22

Polymer-Based Gene & Drug Delivery Systems

Polymers for DDS

X. M. Liu, Y. Ohya, Y. Wang, *Organizers*
T. Fujiwara, *Organizer, Presiding*
L. Zhu, *Presiding*

8:00 Introductory Remarks.

8:05 POLY 49. Macromolecular therapeutics and combination therapies. **J. Hedrick**, N. Park, Y. Yang



TECHNICAL PROGRAM

8:40 POLY 50. Disulfiram copper nanoparticles prepared with a Stabilized Metal Ion Ligand Complex (SMILE) method for cancers treatment. **F. Li**, W. Chen, w. yang, P. Chen, Y. Huang

9:00 POLY 51. Block-copolymer-based polyion complexes for utilization of proteins and inorganic nanoparticles. **A. Kishimura**, Y. Liu, B. KC, T. Egashira, T. Mori, Y. Katayama

9:20 POLY 52. Hydrogel microparticles for drug delivery: Effects of shape and peptide conjugation. **E.P. Kharlampieva**

9:40 Intermission.

10:00 POLY 53. Polymer prodrug nanocarriers for anticancer therapy. **J. Nicolas**

10:20 POLY 54. Triggerable self-immolative nanoparticles for drug delivery. **E.R. Gillies**, B. Fan

10:40 POLY 55. Biodegradable irreversible thermo-gelling polymer systems for drug delivery and other medical applications. **Y. Ohya**, Y. Yoshizaki, T. Nagata, Y. Yoshida, K. Takata, A. Kuzuya

11:00 POLY 56. Post-modifications of recombinant polypeptides for the design of solvent-free self-assembled drug nanocarriers. **E.B. Garanger**, M. Bravo Anaya, S. Lecommandoux

11:20 POLY 57. Polymer zwitterion-temozolomide conjugates for glioblastoma treatment. **S. Ward**, M. Skinner, B. Saha, T. Emrick

Antimicrobial & Cell-Penetrating Polymers

Sponsored by PMSE, Cosponsored by POLY‡

SUNDAY AFTERNOON

Section A

Rosen Centre Hotel
Signature 2

ACS Award in Polymer Chemistry in Honor of Tim Swager

M. Jeffries-EI, S. A. Sydlik, *Organizers, Presiding*

1:00 POLY 58. Dehydration polymerization for poly(hetero)arene conjugated polymers. **D. Schipper**

1:30 POLY 59. New advances in polymer electrolytes. **G.W. Coates**

2:00 POLY 60. Design and synthesis of conjugated polymers based on benzo[1,2-*b*:4,5-*b'*] and Naphtho[2,1-*b*:6,5-*b'*]chalcogenophenes. **M. Jeffries-EI**, C. Gott, E. Muller, A. Brown

2:30 Intermission.



TECHNICAL PROGRAM

2:45 POLY 61. Matchmaking in catalyst-transfer polymerization. **A.J. McNeil**

3:15 POLY 62. Using ROMP to prepare polymers with controlled structures. **R.H. Grubbs**

3:45 POLY 63. 3D printing stem cell instructive Functional Graphenic Materials (FGM) for bone regeneration scaffolds. **S.A. Sydlik**, B. Holt, A. Arnold

4:15 POLY 64. **Award Address** (ACS Award in Polymer Chemistry sponsored by the ExxonMobil Chemical Company). Polymers with unconventional structure and function. **T.M. Swager**

Section B

Rosen Centre Hotel
Salon 12

Synthesis & Properties of Densely Grafted Polymers

J. G. Kennemur, J. B. Matson, G. Stein, R. Verduzco, *Organizers*
K. Beers, *Presiding*

1:00 POLY 65. Striving for perfection: “Defect”-free brush polymer networks for improved metrology. J.M. Sarapas, T.T. Duncan, E. Rettner, E. Chan, **K. Beers**

1:30 POLY 66. Film surface fluctuation dynamics and surface segregation in the limit of dense branching. **M.D. Foster**

2:00 POLY 67. Graft copolymers and bottlebrushes at surfaces for tuning physicochemical and tribological properties of materials. G. Morgese, W. Yan, N. Spencer, M. Zenobi-Wong, **E. Benetti**

2:20 POLY 68. Enthalpy and entropy-driven segregation of mixed bottlebrush polymers in linear polymer matrices. **H. Mei**, T. Laws, J. Li, A. Mah, G. Stein, R. Verduzco

2:40 POLY 69. Interfacial engineering in metal-organic framework-based mixed matrix membranes using covalently grafted polyimide brushes. **T. Li**, H. Wang

3:00 Intermission.

3:30 POLY 70. Structure and properties of liquid crystalline bottlebrush block copolymers. **C.O. Osuji**, M. Gopinadhan, Y. Choo, D. Ndaya, R. Bosire, Y. Rokhlenko, K. Kawamoto, R. Kasi, J.A. Johnson

4:00 POLY 71. Crystallizable α -olefin molecular bottlebrushes: Microstructure evolution during extensional deformation. **C.R. Lopez-Barron**

4:30 POLY 72. Toughness and physical aging in sustainable graft block polymers. **I. Haugan**, B. Lee, M.J. Maher, H.J. Schibur, A. Zografos, S. Jones, M.A. Hillmyer, F.S. Bates

Section C

Rosen Centre Hotel
Salon 19



TECHNICAL PROGRAM

The Fate of Plastics in Water

R. T. Mathers, S. A. Miller, *Organizers, Presiding*
A. P. Dove, U. Natarajan, M. A. Pasquinelli, *Presiding*

1:15 POLY 73. Fate of microplastics in inland waterways. C. Wisinger, L. Maynard, J. Czuba, **J.R. Barone**

1:55 POLY 74. Increasing the water-degradability of PLA. **G. Short**, J. Smith, S.A. Miller

2:15 POLY 75. Elucidating a hydrophobicity trend for oxygen containing functional groups in polymers. **R.T. Mathers**

2:45 POLY 76. Corrosion behavior of biopolyamides derived from itaconic acid. **T. Kaneko**, M. Ali

3:25 Intermission.

3:40 Panel Discussion.

Section D

Rosen Centre Hotel
Salon 23

General Topics: New Synthesis & Characterization of Polymers

D. Garcia, *Organizer*
F. Horkay, R. Shankar, *Presiding*

1:00 POLY 77. Supramolecular polymer-based nanomaterials as a universal combination drug delivery strategy. **J.C. Barnes**

1:20 POLY 78. Oxidative stability of polypropylene for biomedical applications. **R. Wade**, J.W. Kiel, M.T. Reitman

1:40 POLY 79. Chemo-enzymatic synthesis and free radical polymerization of renewable acrylate monomers from cellulose-based lactones. **F. Diot-Néant**, E. Rastoder, S.A. Miller, F. Allais

2:00 POLY 80. Insight into cartilage supramolecular structure and biological function. **F. Horkay**, P.J. Basser

2:20 POLY 81. Design and application of functionalized porous organic polymers in CO₂ adsorption and conversion. **Z. Yang**, I. Popovs, S. Dai

2:40 POLY 82. Synthesis of morphology-tunable functional porous polymers from diblock copolymers hyper-cross-linking self-assembly strategy. **X. Yang**, K. Huang

3:00 POLY 83. Synthesis and photophysical properties of novel fluorescent fluorene-containing conjugated polymers and their application for the detection of common bisphenols. **D.R. Jones**, R. Vallee, M. Levine



TECHNICAL PROGRAM

3:20 POLY 84. Chemical recyclability of polar vinyl polymers derived from renewable methylene butyrolactones. **R.A. Gilsdorf**, E.Y. Chen

3:40 POLY 85. Synthesis of thermo-responsive polymer grafted cellulose nanocrystal and its application for polymer electrolyte. **R. Kato**, S. Patel, S.J. Rowan

4:00 POLY 86. Side-chain flexibility competes with hydrogen bonding on properties of supramolecularly crosslinked polyesters. **Q. Liu**, C. Wang, Y. Guo, A. Joy

4:20 POLY 87. Synthesis and application of innovative multifunctional polyol-siloxane surfactants. **T. Daenzer**, H. Frey

4:40 POLY 88. Thiocarbonyl platform for degradable radical polymerization. **R.A. Smith**, O. McAteer, G. Fu, M. Xu, W. Gutekunst

Section E

Rosen Centre Hotel
Salon 20

New Frontiers in Aerospace Polymers: Advances & Challenges in Experiments & Simulations

Additive Manufacturing for Aerospace Application

Cosponsored by PMSE

Financially supported by Air Force Research Laboratory; Bruker Instruments; Anasys Instruments; Boeing

M. A. Meador, D. Nepal, J. S. Wiggins, *Organizers*

S. E. Morgan, V. Varshney, *Presiding*

1:00 POLY 89. Additive manufacturing for air force applications: Design and characterization of advanced inks and filament feedstock. **H. Koerner**

1:30 POLY 90. Polymer viscosities from molecular simulation: Application to polymers for 3D printing. T. Roman, J. Rogers, N. Lee, J. Kim, J. Reid, I.M. Khan, G. Sapateh, R.J. Berry, **D. Bernhardt**

2:00 POLY 91. Additive manufacturing of thermosetting polymers using frontal polymerization. **J.E. Aw**, N.A. Parikh, X. Zhang, J.S. Moore, P.H. Geubelle, N.R. Sottos

Section F

Rosen Centre Hotel
Salon 21

Poly(2-oxazoline)s & Polypeptoids

R. Hoogenboom, H. Schlaad, R. N. Zuckermann, *Organizers*

G. Delaittre, K. Kempe, *Presiding*

1:20 POLY 92. Synergy of experiment and theory toward well-defined poly(2-oxazoline) synthesis. P. Van Steenberge, R. Hoogenboom, **D.R. D'hooge**



TECHNICAL PROGRAM

1:50 POLY 93. Polypept(o)ides: Combining polypeptides and polypeptoids in polymers. **M. Barz**

2:20 POLY 94. New stimuli-responsive materials via the Spontaneous Zwitterionic Copolymerisation (SZWIP) of 2-oxazolines. **K. Kempe**

2:50 Intermission.

3:05 POLY 95. Straightforward route to new poly(2-oxazoline)s via acylation of well-defined polyethyleneimine. **O. Sedlacek**, R. Hoogenboom

3:25 POLY 96. When α -amino acid NTAs meet nucleophiles. **J. Ling**

3:55 POLY 97. End-functional poly(2-ethyl-2-oxazoline)s for surface grafting and nanoparticle stabilization. G. Gil Alvarado, D. Le, M. Glassner, H. Nguyen, J.A. Johnson, R. Hoogenboom, **G. Delaitre**

4:25 POLY 98. Development of a two-dye-system based on PMMA-graft-OEtOx graft copolymers. **I. Muljajew**, C. Weber, U.S. Schubert

Section G

Rosen Centre Hotel
Salon 22

Polymer-Based Gene & Drug Delivery Systems

Polymers for DDS

X. M. Liu, Y. Ohya, Y. Wang, *Organizers*
T. Fujiwara, *Organizer, Presiding*
F. Li, *Presiding*

1:00 POLY 99. Synthetic and compositional control of multicomponent copolymers to promote drug solubility, bioavailability, and delivery. **T.M. Reineke**

1:35 POLY 100. MMP2-sensitive tumor-targeted drug delivery and sensitization. **L. Zhu**

1:55 POLY 101. Organic-inorganic nanohybrid as magnetically navigated nanocarrier for biologicals. **Y. Sasaki**, R. Kawasaki, R. Mizuta, N. Kinoshita, K. Akiyoshi

2:15 POLY 102. PAMAM-poly(lactide), “Janus-type” hybrids as next-generation biomaterials. **D.L. Watkins**

2:35 POLY 103. Polyanhydrides from radical-mediated thiol-ene polymerizations: From synthesis to drug delivery. **D.A. Shipp**

2:55 Intermission.

3:15 POLY 104. Using grafted functional polyesters for drug delivery systems. **J. Kressler**, K. Maeder



TECHNICAL PROGRAM

3:35 POLY 105. Next-generation opioid antidotes: Covalent nanoparticles for the delivery of Mu opioid antagonists. A. Kassick, M. Feasel, B. Kolber, N. Tomycz, **S. Averick**

3:55 POLY 106. Enhancement of cancer vaccine by modification of antigenicity for cancer cells. **S. Mochizuki**, A. Moritaka, K. Sakurai

4:15 POLY 107. Poly(2-alkyl-2-oxazoline) conjugates of doxorubicin bound via pH-sensitive hydrazone linker: Synthesis, *in vitro*, and *in vivo* evaluation. **O. Sedlacek**, A. Van Driessche, M. Hruby, B. De Geest, R. Hoogenboom

4:35 POLY 108. Quantifying drug cargo partitioning in pluronic block copolymer micelles. **X. Li**, T. Cooksey, M.L. Robertson, L.A. Madsen

Antimicrobial & Cell-Penetrating Polymers

Sponsored by PMSE, Cosponsored by POLY†

MONDAY MORNING

Section A

Rosen Centre Hotel
Signature 2

ACS Award in the Chemistry of Materials in honor of Krzysztof Matyjaszewski

J. Pyun, *Organizer*

J. Lutz, N. V. Tsarevsky, *Presiding*

8:10 POLY 109. Photo-induced structural transitions in block copolymers. **T.P. Lodge**, C. Hall, C. Rivera, C. Seitzinger, Y. Hirose

8:35 POLY 110. Precision synthesis of polyrotaxanes using artificial molecular machines. **J.F. Stoddart**

9:00 POLY 111. Advances and applications of surface-initiated atom transfer radical polymerization for functional material design. **M.R. Bockstaller**

9:25 POLY 112. Polymer-enhanced biomacromolecular systems. **A.J. Russell**, K. Matyjaszewski

9:50 Intermission.

10:05 POLY 113. Encoding mechanics of ultra-soft tissues in silicone. **S. Sheiko**

10:30 POLY 114. DFT studies of structural basis of activity of Cu-based ATRP catalysts. **T. Kowalewski**

10:55 POLY 115. Exploring new catalysts and monomers in catalyst-transfer polycondensation. **K.J. Noonan**



TECHNICAL PROGRAM

11:20 POLY 116. ATRP-inspired carbon-halogen activation in organic synthesis. **M. Coote**, B. Noble, P. Norcott, K. Fung, I. Russell

Section B

Rosen Centre Hotel
Salon 12

ACS Award for Affordable Green Chemistry in Honor of Richard Gross

M. A. Hillmyer, *Organizer*
H. N. Cheng, *Presiding*

8:30 Introductory Remarks.

8:35 POLY 117. Development of new methods for the synthesis of benign polymeric materials. **G.W. Coates**

9:10 POLY 118. Designing infinitely recyclable 'green' polymers with tailored properties built upon a 'gene' for full chemical recyclability. **E.Y. Chen**

9:45 POLY 119. Biopolymer blends as a versatile product platform for green polymer chemistry. **H.N. Cheng**

10:20 POLY 120. Bioconjugates by ATRP. **K. Matyjaszewski**

10:55 POLY 121. Award Address (ACS Award for Affordable Green Chemistry sponsored by The Dow Chemical Company and endowed by Rohm and Haas Company). Biocatalytic routes to tunable building blocks, surfactants and polymers. **R.A. Gross**

Section C

Rosen Centre Hotel
Salon 19

Transport in Polymer Membranes

Morphology, Solid State & Physical Properties of Membranes

Cosponsored by PMSE[‡]
C. M. Stafford, *Organizer*
M. D. Dadmun, T. Saito, *Organizers, Presiding*

8:00 POLY 122. Ion transport in polyelectrolyte multilayers through the glass transition. **S. Abou Shaheen**, M. Yang, J.B. Schlenoff

8:20 POLY 123. Comparative study of electrical conductivity behavior correlated to hydrogen bonding organization between bis-MPA based hyperbranched polymer and dendrimer. **B. Chen**, J.A. Giesen, M.K. Hassan, S.M. Grayson, S. Nazarenko



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

8:40 POLY 124. Molecular-level control over ion transport in membranes comprised of polymers of intrinsic microporosity. **B. Helms**, M. Baran, S. Sahu, M. Carrington, S. Meckler, M. Braten, A. Baskin, D. Prendergast

9:00 POLY 125. Ion transport in precise polymers with layered and disordered aggregates. **K.I. Winey**

9:30 POLY 126. High-temperature metathesis polycondensation chemistry. **K.B. Wagener**, J. Pribyl, T.W. Gaines, M.H. Bell, G. Hester, N. Gallman

9:50 POLY 127. Solvent penetration into structured ionomer membranes. M. Senanayake, D. Perahia, D. Aryal, **G.S. Grest**

10:10 Intermission.

10:40 POLY 128. Cation conduction in solvent-free ionomers for rechargeable batteries. J. Liu, B. Park, **J.L. Schaefer**

11:10 POLY 129. Stretchable solid polymer electrolytes based on poly(acrylic acid) crosslinking with silica nanoparticles. **Y. Song**, U. Choi

11:30 POLY 130. Elastic single-ion conducting polymer electrolyte. **P. Cao**, B. Li, G. Yang, J. Nanda, A.P. Sokolov, T. Saito

11:50 POLY 131. Superionic conductive polymer electrolyte for solid lithium-metal batteries with long cycle life. **Y. Zhu**

Section D

Rosen Centre Hotel
Salon 23

Excellence in Graduate Polymer Research

Biobased, Degradable & Chain-Exchange Polymers

Cosponsored by PRES, PROF[‡], SOCED[‡] and YCC[‡]
Financially supported by Industrial Advisory Board; TOSOH; Wiley
H. Cheng, *Organizer*
C. Coltrain, C. J. Ellison, *Presiding*

8:25 Introductory Remarks.

8:30 POLY 132. Amino acid-based poly(ester urea)s for soft-tissue repair applications. **N. Dreger**

8:55 POLY 133. Covalently crosslinked coacervate: Immobilization and stabilization of proteins with enhanced enzymatic activity. **M. Zhao**, S. Cho, N. Zacharia

9:20 POLY 134. Efficient synthesis of novel glycosaminoglycan analogs. **C. Gao**, K.J. Edgar

9:45 POLY 135. Improving mechanical properties of fatty acid-derived thermoplastic elastomers by incorporating a transient network. **W. Ding**, M.L. Robertson



TECHNICAL PROGRAM

10:10 Intermission.

10:25 **POLY 136.** Harnessing imine reactivity for dynamic topological and functional transformations. **M.B. Sims**, K.Y. Patel, M. Bhatta, S. Mukherjee, J.J. Lessard, L. Bai, B.S. Sumerlin

10:50 **POLY 137.** Reprocessable polymer networks based on dynamic chemistry with concurrent dissociative and associative mechanisms: Judicious design leading to excellent reprocessability. **L. Li**, X. Chen, J.M. Torkelson

11:15 Remarks by **B. Charpentier**, 2019 ACS President.

11:30 **POLY 138.** Kinetic control of block polymer micelles: Cavitation induced exchange and templates for nanomaterials. **K.A. Lantz**, A. Sarkar, K.C. Littrell, T. Li, K. Hong, W. van den Bergh, N.B. Clamp, M. Stefik

Section E

Rosen Centre Hotel
Salon 20

Industrial Innovations in Polymer Science

Cosponsored by I&EC
M. O. Hunt, *Organizer*
H. A. Brown, B. Rodier, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 **POLY 139.** Theoretical studies on ring-opening polymerizations by alkoxides and (thio)ureas. **G.O. Jones**, B. Lin, X. Zhang, J. Hedrick, R.M. Waymouth

8:35 **POLY 140.** Computational mini-plant: Industrial applications of quantum mechanical calculations. **I. Konstantinov**, S. Ewart, A. Krasovskiy, H.A. Brown, S. Munjal

9:05 **POLY 141.** Data-based decision-making in industrial polymer problem solving. **J. Rancourt**, B. Caba

9:35 Intermission.

10:05 **POLY 142.** From lab to market: Polyimide aerogels. **D.J. Irvin**, G.D. Poe

10:35 **POLY 143.** Injectable microgel for soft tissue repair. **S. Poleon**

11:05 **POLY 144.** Contact lenses: More than meets the eye. **M.R. Clark**

11:35 Concluding Remarks.

Section F

Rosen Centre Hotel
Salon 21



TECHNICAL PROGRAM

Poly(2-oxazoline)s & Polypeptoids

R. Hoogenboom, R. N. Zuckermann, *Organizers*
H. Schlaad, *Organizer, Presiding*
F. Wiesbrock, *Presiding*

8:10 POLY 145. Bio-sourced chelating poly(2-oxazoline)s. **H. Schlaad**, N. Lüdecke

8:40 POLY 146. Green light photoswitchable poly(2-isopropenyl-2-oxazoline) supramolecular hydrogels. **X. Xu**, V. Jerca, R. Hoogenboom

9:00 POLY 147. Gradient copolymers from aliphatic and aromatic 2-oxazolines for drug delivery. S. Datta, N. Petrenčíková, P. Šrámková, Z. Kroneková, A. Jutková, D. Jancura, **J. Kronek**

9:30 Intermission.

9:45 POLY 148. Upscaling poly(2-oxazoline) synthesis in continuous flow mode: Beyond microwave synthesizers. **V. R de la Rosa**, E. Baeten, R. Hoogenboom, T. Junkers

10:15 POLY 149. Synthesis and self-assembly of carbohydrate-conjugated poly(2-oxazoline)s: Polymer vesicles with molecular permeability towards therapeutic nanofactories. **T. Nishimura**, N. Sumi, Y. Koda, Y. Sasaki, K. Akiyoshi

10:35 POLY 150. Messenger RNA loaded polyplex micelles having hydrophobic core protective layer composed of thermo-switchable poly(oxazoline) for promoted gene expression. **S. Osawa**, K. Osada, K. Kataoka

10:55 POLY 151. Thermoresponsive, biodegradable polyesters: Tunable properties and efficient protein encapsulation. **M. Cruz**, M. Kundu, T. Leeper, A. Joy

11:15 POLY 152. Merging dielectric stability and ubiquitous adhesion: Poly(2-oxazoline)s in microelectronics and high-voltage engineering. **F. Wiesbrock**, A. Eibel, P. Marx, R. Hofmann

Section G

Rosen Centre Hotel
Salon 22

Polymer-Based Gene & Drug Delivery Systems

New Therapeutics & Gene Delivery

T. Fujiwara, X. M. Liu, Y. Wang, *Organizers*
Y. Ohya, *Organizer, Presiding*
C. Scholz, *Presiding*

8:00 POLY 153. Self-assembling nanodrugs for novel antioxidant therapeutics. **Y. Nagasaki**

8:35 POLY 154. Transdermal delivery of polymer nanoparticles via faint electricity. **K. Kogure**, Y. Nagasaki



TECHNICAL PROGRAM

8:55 POLY 155. Redox-responsive PEGylated macrophotosensitizer nanoparticles for enhanced near-infrared imaging-guided photodynamic therapy. **L. Yan**

9:15 POLY 156. Metabolism-controlled boron delivery systems composed of biocompatible polymers and boronophenylalanine for neutron capture therapy. **T. Nomoto**, Y. Inoue, Y. Yao, M. Suzuki, K. Kanamori, H. Takemoto, M. Matsui, K. Tomoda, N. Nishiyama

9:35 POLY 157. Enzyme-Directed Assembly of Particle Immunotherapeutics (EDAPI): A strategy for engineering tumor microenvironments for cancer therapy. **C. Battistella**, M.P. Thompson, T. Hayashi, C.E. Callmann, D.A. Carson, N.C. Gianneschi

9:55 Intermission.

10:15 POLY 158. Nanostructured DNA for the *in vivo* delivery of biomolecules and cells. **M. Nishikawa**

10:35 POLY 159. Modular non-viral gene delivery vectors as probes to study the evolution of DNA-polymer complexes within mammalian cells. t. suk-in, C. Marks, S. Ross, r. bellin, **S. Granados Focil**

10:55 POLY 160. Targeted three-layered micelles and injectable hydrogels for systemic and local gene delivery systems. **T. Fujiwara**, O.M. Merkel

11:15 POLY 161. Well-defined poly(ethylene glycol)-*b*-poly(ϵ -caprolactone) based diblock polymeric biomaterials for drug and gene delivery. **A. Jafari**, G. Zhang, L. Yan, M. Mohamed, Y. Wu, B.A. Pfeifer, C. Cheng

11:35 POLY 162. Effects of protonation and salt concentration on the structure of polyethylenimine (PEI) in water. **C. Gallops**, J. Ziebarth, Y. Wang

Antimicrobial & Cell-Penetrating Polymers

Sponsored by PMSE, Cosponsored by POLY†

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Sponsored by PROF, Cosponsored by AGFD, ANYL, BIOL, BIOT, CARB, CELL, CHED, CMA, COLL, COMP, ENVR, GEOC, I&EC, MEDI, MPPG, NUCL, ORGN, PHYS, PMSE, POLY, PRES, WCC and YCC

PolyEd: Incorporating Polymer Chemistry in Undergraduate & High School Curricula

Sponsored by CHED, Cosponsored by POLY

MONDAY AFTERNOON

Section A



TECHNICAL PROGRAM

Rosen Centre Hotel
Signature 2

ACS Award in the Chemistry of Materials in honor of Krzysztof Matyjaszewski

J. Pyun, *Organizer*
K. Beers, B. S. Sumerlin, *Presiding*

1:00 POLY 163. Utilizing functional monomers with self-accelerating reactions to explore polymers with new structures and functions. **H. Gao**

1:20 POLY 164. Rational design of multicomponent bottlebrush block copolymers for nanotemplating. **M. Zhong**, A. Le, R. liang, X. Fu

1:40 POLY 165. Studying kinetics to design and tailor dynamically crosslinked polymer materials. **D. Konkolewicz**, P. Chakma, B. Zhang, Z. Digby, J. Ke, J. Sparks

2:00 POLY 166. Metallo-polyelectrolytes: Chemistry, materials, and unknown. **C. Tang**

2:20 POLY 167. Hypervalent iodine reagents with (pseudo)halide, carboxylate, or tetrazolate ligands in the synthesis of functional polymers. **N.V. Tsarevsky**

2:40 Intermission.

2:55 POLY 168. Selective deuteration of polyethylene via polyhomologation. W. Farrell, S.V. Orski, A.K. anthony.kotula@nist.gov, **K. Beers**

3:20 POLY 169. Dynamic-covalent chemistry for functional diversification, vitrimers, and other self-healing materials. J.J. Lessard, M.B. Sims, L.F. Garcia, C.P. Easterling, K.C. Bentz, S. Arencibia, D.A. Savin, **B.S. Sumerlin**

3:45 POLY 170. Design of high-precision polymers by multistep synthesis. **J. Lutz**

4:10 POLY 171. Artificial enzymes via ATRP from [2Fe-2S] metallopolymers for H₂ production via water splitting. **J. Pyun**, M. Karayilan, K. Clary, D.L. Lichtenberger, R.S. Glass

4:35 POLY 172. Award Address (ACS Award in the Chemistry of Materials sponsored by DuPont). Functional materials by ATRP: From precise synthesis to new applications. **K. Matyjaszewski**

Section B

Rosen Centre Hotel
Salon 12

Synthesis & Properties of Densely Grafted Polymers

J. G. Kennemur, G. Stein, R. Verduzco, *Organizers*
J. B. Matson, *Organizer, Presiding*



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

1:00 POLY 173. Precise control over structure and properties in brush polymers. **R.H. Grubbs**

1:45 POLY 174. Coarse-grained simulation of the dilute solution structure of bottlebrush polymers. S. Dutta, M. Wade, D. Walsh, D. Guironnet, S. Rogers, **C.E. Sing**

2:15 POLY 175. Alkyl wedge-type polymer architectures and their applications as photonic crystals. **B. Boyle**, G. Miyake

2:35 POLY 176. Aqueous self-assembly of amphiphilic cylindrical and cone-shaped (tapered) bottlebrush polymers prepared by sequential-addition of macromonomers ring-opening metathesis polymerization (SAM-ROMP). **J.B. Matson**

2:55 POLY 177. Worm-to-globule shape transition of thermosensitive binary heterografted molecular bottlebrushes in water. **B. Zhao**

3:15 POLY 178. Grafting linear and linear-hyperbranched block copolymers by continuous flow chemistry polymerizations. **R.C. Advincula**

Section C

Rosen Centre Hotel
Salon 19

Transport in Polymer Membranes

Block Copolymers, Morphology Control & Poly(ionic Liquids)

Cosponsored by PMSE[‡]

M. D. Dadmun, T. Saito, C. M. Stafford, *Organizers*

P. Cao, M. A. Hickner, *Presiding*

1:00 POLY 179. Manipulating monomer segment distributions to tune self-assembly and macromolecular properties in ion-conducting block copolymer systems. **T.H. Epps**, M.A. Morris, C.K. Shelton, P. Ketkar

1:30 POLY 180. Morphology and ion dynamics in oligomeric ethylene oxide functionalized block copolymer electrolytes. **D.A. Waldow**, J. Harrison, R. Giridharagopal, D.S. Ginger

1:50 POLY 181. Exploring ionic conduction mechanism in the nanoscale by self- assembled block copolymer electrolytes films. **D. Sharon**, P. Bennington, S. Patel, P.F. Nealey

2:10 POLY 182. Architecture and polarity control of precise network polymerized ionic liquids to understand aggregation and ionic conductivity. **C. Evans**, Q. Zhao, C. Shen

2:30 Intermission.

3:00 POLY 183. Improving single-ion conductivity of polymer electrolyte by softening backbone. **S. Zhao**, P. Cao, T. Saito, A.P. Sokolov

3:20 POLY 184. Effect of relative humidity on the ionic conductivity of poly(ionic liquid) networks containing variable counteranions. **K.M. Miller**, R.D. Johnson, N.C. Bontrager, S.A. Radomski



TECHNICAL PROGRAM

3:40 POLY 185. Developing a new approach to describe ion sorption and transport in Nafion membranes. **R. Sujanani**, J. Kamcev, E. Jang, D.R. Paul, B.D. Freeman

4:00 POLY 186. Biomimetic neurons using polyelectrolytes: Experimental implications on current models. **S. Kozawa**, L. Kreider, G. Tierney, A. Venkataswamy, A.Y. Walker, G.E. Wnek

4:20 POLY 187. Platinum-acetylide polymers: An investigation of ultrafast photoinduced charge transfer. **R. He**, S. Valandro, K.S. Schanze

Section D

Rosen Centre Hotel
Salon 23

Excellence in Graduate Polymer Research

New Structures & Applications

Cosponsored by PRES, PROF, SOCED and YCC
Financially supported by Industrial Advisory Board; TOSOH; Wiley
H. Cheng, *Organizer, Presiding*
C. J. Ellison, *Presiding*

1:00 Introductory Remarks.

1:15 POLY 188. Assembling graphene oxide at fluid-fluid interface: A new way to architect hybrid structures for advanced application. **P. Wei**, E. Pentzer

1:40 POLY 189. Polymer metal-organic cage gels for water purification. **J. Zhao**, J.A. Johnson

2:05 POLY 190. Tuning mechanical properties of polymer brush surfaces to dictate wrinkle morphologies. **C. Reese**, W. Guo, B. Thompson, C.M. Stafford, D.L. Patton

2:30 POLY 191. Facile synthesis of carbon flower particles from a novel polyacrylonitrile system. **S. Chen**, Z. Bao

2:55 Intermission.

3:10 POLY 192. Photopolymer design for additive manufacturing of elastomers. **P. Scott**, V. Meenakshisundaram, M. Hegde, J.M. Serrine, N.A. Chartrain, C. Kasprzak, K. Feller, C.B. Williams, T.E. Long

3:35 POLY 193. Controlled phase separation and thermo-mechanical properties in hybrid radical/cationic systems using photopolymerization. **E. Hasa**, A. Guymon, J.W. Stansbury, J.L. Jessop

4:00 POLY 194. Chalcogenide Hybrid Inorganic/organic Polymers (CHIPs): A unique class of optical polymers for IR imaging and photonics. **T. Kleine**, R.S. Glass, R.A. Norwood, J. Pyun

Section E

Rosen Centre Hotel
Salon 20



TECHNICAL PROGRAM

Industrial Innovations in Polymer Science

Cosponsored by I&EC
M. O. Hunt, *Organizer*
H. A. Brown, B. Rodier, *Organizers, Presiding*

1:00 Introductory Remarks.

1:05 POLY 195. Increased performance in liquid sound damper formulations through controlled interaction between polymer dispersions and inorganic surfaces. **J. Bohling**, J. Gimbal, J. Gallagher, S. Whitehouse, J. Reffner

1:35 POLY 196. Hydrophobic polymers for improved barrier properties in industrial coatings. **D.N. Haase**

2:05 POLY 197. Effectiveness of demulsifying agents in breaking water-in-crude oil emulsions. **R.M. Jenkins**, T. Kuo, D. Miller, K. Whitaker, A. Schmitt, M. Tulchinsky, H. Wiles, T. Kalantar

2:35 Intermission.

3:05 POLY 198. Polymeric substrates with attached controlled radical initiators. **J.K. Rasmussen**, S.B. Roscoe, G.W. Griesgraber, D.J. O'Neal, E.P. Narveson

3:35 POLY 199. Sustainable plastics: Using polymer stabilizers to yield recyclable polyolefins. **K.M. Knauer**, R.E. King

4:05 POLY 200. Tailored EPDM architecture for automotive extruded profiles. **J. Tuberquia**, C. Li Pi Shan, S. Wu, G. Li, L. Nguyen

4:35 Concluding Remarks.

Section F

Rosen Centre Hotel
Salon 21

Poly(2-oxazoline)s & Polypeptoids

R. Hoogenboom, H. Schlaad, R. N. Zuckermann, *Organizers*
R. Becer, E. Benetti, *Presiding*

1:20 POLY 201. Poly(2-oxazoline) derivatives: Their applications from gene delivery to engine oil additives. **R. Becer**

1:50 POLY 202. Smart polymers based on N-isopropylacrylamide and 2-oxazolines. **J. Rueda**, S. Zschoche, D. Schmaljohann, M. Binner, A. Janke, K. Arndt, S. Lehmann, B. Voit

2:20 POLY 203. Sequence-selective dynamic covalent assembly of information-bearing oligopeptoids. **T.F. Scott**, S.C. Leguizamón

2:50 Intermission.



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

3:05 POLY 204. Designing amphiphilic peptoids for bio-inspired synthesis of hybrid materials. **C. Chen**

3:35 POLY 205. Poly(2-oxazoline)s on surfaces: Chemical and topological design, properties, and applications. G. Morgese, **E. Benetti**

4:05 POLY 206. Antifouling peptoid brushes: From polysarcosine to zwitterionic sequences. D.L. Cheung, **K. Lau**

4:25 POLY 207. Modification of poly(2-oxazoline)s with pendant ester groups: a kinetic investigation. **J. Van Guyse**, R. Hoogenboom

Section G

Rosen Centre Hotel
Salon 22

Polymer-Based Gene & Drug Delivery Systems

Gene Delivery

T. Fujiwara, X. M. Liu, Y. Ohya, *Organizers*
Y. Wang, *Organizer, Presiding*
E. P. Kharlampieva, *Presiding*

1:00 POLY 208. Beta-glucans/DNA complexes for immunocyte targeting delivery of therapeutic oligonucleotides. **K. Sakurai**

1:35 POLY 209. Guanylurea-functionalized conjugated polymers for efficient gene knockdown in normal human bronchial epithelium cells. M. Ahmed, R. Dutta, P. Manandhar, H. Unwalla, **J. Moon**

1:55 POLY 210. Poly(amino acid)-based gene delivery systems: The story starts after the synthesis. **C. Scholz**, D. Ulkoski

2:15 POLY 211. Gene expression of aspect ratio-controlled polyplexes based on the effect of multi-arm poly(ethylene glycol). **A. Harada**, E. Yuba

2:35 Intermission.

2:55 POLY 212. Enzymatic synthesis of aptamer-targeted polynucleotide drugs for cancer therapy. L. Tang, S. Deshpande, Y. Yang, R. Gu, A. Chilkoti, **S. Zauscher**

3:15 POLY 213. RAFT polymerization for the synthesis of tertiary amine-based diblock copolymer nucleic acid delivery vehicles. **A.E. Smith**, T.A. Brooks, A.K. McClellan, T. Hao

3:35 POLY 214. Cationic star-shaped glycopolymer brushes for targeted gene delivery. **R. Liu**, A. Blakney, Y. Gokhan, P. McKay, R. Shattock, R. Becer

3:55 POLY 215. Polyplex interaction strength impacts potency during cancer immunotherapy. **S.J. Tsai**, J. Andorko, X. Zeng, J. Gammon, C. Jewell



TECHNICAL PROGRAM

4:15 POLY 216. Encapsulation and ultrasound-triggered release of G-quadruplex DNA in hydrogel microcapsules. **A. Alford**, N. Gupta, V.A. Kozlovskaya, D.E. Graves, E.P. Kharlampieva

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Sponsored by PROF, Cosponsored by AGFD, ANYL, BIOL, BIOT, CARB, CELL, CHED, CMA, COLL, COMP, ENVR, GEOC, I&EC, MEDI, MPPG, NUCL, ORGN, PHYS, PMSE, POLY, PRES, WCC and YCC

Antimicrobial & Cell-Penetrating Polymers

Sponsored by PMSE, Cosponsored by POLY‡

Chemistry in Space: Future Directions

Sponsored by YCC, Cosponsored by AGFD, ANYL, BIOT, BMGT, CHAS, ENVR, FLUO, GEOC, HIST, I&EC, MEDI, POLY and PROF

PolyEd: Incorporating Polymer Chemistry in Undergraduate & High School Curricula

Sponsored by CHED, Cosponsored by POLY

Undergraduate Research Posters

Polymer Chemistry

Sponsored by CHED, Cosponsored by PMSE, POLY and SOCED

MONDAY EVENING

Section A

Orange County Convention Center
West Hall C

Sci-Mix

A. Pritzlaff, *Organizer*

8:00 - 10:00



TECHNICAL PROGRAM

30, 81, 84, 89, 134, 137, 150-151, 181, 183, 189, 192. See previous listings.

225, 227-228, 230, 235, 238, 248, 254-255, 257, 267, 287, 289, 309, 326, 333-335, 337, 341-342, 356, 366, 368, 385-386, 394, 402, 416, 418, 435, 437, 459, 462, 474-476, 491, 494, 499, 502, 514, 526, 531-532, 536, 539, 543, 556-567, 573, 574, 608, 639, 662. See subsequent listings.

Revamping Practical Chemistry Teaching for the New Frontier

Sponsored by CHED, Cosponsored by PMSE, POLY and RUBB

TUESDAY MORNING

Section A

Rosen Centre Hotel
Signature 2

Carl S. Marvel Award for Creative Polymer Chemistry Award in Honor of Matt Becker

Biomaterials Take Form

Cosponsored by PMSE
A. P. Dove, *Organizer, Presiding*

8:00 POLY 217. Novel biomaterials from sustainable sources. **A.P. Dove**

8:25 POLY 218. Applications of redox-switchable catalysts for the synthesis of advanced polymeric materials. **J.A. Byers**, M. Qi, K.R. Delle Chiaie, J. Kehl, M. Thompson, S. Gonsales

8:50 POLY 219. Collages of arts and science. **G.R. Newkome**

9:15 POLY 220. C–H functionalization of polyolefins. **F.A. Leibfarth**, J. Williamson, C. Na, E.J. Alexanian

9:40 POLY 221. Compression-activated fluorescence in polymeric networks. C. Kabb, C. O'Bryan, C. Morley, T.E. Angelini, **B.S. Sumerlin**

10:05 Intermission.

10:30 POLY 222. Enzyme-responsive peptide-polymer progelators for minimally invasive delivery to the heart post-myocardial infarction. **N.C. Gianneschi**, A. Carlini, K. Christman

10:55 POLY 223. Brush-like polymers and computationally driven design of soft materials. **A.V. Dobrynin**

11:20 POLY 224. Exploring the power of PISA. **R.K. O'Reilly**



TECHNICAL PROGRAM

11:45 POLY 225. Predicting 3D printability of functional polymers: balancing rheology with reactivity. **T.E. Long**, G. Adikari Appuhamillage, J.M. Sirrine, M. Hegde, J. Herzberger, D.A. Rau, X. Chen, C.B. Arrington, M.F. Cashman, P. Scott, E. Wilts, V. Meenakshisundaram, N.A. Chartrain, C.B. Williams

Section B

Rosen Centre Hotel
Salon 12

Polymer Bioconjugates for a Changing World

Cosponsored by BIOT
D. Konkolewicz, R. C. Page, J. K. Pokorski, *Organizers*
J. Kaar, *Organizer, Presiding*
C. Boyer, *Presiding*

8:00 POLY 226. Semi-discrete protein-RAFT polymer conjugates and single-enzyme nanogels. A. Beloqui, G. Gil Alvaradejo, E. Miceli, J. Morgenstern, J. Hubbuch, **G. Delaittre**

8:20 POLY 227. Practical synthesis of complex glycopolymers using water-soluble amino-oxy functional scaffolds. **A. Laezza**, S. Richards, M.I. Gibson

8:40 POLY 228. Photoinduced reversible-deactivation radical polymerization (photoRDRP): Shedding light on structure and function of protein-like polymers. **H. Sun**, W. Choi, N.C. Gianneschi

9:00 POLY 229. Covalently linking natural products and synthetic polymers by ATRP. **K. Matyjaszewski**

9:30 POLY 230. Aqueous high throughput photomediated controlled/living radical polymerization (PET-RAFT): tailoring for bioconjugation. **C. Boyer**

10:00 Intermission.

10:30 POLY 231. Synthesis and biological applications of hydrophilic glycodendrimers. **K.D. McReynolds**

10:50 POLY 232. Bioconjugation strategies to combine polymers with proteins and living cells. M. Hasan, L. Wilkins, R. Tomás, A. Fayer, B. Martyn, **M.I. Gibson**

11:20 POLY 233. Automated engineering of well-defined and protein-like biofunctional polymers. **A.J. Gormley**, R. Chapman

Section C

Rosen Centre Hotel
Salon 19

Transport in Polymer Membranes

Flow Batteries & Alkaline Fuel Cells



TECHNICAL PROGRAM

Cosponsored by PMSE[‡]
M. D. Dadmun, T. Saito, C. M. Stafford, *Organizers*
B. Helms, J. L. Schaefer, *Presiding*

8:00 POLY 234. Role of the electrolyte on the structure/transport relationships of PFSA membranes for redox flow batteries. **D.I. Kushner**, A. Kusoglu, A.Z. Weber

8:20 POLY 235. Interplay of electrostatic interactions, nanoparticle dispersion, and ion transport in ionomer nanocomposites for vanadium redox flow batteries. **A.B. Jansto**, A. Balwani, T. Martin, R.L. Jones, E.M. Davis

8:40 POLY 236. Sulfonated poly(biphenyl alkylene)s as ion exchange membranes for alkaline redox flow batteries. **S. Granados Focil**, v. Gutierrez-venegas

9:00 POLY 237. New ion transport membranes for large-scale energy storage. **M.A. Hickner**

9:30 POLY 238. Uncovering how the nanoparticle–polymer interface affects segmental dynamics and water transport in ionomer nanocomposites. **A. Balwani**, A.B. Jansto, A. Faraone, E.M. Davis

9:50 POLY 239. Fluorocarbon-based ionomers with single- and multi-acid side chains at nanoscale interfaces: What matters. S. Farzin, T. Johnson, C. Nguyen, J. Turner, **S.K. Dishari**

10:10 Intermission.

10:40 POLY 240. Ion transport in anion exchange membranes for alkaline fuel cells. **Y.A. Elabd**

11:10 POLY 241. Highly conductive, chemically stable, hydroxide conducting membranes based on poly(norbornene). G. Huang, M. Mandal, **P. Kohl**

11:30 POLY 242. Effect of phosphonated triazine monomer additive in disulfonated poly(arylene ether sulfone) composite membranes for proton exchange membrane fuel cells. **T.N. Thompson**

11:50 POLY 243. Structure-transport relationships of perfluorosulfonic acid membranes in dry-hot conditions: The impact of side-chain chemistry. **X. Luo**, A. Kusoglu

Section D

Rosen Centre Hotel
Salon 23

Excellence in Graduate Polymer Research

Approaches to Polymer Synthesis

Cosponsored by PRES, PROF, SOCED and YCC
Financially supported by Industrial Advisory Board; TOSOH; Wiley
H. Cheng, *Organizer, Presiding*
T. E. Long, *Presiding*

8:30 POLY 244. Real-time measurement of analyte partitioning and polymer brush conformation change. **K.A. Miller**, S. Wetzler, L. Kisley, A. Stanton, N.W. Reed, R.C. Bailey, P.V. Braun



TECHNICAL PROGRAM

8:55 POLY 245. Living metathesis & metallotropy polymerization gives conjugated polyenynes from multialkynes: How to design sequence-specific cascades for polymers. **C. Kang**, T. Choi

9:20 POLY 246. Leveraging low ring strain: The path towards precision polypentenamers. **W. Neary**, B.A. Fultz, J.G. Kennemur

9:45 POLY 247. Macromolecular engineering through metal-free ring-opening metathesis polymerization. **P. Lu**, A.J. Boydston

10:10 Intermission.

10:25 POLY 248. Flow-enabled control over macromolecule architecture. **D. Walsh**, D. Guironnet

10:50 POLY 249. Postpolymerization modification strategy to solid state block polyelectrolytes. **D.J. Goldfeld**, E. Silver, M.R. Radlauer, M.A. Hillmyer

11:15 POLY 250. Development of strongly reducing phenoxazine organic photoredox catalysts and their application in organocatalyzed atom transfer radical polymerization. **B. McCarthy**

Section E

Rosen Centre Hotel
Salon 20

New Frontiers in Aerospace Polymers: Advances & Challenges in Experiments & Simulations

Bioinspired Materials for Aerospace Composite

Cosponsored by PMSE

Financially supported by Air Force Research Laboratory; Bruker Instruments; Anasys Instruments; Boeing

M. A. Meador, J. S. Wiggins, *Organizers*

D. Nepal, *Organizer, Presiding*

S. Rahatekar, *Presiding*

10:30 POLY 251. Cellulose nanocrystals: A versatile macromolecule for aerospace applications. **V.A. Davis**

11:00 POLY 252. Substitution of formaldehyde in phenolic networks for ablative composites. **S. Caillol**

11:20 POLY 253. Synthesis of biorenewable polyphenols from cardanol: Precursors to high-performance materials. **J. Muldoon**, m. garrison, B.G. Harvey

Section F

Rosen Centre Hotel
Salon 21

Undergraduate Research in Polymer Science



TECHNICAL PROGRAM

S. E. Morgan, *Organizer*
S. Nazarenko, *Presiding*

8:00 Introductory Remarks.

8:15 **POLY 254.** Sustainable polymers in society: Demos of renewable polymers manufacture in the lab for HS students from a chemical/environmental engineering summer camp. **L.A. Lucia**, R.A. Venditti, H. Jameel, M. Byrd, L. Pal, J. Piercy, J. Pawlak, S. McAlexander

8:30 **POLY 255.** Combining thiol-ene and acetal chemistries to synthesize degradable, environmentally friendly networks. B.M. Alameda, **N. Pierini**, D.L. Patton

8:45 **POLY 256.** Crosslinked biodegradable thermoset polymer films based on sodium alginate. **K.D. Barz**, T. Filipova

9:00 **POLY 257.** Synthesis and assembly of zwitterionic PMPC-based block copolymers. **J.D. Mitchell**, J. Ting, A.E. Marras, A. Herzog-Arbeitman, M.V. Tirrell

9:15 **POLY 258.** Water content in polyelectrolyte complex coacervates. **K. Wilcox**, N. Zacharia

9:30 Intermission.

10:00 **POLY 259.** Tuning the pKa of poly(lysine): Enhancing stimuli-responsiveness of peptide block copolymers. **A.K. Nason**, B.E. Barnes, D.A. Savin

10:15 **POLY 260.** Assessing warping issues with 3D printed ceramic models using SLA 3D printers. **L. Rodriguez**, N. Ruzycki

10:30 **POLY 261.** Development of a powder melt extrusion 3D printer. **T. Mensch**, B. Boyle, G. Miyake

10:45 **POLY 262.** Print parameter effects on porcelain ceramic print shrinkage in stereolithography printers. **D. Alvarez**, N. Ruzycki

11:00 **POLY 263.** Tailoring buckling instabilities in ultrathin polymer brush surfaces. **B.J. Thompson**, C.M. Reese, D.L. Patton

11:15 **POLY 264.** Mechanical actuation in polymeric bilayers. **C. Wisinger**, L. Maynard, J.R. Barone

11:30 **POLY 265.** Toward an understanding of dielectric breakdown through incorporating defects into polyetherimides. **J. Lockwood**

Section G

Rosen Centre Hotel
Salon 22

Polymer-Based Gene & Drug Delivery Systems

Processing & Formulation for DDS



TECHNICAL PROGRAM

T. Fujiwara, Y. Ohya, Y. Wang, *Organizers*
X. M. Liu, *Organizer, Presiding*
D. L. Watkins, *Presiding*

8:00 POLY 266. Oral multiparticulates as a platform approach for pediatric drug development. **M. Santangelo**, J.A. Bartlett

8:20 POLY 267. Advancements in softgels as a drug-delivery system. **N. Elkarim**

8:40 POLY 268. Progress in the development of high-solids, quick-set pharmaceutical tablet coatings. **T.H. Kalantar**, M. Ladika, H. Shao, S. Dean, K. Harris, P. Sheskey, K. Coppens, K. Balwinski, D. Holbrook

9:00 POLY 269. Intracellular delivery of biomolecules via freeze concentration using polyampholyte nanocarriers. **K. Matsumura**, S. Ahmed

9:20 POLY 270. Blood-brain barrier crossing nanoparticle for the delivery of antiretrovirals for targeting HIV-infected brain reservoirs. **N. Kolishetti**, M. Kamran, A. Shah, B. Surnar, M. Nair, S. Dhar

9:40 Intermission.

10:00 POLY 271. Development of a novel 3D printed, drug-eluting, biodegradable ring for treatment of eosinophilic esophagitis. **A. Prasher**, R. Shrivastava, D. Dahl, P. Sharma, S.R. Benhabbour

10:20 POLY 272. High-capacity matrix excipients for controlled drug release: surpassing the state-of-the-art. **V. R de la Rosa**, A. Samaro, V. Van Hoorne, A. Tigrine, M. Purino, M. Vergaalen, B. Monnery, C. Vervaeet, R. Hoogenboom

10:40 POLY 273. Microfluidic synthesis of drug-loaded PLGA microparticles: A greener approach. **M.J. Owen**, J.H. Yik, D.R. Haudenschild, G. Liu

11:00 POLY 274. Effect of dexamethasone on ambient temperature 3D printing, rheology, and degradation of a low modulus polyester. **T. Jain**, D. Saylor, C. Piard, Q. Liu, J. Fisher, I. Isayeva, A. Joy

11:20 POLY 275. Active loading and triggered release of charged molecules with porous nanocapsules. **W. Zhang**, S. Shmakov

Applied Materials for New Frontiers: Ten Years of ACS Applied Materials & Interfaces

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TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

GSSPC: Artificial Molecular Machines & the Next Generation of Molecular Control

Sponsored by CHED, Cosponsored by COLL, I&EC, ORGN‡, PHYS, POLY and PRES

TUESDAY AFTERNOON

Section A

Rosen Centre Hotel
Signature 2

Carl S. Marvel Award for Creative Polymer Chemistry Award in Honor of Matt Becker

Biomaterials' Take on Function

Cosponsored by PMSE
A. P. Dove, *Organizer*
K. L. Wooley, *Presiding*

1:00 POLY 276. Highly branched polymers prepared via ring-opening metathesis polymerization of macromonomers: Syntheses and applications as prodrugs and biological imaging agents. **J.A. Johnson**

1:25 POLY 277. Block copolymers of polysaccharides and conventional polymers as compatibilizers in blends of bio-derived polymers. **J.B. Matson**, K. Arrington, A. Volokhova

1:50 POLY 278. Polymers at surfaces: Growth and detachment. **H.A. Klok**

2:15 POLY 279. Controlled polymer assemblies promote drug delivery and cellular genome editing. **T.M. Reineke**

2:40 Intermission.

3:05 POLY 280. Next-generation click chemistry for block copolymer synthesis. **C.J. Hawker**

3:30 POLY 281. Striving for perfection: Model materials for short chain branched polyolefins. S.V. Orski, W. Farrell, **K. Beers**

3:55 POLY 282. Modeling the rheological behavior of sulfonated polystyrene ionomers. **R.A. Weiss**, C. Huang

4:20 POLY 283. Celebration of the accomplishments of Matthew L. Becker: From peptide-polymer conjugates and peptide-functionalized shell crosslinked knedel-like nanoparticles (SCKs) as a Ph.D. student to a diverse range of biologically-active functional polymer materials. **K.L. Wooley**

4:45 POLY 284. New resorbable materials and inks are needed if additive manufacturing will really change medicine. **M. Becker**

Section B



TECHNICAL PROGRAM

Rosen Centre Hotel
Salon 12

Polymer Bioconjugates for a Changing World

Cosponsored by BIOT
J. Kaar, D. Konkolewicz, R. C. Page, J. K. Pokorski, *Organizers*
R. Chapman, A. Simakova, *Presiding*

1:00 POLY 285. Grafting through method for implanting of lysozyme enzyme in molecular brush for improved biocatalytic activity and thermal stability. **X. Wang**, N.S. Yadavalli, A.M. Laradji, S. Minko

1:20 POLY 286. Using orthogonal grafting-from strategies to access well-defined 2-polymer, 1-protein bioconjugates. **K. Burridge**, M.M. Kearns, T. Wright, D. Konkolewicz, R.C. Page

1:40 POLY 287. Molecular sieving on the surface of nano-armored protein. **B. Kaupbayeva**, H. Murata, A. Lucas, K. Matyjaszewski, J.S. Minden, A.J. Russell

2:00 POLY 288. Ideal protein materials with genetic code expansion. **R.A. Mehl**, R.M. Bednar

2:30 POLY 289. Oxygen tolerant polymerisation for the design of biomaterials. **R. Chapman**

3:00 Intermission.

3:30 POLY 290. New conjugation approach to covalently crosslink and bond silk proteins on polymers for optical materials. **L. Bast**, N. Bruns

3:50 POLY 291. Cell surface conjugation of polymer nano- and microparticles. **H.A. Klok**

4:20 POLY 292. Polypept(o)ide-based cylindrical polymerbrushes as multifunctional nanocarriers. **C. Seidl**, M. Schinnerer, M. Barz

4:40 POLY 293. Exploiting the benefits of homogeneous and heterogeneous biocatalysis: Tuning the molecular interaction of enzymes with solvents via polymer modification. **J. Kaar**

Section C

Rosen Centre Hotel
Salon 19

Transport in Polymer Membranes

Gas Separation

Cosponsored by PMSE†
M. D. Dadmun, C. M. Stafford, *Organizers*
T. Saito, *Organizer, Presiding*
Z. P. Smith, *Presiding*



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- 1:00 POLY 294.** Enhancing CO₂/N₂ selectivity of addition-type polynorbornenes. **B.K. Long**, C. Maroon, J. Townsend, K.R. Gmernicki, D.J. Harrigan, B.J. Sundell, J.A. Lawrence, S.M. Mahurin, K.D. Vogiatzis
- 1:20 POLY 295.** Tailored CO₂-philic polymers for high flux CO₂ separation. T. Hong, P. Cao, B. Li, S. Zhao, A.P. Sokolov, **T. Saito**
- 1:40 POLY 296.** Multiscale modeling of time-dependent CO₂ and N₂ permeation through a glassy polymer at steady and non-steady state. **M. Soniat**, M. Tesfaye, D. Brooks, N.D. Humphrey, L. Weng, B. Merinov, W.A. Goddard, A.Z. Weber, F.A. Houle
- 2:00 POLY 297.** Characterization of high-performance membrane polymers for gas separation using broadband dielectric spectroscopy. **M. Boehning**, H. Yin, A. Schönhals
- 2:20** Intermission.
- 2:50 POLY 298.** Toward role of two-dimensional nanomaterials for polymeric membrane materials. **H. Park**
- 3:20 POLY 299.** Polymers with ether-oxygen-rich branches with superior membrane CO₂/N₂ separation properties. **H. Lin**
- 3:40 POLY 300.** Photocurable polyethylene glycol containing thiol-ene membranes for efficient separation of CO₂ from light gases. **S. Nazarenko**, V. Vasagar, J.M. Schekman, M. Khraisheh, M.A. AlMa'adeed, M.K. Hassan
- 4:00 POLY 301.** Synthesis and characterization of polyimides containing bulky ethyl substituents for propylene/propane separation. **S. Yoo**, H. Park
- 4:20 POLY 302.** Anti-plasticization of polyimide membrane for olefin/paraffin separation using 2D nanofillers. **J. Lee**, F. Moghadam

Section D

Rosen Centre Hotel
Salon 23

Excellence in Graduate Polymer Research

Conjugated & Electroactive Polymers

Cosponsored by PRES, PROF, SOCED and YCC
Financially supported by Industrial Advisory Board; TOSOH; Wiley
H. Cheng, *Organizer*
C. Coltrain, T. E. Long, *Presiding*

- 1:00 POLY 303.** Structural and optoelectronic landscape of semiconductor:ferroelectric blends. **A. Khirbat**, I. Bargigia, A. Levitski, M. Losego, C. Silva, G.L. Frey, L.J. Richter, N. Stingelin
- 1:25 POLY 304.** Synthesis and strategic design of solution-processable diketopyrrolopyrrole copolymer semiconductors for enhanced performance in n-channel organic field effect transistors. **C. Buckley**, E. Reichmanis
- 1:50 POLY 305.** Ester-functionalized, wide band-gap conducting polythiophene for organic field effect transistors. **R. Gunawardhana**, C. Bulumulla, P.L. Gamage, M.C. Biewer, M.C. Stefan



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

2:15 POLY 306. Organic conductive polymers as printed electronics on fabrics for wearable electronics. **S. Sinha**, Z. Li, Y. Noh, K. Chon, Y. Cao, G. Sotzing

2:40 Intermission.

2:55 POLY 307. Design of nanostructured, self-doped block polymer electrolytes for lithium-ion battery electrolytes. **M.A. Morris**, T.H. Epps

3:20 POLY 308. Combined computational and experimental study on the effects of side-chain architecture of polythiophene derivatives on structure and ionic conduction. **J. Onorato**, B. Dong, C. Nowak, J. Strzalka, F. Escobedo, C.K. Luscombe, P.F. Nealey, S. Patel

3:45 POLY 309. Aramid nanofiber composite separators for high performance lithium-sulfur batteries. **A.E. Emre**, A. Gerber, N. Kotov

Section E

Rosen Centre Hotel
Salon 20

New Frontiers in Aerospace Polymers: Advances & Challenges in Experiments & Simulations

Multifunctional Composite for Aerospace

Cosponsored by PMSE

Financially supported by Air Force Research Laboratory; Bruker Instruments; Ansys Instruments; Boeing

M. A. Meador, D. Nepal, *Organizers*

J. S. Wiggins, *Organizer, Presiding*

H. Koerner, *Presiding*

1:30 POLY 310. Flexible polyimide aerogels with aliphatic links in the backbone structure for conformal antenna application. **H. Guo**, M. Meador, D. Tresp, B. Dosa, L. McCorkle

1:50 POLY 311. Multifunctional polymers and composites for aerospace applications. **T. Williams**

2:20 POLY 312. Boron nitride nanotube polymer composites for aerospace applications. **M. Jakubinek**, Y. Martinez-Rubi, B. Ashrafi, J. Guan, M. Rahmat, K. Kim, C. Kingston, B. Simard

2:40 POLY 313. Polymer aerogel nanocomposites via functionalized nanoparticles. **J.R. Alston**, H. Harrison, F. Kabir, A. Kelkar

Section F

Rosen Centre Hotel
Salon 21

Undergraduate Research in Polymer Science



TECHNICAL PROGRAM

Cosponsored by PMSE
S. E. Morgan, *Organizer*
H. Broadhead, *Presiding*

1:00 POLY 314. Synthesis of cyclobutane-containing building blocks from sorbic acid using photoenergy. **M. Mabin**, Z. Wang, Q.R. Chu

1:15 POLY 315. Effects of functionalized carbon nanostructures on material properties of nylon 6 and CNT dispersion. **J. Robinson**, M. Roth, M.K. Shukla, G. Subramanian

1:30 POLY 316. One-dimensional photonic crystals from ultra-high refractive index chalcogenide hybrid inorganic/organic polymers (CHIPs). **K. Konopka**, T. Kleine, R.A. Norwood, J. Pyun

1:45 POLY 317. Synthesis and characterization of novel Polyhedral Oligomeric Silsesquioxane (POSS) benzoxazine reactive diluents. **V.C. Torres**, W.K. Fuchs, J.S. Wiggins

2:00 POLY 318. Manipulation of isotropic-nematic phase transitions in aqueous liquid crystals. **J. Stelzel**, G. Parkinson, P.S. Russo

2:15 POLY 319. Gold catalyzed polymerization reactions of unsaturated substrates. **S. Stanciu**, E.R. King, J. Tropp, N. Eedugurala, L.E. Gonce, J.D. Azoulay

2:30 POLY 320. Synthesis of di- and trisallylide monomers for ring-opening polymerization. **M. Maday**, M.D. Scholten

2:45 Intermission.

3:15 POLY 321. Copper ion encapsulation via micelles of diblock copolymers. **A.E. Ringuette**, C. Chen, L.L. Cai, N.J. Lee, C. Ho, J.J. Lee, S.L. Goh, C. Goh

3:30 POLY 322. Unraveling the kinetic growth mechanism of single-chain nanoparticles with Diels-Alder chemistry. **S.E. Gosting**, E. Wilborn, C.G. Gregory, T. Page, W. Ramos, M. Hunter, P.J. Costanzo

3:45 Panel Discussion.

Applied Materials for New Frontiers: Ten Years of ACS Applied Materials & Interfaces

Sponsored by MPPG, Cosponsored by COLL[‡], INOR[‡], PMSE[‡] and POLY[‡]

Exploring the Frontiers of Chemistry through NASA Research

Living There: Science for the Future of Manned Space Exploration

Sponsored by COMSCI, Cosponsored by ANYL, BIOL[‡], BIOT, CELL, COLL, ENFL[‡], I&EC[‡], INOR[‡], NUCL[‡], PHYS[‡], PMSE[‡] and POLY[‡]



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Sponsored by PROF, Cosponsored by ENVR, GEOC, I&EC, MEDI, MPPG, NUCL, ORGN, PHYS, PMSE, POLY, WCC and YCC

GSSPC: Artificial Molecular Machines & the Next Generation of Molecular Control

Sponsored by CHED, Cosponsored by COLL, I&EC, ORGN†, PHYS, POLY and PRES

TUESDAY EVENING

Section A

Orange County Convention Center
West Hall C

Dispersivity in Block Copolymers: Synthesis, Characterization, Modeling & the Effects on Self-Assembly

Posters

Cosponsored by PMSE

W. Gao, P. D. Hustad, M. K. Mahanthappa, M. L. Robertson, *Organizers*

5:00 - 7:00

POLY 323. Thermo-responsive block copolymers in stabilizing and controlling catalytic efficiency of gold nanoparticles. **S. Bera**, D. Dhara

POLY 324. Synthesis of triple-responsive, amphiphilic block copolymers for potential drug-delivery applications. **P. Poddar**, S. Maiti, D. Dhara

POLY 325. Study on self-assembly structure of nanorod surfactant between block copolymer and aqueous solution using interfacial energy and polymer stretching energy. **C. Nam**, K. Ku, J. Ryu, W. Lee

POLY 326. Tailor-made thermoplastic elastomers via modulation of molecular weight distributions. **S.I. Rosenbloom**, D.T. Gentekos, B.P. Fors

POLY 327. Synthesis and characterize of the dual-thermo- responsive diblock copolymer. **D. Zhao**, R. Rajan, K. Matsumura

POLY 328. Phase behavior and structural determinants of multifunctional tripodal mesogens prepared via the Passerini three-component reaction. **S. Song**, D. Sahoo, M. Kumar, D.A. Barkley, P.A. Heiney, J.G. Rudick

POLY 329. Computational investigation on carbon nanotube-composite interactions using the ReaxFF reactive force field. **B. Damirchi**, A.C. van Duin



TECHNICAL PROGRAM

POLY 330. Oriented block copolymer domains in fibers. **Z. Zhou**

POLY 331. Effect of MFC size-concentration in the structure of PVA hydrogels. **W.E. Magalhães**, G.G. Goetten de Lima, B. Ferreira, M. de Matos, C. Jordão, F. Claro

POLY 332. One-pot synthesis and properties of high molecular weight multiblock copolymer via RAFT emulsion polymerization. **F. Jinwei**

POLY 333. Local internal morphologies in diblock copolymer thin films revealed by combined nanoscale infrared microscopy and mechanical mapping. **K. Ho**, S.S. Kim, L. Gilburd, S. de Beer, G.C. Walker

Section A

Orange County Convention Center
West Hall C

Excellence in Graduate Polymer Research

Posters

H. Cheng, *Organizer*

5:00 - 7:00

POLY 334. External control in atom transfer radical polymerization. **S. Dadashi Silab**, K. Matyjaszewski

POLY 335. Accelerated CuAAC coupling reaction fulfilled the synthesis of ultrahigh densely grafted polymers by grafting-onto strategy. **W. Gan**, Y. Shi, B. Jing, X. Cao, H. Gao

POLY 336. Inverse vulcanization of sulfur and charged monomers to enhance solubility and create inexpensive metal binding materials. **M. Eder**, C. Jenkins

POLY 337. Light-switchable silicon-based polymers with high thermal stability and surface areas. **N. Hu**, T. May, J.C. Furgal

POLY 338. Bouligand nanocomposites: Self-assembly of cellulose nanocrystals with thermoresponsive polymer. **H. Vu**, B. Natarajan, J. Woodcock, J. Obrzut, S. Seethamraju, J. Gilman, E. Coughlin

POLY 339. pDVB old polymer new tricks: Coupling of organic and inorganic chemistry for nanoparticle synthesis and noninvasive optogenetics applications. **E. Zhang**, A.A. Dickey, M. Burdette, M. Rich, K. Cannon, I. Bandera, M. Bolding, J. Ballato, J.W. Kolis, S.H. Foulger

POLY 340. Elucidating the relationship between the states of water and transport properties of ions in swollen polymer networks. **T. Tran**, C. Lin, H. Lin

POLY 341. Vapor-phase infiltration of metal oxides into microporous polymers for solvent stable nanofiltration membranes. **F. Zhang**, E. McGuinness, Y. Ma, M. Losego, R.P. Lively



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

POLY 342. Design and synthesis of functional sugar poly(orthoester) nanomaterials with ultra-low immunogenicity. **S. Maiti**, S. Manna, A. Esser-Kahn, W. Du

POLY 343. Bioadvantaged hydrophobic nylon-6,6 copolymers. **S. Abdolmohammadi**, N. Hernandez, J. Tessonier, E.W. Cochran

POLY 344. Computational study on the peroxide crosslinking of polyethylene using ReaxFF reactive force field. **D. Akbarian**, W. Woodward, A.C. van Duin

Section A

Orange County Convention Center
West Hall C

General Topics: New Synthesis & Characterization of Polymers

Posters

D. Garcia, *Organizer*

5:00 - 7:00

POLY 345. Measurement and control of odor contributors in waterborne architectural coatings. **J. Bohling**, M. Gallagher, P. Doll, J. Xu, D. Lin, J. Zou

POLY 346. Polycarbonate/polypeptide hybrid copolymers for soft tissue adhesives. **J. Wilson**, A. Heise

POLY 347. Pyrrole-based donor-acceptor conjugated molecules for organic electronics. **P.L. Gamage**, A.K. Fiedler, M.C. Stefan, M.C. Biewer

POLY 348. Interpenetrating polymer networks consisting of poly vinyl pyridine and poly phenylene oxide for use in organic electronics. T. Hussain, B. Parody, **G.D. Phelan**

POLY 349. Developing a platform to evaluate photoswitches and their mechanical work. **F. Stricker**, J. Read de Alaniz

POLY 350. Multifunctional sulfonamide-based polymers for water purification. **B. Hall**, E. Shelton, M.D. Schulz

POLY 351. Synthesis and characterization of polysulfone-based polymers for water remediation applications. **C. Morales Guzman**, E. Nicolau

POLY 352. Preparation and characterization of PEEK polymer electrolyte membranes with imidazolium group for anion exchange fuel cell. **S. Nam**

POLY 353. Ion exchange hybrid membranes with improved ion exchange capacity using ion exchange particles. **S. Nam**

POLY 354. Novel triazole-based semifluorinated sulfonated polyimides: Investigation of proton exchange membrane properties. **A. Singh**, S. Banerjee



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- POLY 355.** Towards fine-tuning the hydrophilicity and hydrophobicity of PVDF block copolymers. V. Vasu, **A. Dutta**, A.D. Asandei
- POLY 356.** Metal-free, highly soluble, fully aromatic fluorinated ladder polymer. **J.R. Molina**
- POLY 357.** Cross-linked polymerization of carbodiimides to explore liquid crystalline behavior. **C.U. Jayarathna**, B.M. Novak
- POLY 358.** Synthesis of bottlebrush (co)polymers via direct "click" polymerization of macromolecules. **Y. Wang**, Y. Fu
- POLY 359.** Performing Ring Opening Metathesis Polymerization (ROMP) reactions under flow conditions. **S. Subnaik**, C.E. Hobbs
- POLY 360.** Biobased cyclobutane-containing building blocks: Synthesis of cyclobutane diacid for novel polyesters. **R.K. Shahni**, Z. Wang, Q.R. Chu
- POLY 361.** Development of an initiator with post-polymerization photo-cleavage capabilities. **M.S. Baker**, C. Ludwig
- POLY 362.** Synthesis of acid-degradable star polymers by chain-growth CuAAC polymerization of AB monomers from active core. **W. Gan**, X. Cao, H. Gao
- POLY 363.** Rediscovery of s-tetrazines: UV absorbing additive, chemical blowing agent, and crosslinker. **W. Sun**, R. Bagge, R. Nanayakkara, D.A. Loy
- POLY 364.** Simple toolbox for building dendritic and polyisoprene based multidentate phosphine ligand structures and their Pd(0) complexes. **J.C. von Irmer**, M. Rehahn
- POLY 365.** Utilizing dynamic sulfur bonds to modify polysulfide. **P.M. Walker**, C. Jenkins
- POLY 366.** Probing the mechanism of thermally driven thiol-Michael dynamic covalent chemistry. **B. Zhang**, P. Chakma, M.P. Shulman, J. Ke, Z. Digby, D. Konkolewicz
- POLY 367.** Synthesizing laccol polymer and its copolymers using lacquer sap *Toxicodendron succedanea* for radiation hard applications via cationic polymerization and characterizing the materials. **I.H. Marasinghe Arachchilage**, M. Patel, j. harmon
- POLY 368.** Development of a cheap, efficient and stable "click" platform to access complex polymer architectures. **S. Bailey**, J. Read de Alaniz, E. Discekici
- POLY 369.** Hydrothermal polymerization of composition- and morphology-tunable polyimide microparticles. **T. Kim**, K. Lee, S. Kwak, B. Kim
- POLY 370.** Synthesizing macromonomers for brush polymers via anionic polymerization strategies. **R.M. Pearson**, G. Miyake
- POLY 371.** Bio-based benzoxazine monomers derived from di-furan-amine, vanillin, and phenol. **M. YU**, G.R. Palmese, J. La Scala
- POLY 372.** Analysis of various synthetic procedures to generate poly(S-r-DVB) by inverse vulcanization. **A. Fistrovich**, C. Jenkins



TECHNICAL PROGRAM

POLY 373. Effect on dispersity of end-capping in ATRP-grown surface-initiated brushes. **N.H. Vy**, D.H. Adamson

POLY 374. Butadiene ATRP with group 8 transition metal catalysts. V. Vasu, M. Johnson, W. Bannerman, **A. Dutta**, A.D. Asandei

Section A

Orange County Convention Center
West Hall C

New Frontiers in Aerospace Polymers: Advances & Challenges in Experiments & Simulations

Posters

Cosponsored by PMSE

Financially supported by Anasys Instruments; Bruker Instruments; Boeing; Air Force Research Laboratory
M. A. Meador, D. Nepal, J. S. Wiggins, *Organizers*

5:00 - 7:00

POLY 375. Rheological and processability improvements in polyethersulfone-POSS nanocomposites. **R. Shankar**, M. Woellner, A.F. Lopez, L. Kemp, S.E. Morgan

POLY 376. High-temperature polybenzoxazine resins for aerospace applications. **C.L. Crickmore**, D.A. Rider

POLY 377. Boron-containing hybrid organic-inorganic polymers: synthesis and characterization. **J. Heckler**, T. Pruyn

Section A

Orange County Convention Center
West Hall C

Poly(2-oxazoline)s & Polypeptoids

Posters

Cosponsored by PMSE

R. Hoogenboom, H. Schlaad, R. N. Zuckermann, *Organizers*

5:00 - 7:00

POLY 378. New methylene blue removal agents based on N,N-dimethylacrylamide and 2-oxazoline macromonomer. **F. Santillan**, J. Rueda

POLY 379. Removal of phenolic compounds from water solutions using porous poly(2-oxazoline)s obtained using high internal phase emulsion (HIPE) polymerization. **M. Ceglowski**, R. Hoogenboom

POLY 380. What is the shoulder? Understanding the appearance of the higher molecular weight fraction in the size exclusion chromatography from the synthesis of poly(2-alkyl-2-oxazoline)s. **d. bera**, R. Hoogenboom



TECHNICAL PROGRAM

POLY 381. Synthesis and characterization of thiol and aldehyde functionalized poly(2-oxazoline)s. **M. Purino**, A. Tigrine, V. R de la Rosa, R. Hoogenboom

POLY 382. Well-defined star-shaped poly(2-oxazolines). **X. Xu**, V. Jerca, R. Hoogenboom

POLY 383. Block copolymers of poly(-2-oxazoline)s and polyesteramides. **I. Muljajew**, M. Dirauf, C. Weber, U.S. Schubert

Section A

Orange County Convention Center
West Hall C

Polymer-Based Gene & Drug Delivery Systems

Posters

T. Fujiwara, X. M. Liu, Y. Ohya, Y. Wang, *Organizers*

5:00 - 7:00

POLY 389. Synthesis and optimisation of lipid-hybrid nanoparticles loaded with a mixture of two antiretroviral drugs for the treatment of HIV: Application in nanomedicine. **H.H. Elkateb**, T. McDonald

POLY 390. Investigation of the tumor penetration capability of PVCL/OEGA/GMA nanogels using a multicellular tumor spheroid model. **C. Zhang**, E. Gau, W. Sun, A. Pich, X. Shi

POLY 391. pH-Triggered amphiphilic polycarbodiimides as nanocarriers. **E.H. De Silva**, B.M. Novak, M.C. Stefan, A.T. Brown, K.J. Balkus

POLY 392. pH-Dependent dissolution of enteric polymers: A misconception? Implications for pH-dependent drug delivery. **J. Al-Gousous**, H. Ruan, J. Blechar, K. Sun, N. Salehi, P. Langguth, N. Job, R. Loebenberg, E. Lipka, M. Bermejo, G.E. Amidon, G.L. Amidon

POLY 393. Design and development of dual-headed nanosystems: Drug delivery applications. **G. Kaur**, N. Majeti

POLY 394. Adipose-derived stem cell delivery system using temperature-responsive biodegradable injectable hydrogel. **Y. Yoshizaki**, H. Takai, S. Fujiwara, M. Ii, H. Uchida, S. Nemoto, A. Kuzuya, Y. Ohya

POLY 395. Multilayer hydrogel capsules for encapsulation of small molecules. **V.A. Kozlovskaya**, E.P. Kharlampieva

POLY 396. Multilayer microcapsules from MRI-compatible poly(N-vinylcaprolactam)-co-ruthenium copolymer with ultralow magnetic susceptibility. **N. Mitchell**, A. Alford, V.A. Kozlovskaya, E.P. Kharlampieva

POLY 397. Porous polymeric microparticles for delivery of agents to control myopia progression. **M. Mohammadiroudbari**, V.A. Kozlovskaya, E.P. Kharlampieva

POLY 398. Efficient pro-oxidant cancer therapy using ROS-responsive thioether-based polymeric nanoparticles. Y. Kim, S. Kim, **M. Shim**



TECHNICAL PROGRAM

POLY 399. Magnetic molecularly imprinted polymer nanovectors as targeted delivery systems for breast cancer treatment. **M. Nerantzaki**, c. wilhelm, J. Fresnais, C. Ménager, N. Griffete

POLY 400. Well-defined pH-responsive PEG-*b*-PHEMA-*b*-PBA based micelles for targeted delivery of doxorubicin. **M. Mohamed**, A. Singh, A. El-Sokkary, M. Akl, P.N. Prasad, C. Cheng

POLY 401. Supramolecular hydrogels based on poly (ethylene glycol)-poly (lactic acid) block copolymer micelles and α -cyclodextrin for potential injectable drug delivery system. **A. Poudel**

POLY 402. Non-viral genome editing based on polymer-derived CRISPR conjugates. **W. Ejaz**, M. Canakci, F. Anson, B. Laliberte, J.A. Hardy, B. Osborn, S. Thayumanavan

Section A

Orange County Convention Center
West Hall C

Polymer Bioconjugates for a Changing World

Posters

Cosponsored by BIOT
J. Kaar, D. Konkolewicz, R. C. Page, J. K. Pokorski, *Organizers*

5:00 - 7:00

POLY 384. Synthesis of laccase polymer hybrids. **M. Kovaliov**, S. Averick

POLY 385. Sub-7 nm patterning platforms through directed self-assembly of metal conjugated biopolymers. **G. Pathiraja**, K. Davis, H.P. Rathnayake, D. Herr

POLY 386. Generation of solution-stable galectin-3 polymer conjugates. **A. Pritzlaff**, D. Rucco, L. Lin, H.A. Lower, D.A. Savin

POLY 387. Investigation of site-specific polymerization techniques *via* genetic incorporation of bioconjugate handles for studies with self-assembling and stimuli-responsive protein-polymer materials. **D. Rucco**, A. Pritzlaff, S. Betters, D.A. Savin

POLY 388. Preparation and characterization of modified chitosan nanoparticles for the adsorption of lead from drinking water. **M.A. Nunez Herrera**, K. Milligan, V.N. Fondong

Section A

Orange County Convention Center
West Hall C

Polymers & Biomimicry

Posters



TECHNICAL PROGRAM

A. N. Dhinojwala, T. Williams, *Organizers*

5:00 - 7:00

POLY 403. Tuning enzyme diffusion and reaction on temporal hydrogel stiffening. **H. Liu**, C. Lin

POLY 404. Charge density and swelling behavior of pH-sensitive polymers with mixed functional groups. **S. Yang**, J. Shyue

POLY 405. Characterizing the structure and dynamics of styrene-maleic acid copolymer-lipid nanoparticles (SMALPS) as a membrane mimetic. **K. Burridge**, I. Sahu, B. Harding, A.P. Bali, G. Dixit, M.T. Dolan, R. Edelmann, C. Dabney-Smith, D. Konkolewicz, G. Lorigan

POLY 406. On-demand softening of hydrogels through SrtA-mediated transpeptidation. D. Moore, **M. Arkenberg**, C. Lin

POLY 407. Robust and transparent superhydrophobic surfaces with high thermal resistance. Y. Park, **H. Lim**

POLY 408. Tetracycline Molecularly Imprinted Polymers (MIP): Synthesis, characterization, and comparison between conventional MIP, MIP@SiO₂, and hollow porous MIP. **R.R. Pupin**, M.T. Sotomayor

Section A

Orange County Convention Center
West Hall C

Synthesis & Properties of Densely Grafted Polymers

Posters

J. G. Kennemur, J. B. Matson, G. Stein, R. Verduzco, *Organizers*

5:00 - 7:00

POLY 409. Aromatic polyamide brushes: Next-generation surface coatings. **C.J. Reese**, E. Graham, A. Kennedy, T.A. Crowe, S.G. Boyes

Section A

Orange County Convention Center
West Hall C

Transport in Polymer Membranes

Posters

M. D. Dadmun, T. Saito, C. M. Stafford, *Organizers*



TECHNICAL PROGRAM

5:00 - 7:00

POLY 410. Fundamental study of interaction between minor gases and a polymeric membrane for carbon dioxide transport. **T. Park**, E. Chung

POLY 411. Molecular diffusion of carbon dioxide through hyperbranched polyethylenimine. **G. Lee**, S. Jang

POLY 412. Stability of polyamide nanofiltration membranes with peracetic acid/hydrogen peroxide disinfection. **M. Ghafari**, N. Dai

POLY 413. Going against entropy: conversion of immiscible polyimide blends to miscible blends for gas separation applications. **C. Karunaweera**, S. Haghiri, S. Panangala, I.H. Musselman, K.J. Balkus, J.P. Ferraris

POLY 414. Leveraging conductivity-enhancing pathways in homopolymer-blended block polymer electrolytes. **M.A. Morris**, R. Nieuwendaal, J. Dura, T.H. Epps

POLY 415. Fuel transport properties of functionalized nanoclay/urethane composites. **J. Sloan**, D. Flanagan, D. Deschepper, H. Feuer

POLY 416. Decomposition mechanisms of novel electrolytes within Li-air batteries for NASA electric aircraft. **R.P. Viggiano**, D. Dornbusch, W.R. Bennett, K. Knudsen, P. Arrechea, J. Lawson

Section A

Orange County Convention Center
West Hall C

Undergraduate Research in Polymer Science

Posters

Cosponsored by PMSE
S. E. Morgan, *Organizer*

5:00 - 7:00

POLY 417. Impact resistant polymers: Investigating polyamides via *cis/trans* isomerization. **K. Kelsall**, J. Garraway, E.S. Sterner

POLY 418. Bicyclic guanidine organocatalysts: A comparison of three structural analogs. **A. Chesness**, M.D. Scholten

POLY 419. Design and synthesis of bio-based click-able polymeric sensors. **D.A. Kure**, C.A. Corley, S.T. Iacono, A.R. Jennings

POLY 420. Improving the recyclability of PET-PE mixed waste streams. **A.F. Bratton**, C.J. Ellison, K.M. Miller

POLY 421. Development and characterization of perfluorocyclopentene-polyhedral oligomeric silsesquioxane polymers of varying side chain length. **E.L. Alvino**, E.C. Lochmaier, S.T. Iacono, A.R. Jennings



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- POLY 422.** Isodimorphic co-crystallization in succinate polyester polyols: Comparison of butanediol and hexanediol copolymer; and blend crystallization structure, kinetics, and compatibility. T. Hunt, M. Stitt, C. Finley, **J. Dvorak, S. Cabrera**, A. Schrock
- POLY 423.** Preparation of perfluoropolyether-modified nanoparticles for improved fluoropolymer filament compatibilization for 3D-printed structural energetics. **B. Martin**, J. Mates, J. McCollum, S.T. Iacono
- POLY 424.** Preparation and characterization of metallized electrospun microfiber fluoropolymer composites for energetic applications. **E. Gazmin**, J. McCollum, J. Mates, S.T. Iacono
- POLY 425.** Polysilazane preceramic polymer formulations of differing crosslink densities. **N.L. Williams**, T. Pruyn, A.R. Jennings
- POLY 426.** Asymmetric catalysis with helical supramolecular benzene 1-monourea-3,5-bisamide polymers. **K. Bone**, M. Raynal
- POLY 427.** Synthesis and characterization of a novel polymer by Sonogashira coupling between cyclopentadithiophenes and difurodiketopyrrolopyrroles for use in organic hybrid solar cells. **H.P. Masching**, J.L. Duffy-Matzner
- POLY 428.** Investigating the photoswitching properties of donor-acceptor Stenhouse adducts in pursuit of light-responsive systems to perform mechanical work. **K. Lindsey, K. Clark, J. Read de Alaniz**
- POLY 429.** Investigating optimal reaction conditions for the synthesis of Polylactic Acid (PLA). **E. Garza, R. Bui**, J. Tormos
- POLY 430.** Development of a 3D-printed microfluidic device for biological applications using LEGO® PDMS molds. **C. Gething**, H.J. Fletcher
- POLY 431.** Poly(4-vinylpyridine-N-oxide) as an oxygen atom transfer reagent. **G. Fata, C. Hutchison**, C.R. Turlington
- POLY 432.** Novel chiral organic catalysts for methacrylate polymerizations. **K.G. Oberle, J.C. Lowe**, C.R. Turlington
- POLY 433.** Investigation of reducing highly cross-linked polysulfides to polythiols. **K. Laws**, C. Jenkins
- POLY 434.** Synthesis and characterization of networked fatty acid based polymers. **M. Maw**, R.W. Kopitzke
- POLY 435.** Understanding the interface of wavelength selective resins for multi-material printing. **R.C. Chavez**, N. Dolinski, C.J. Hawker
- POLY 436.** Phosphonium-containing poly(ionic liquid) networks prepared from thiol-ene 'click' photopolymerization. **S. Sims**, R. Whittaker, K.M. Miller
- POLY 437.** Alternative to commercial plastics: Extraction and polymerization of a biorenewable monomer. **J. Thomas**, S. Shen, S.A. Miller
- POLY 438.** Thermal carbon analysis as a novel tool for examination of transparent polyimide aerogel properties. **T. Berg**, B. Nesper, A. Kubatova, S.L. Vivod
- POLY 439.** Synthesis and characterization of copolymers for the fabrication of novel polymer-MOF crystals. **A.N. Radzanowski**, J.M. Schekman, Y.C. Simon



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- POLY 440.** Synthesis of thermosensitive copolymers for the modification of polysaccharides. **C. Barrios**, C. Jenkins, R. Auzely-Velty
- POLY 441.** Multiblock copolymers from diallylammonium monomers. **A. Biery**, D.M. Knauss
- POLY 442.** Synthesis and characterization of silicone “hybrid” polymers prepared by platinum catalyzed hydrosilylation reactions. **A. Drumm**, J.W. Krumpfer
- POLY 443.** Synthesis of poly(quinoline)s and their derivatives via [4+2]-cycloadditions. K.M. Ryan, **J.W. Krumpfer**
- POLY 444.** Pseudo-polyrotaxane and polyrotaxanes of poly(ethylene glycol) for biomedical applications. **A.M. Alamoudi**, A.M. Abdulrahman, I.M. Khan
- POLY 445.** Biofilm prevention via covalently anchored bacteriophages on polymeric surfaces. **C. Perritt**, G. Sahukhal, H. Broadhead
- POLY 446.** Preparation and characterization of modified chitosan nanoparticle for substained release of bovine serum albumen under physiological conditions. **E.e. Uche**, K. Milligan, V.N. Fondong
- POLY 447.** Effect of hydrogenation on conductivity and glass transition temperature in novel oxanorbornene dicarboximide based polymers. **A. Riedl**, D.A. Waldow
- POLY 448.** Manipulation of molecular topology and composition using Diels-Alder chemistry. **M. Hunter**, M.S. Meyersohn, S.E. Gosting, N. Skinner, P.J. Costanzo
- POLY 449.** Degradable imine-containing core-crosslinked star polymers. M.B. Sims, **J. Rapp**, S. Goodrich, M. Li, B.S. Sumerlin
- POLY 450.** Bismuth (III) subsalicylate as a greener polymerization catalyst in teaching lab experiments. **H. Kolsky**

WEDNESDAY MORNING

Section A

Rosen Centre Hotel
Signature 2

Dispersity in Block Copolymers: Synthesis, Characterization, Modeling & the Effects on Self-Assembly

Disperse Block Polymer Self-Assembly

Cosponsored by PMSE
P. D. Hustad, M. K. Mahanthappa, *Organizers*
W. Gao, M. L. Robertson, *Organizers, Presiding*

8:30 POLY 451. Influence of polymer molecular weight distribution skew on properties. **B.P. Fors**



TECHNICAL PROGRAM

9:00 POLY 452. Tuning the effective interaction parameters or dispersity from the short mid-block in PS-b-PMMA based block copolymers. **J. Bang**, J. Huh

9:30 POLY 453. Importance of polydispersity in quantitative predictions for block copolymer melts. **M.W. Matsen**

10:10 Intermission.

10:30 POLY 454. Shear alignment of sphere-forming ABA triblock copolymers with a polydisperse midblock. W. Ding, C.R. Lopez-Barron, W.R. Burghardt, **M.L. Robertson**

11:00 POLY 455. Morphology and ionic conductivity in lithium salt-doped broad dispersity triblock polymers. **M.K. Mahanthappa**, H. Xu

Section B

Rosen Centre Hotel
Salon 12

Polymer Bioconjugates for a Changing World

Cosponsored by BIOT
J. Kaar, D. Konkolewicz, R. C. Page, J. K. Pokorski, *Organizers*
P. Besenius, K. Burrige, *Presiding*

8:00 POLY 456. Telechelic peptide-polymer conjugates as a toolbox for viromimetic assemblies and thermoresponsive hydrogels. R. Otter, C. Berac, **P. Besenius**

8:30 POLY 457. Polypeptide and protein-based bioconjugates as innovative functional biomaterials. **S. Lecommandoux**, E. garanger, B. Garbay, M. Bravo Anaya

9:00 POLY 458. Deploying light-mediated chemistries for the formation and modulation of biomaterial properties. **A.M. Kloxin**

9:30 POLY 459. Biotemplated polymer synthesis: Controlling polymer structures for biomedical applications. **T. Weil**

10:00 Intermission.

10:30 POLY 460. Tuning properties of microstructured polymer-polypeptide hydrogels. C. Garcia, **K.L. Kiick**

11:00 POLY 461. Zwitterionic versions of poloxamers: Functional nanostructures and bioconjugates. **T. Emrick**

11:30 POLY 462. High-throughput bioconjugate synthesis and screening for biocatalytic applications. **A. Simakova**, G. Lewis, A.K. Fisher, M. Link, K. Matyjaszewski, A.J. Russell

Section C

Rosen Centre Hotel
Salon 19



TECHNICAL PROGRAM

Transport in Polymer Membranes

Gas Separation

Cosponsored by PMSE‡

M. D. Dadmun, T. Saito, C. M. Stafford, *Organizers*

H. Lin, B. K. Long, *Presiding*

8:00 POLY 463. Fundamental study of gas and vapor sorption and transport mechanism in triptycene-based polymers. V. Loiano, Y. Li, S. Luo, Q. Zhang, R. Guo, **M. Galizia**

8:20 POLY 464. High-temperature gas separation properties of sub-micron polybenzimidazole membranes. **M.M. Merrick**, B.D. Freeman

8:40 POLY 465. H₂O and O₂ sorption and diffusion behavior in thermoset polymers with temperature. **M.C. Celina**, E. Linde, N. Giron

9:00 POLY 466. Membrane-based gas separations with a new class of ultrapermeable porous polymers. Y. He, F. Benedetti, S. Lin, C. Liu, Y. Zhao, H. Ye, T.A. Van Voorhis, M. De Angelis, T.M. Swager, **Z.P. Smith**

9:30 POLY 467. Probing the glass transition temperature of polymers of intrinsic microporosity (PIMs) by fast scanning calorimeter. **H. Yin**, Y. Chua, B. Yang, C. Schick, P. Szymoniak, M. Boehning, A. Schönhals

9:50 POLY 468. Engineering microporosity in polymeric membranes for fast and selective gas transport. T. Corrado, **R. Guo**

10:10 Intermission.

10:40 POLY 469. Advancing toward lower energy-intensity gas separations using polymer-derived membranes. **W.J. Koros**

11:10 POLY 470. Water sorption, dilation, and transport in polybenzimidazoles for gas separation membranes. **J.D. Moon**, M. Galizia, H. Borjigin, R. Liu, J.S. Riffle, B.D. Freeman, D.R. Paul

11:30 POLY 471. Thiol-ene networks containing tethered perfluoroalkyl chains: Synthesis and investigation of gas permeation, free volume, and surface properties. **S. Nazarenko**, R. Ramakrishnan, S.W. Wand, V. Vasagar, J. Goetz, B.M. Ameduri, J.W. Rawlins

11:50 POLY 472. Development of novel PDMS membranes for C₃₊ hydrocarbon recovery from natural gas. **J. Yang**, D.J. Harrigan, M.M. Vaidya, M.L. Ostraat, A.A. Bahamdan

Section D

Rosen Centre Hotel
Salon 7

Polymers & Biomimicry

Concepts in Biomimicry



TECHNICAL PROGRAM

A. N. Dhinojwala, *Organizer*
T. Williams, *Organizer, Presiding*

8:00 POLY 473. Biomimetic information displays. **V. Kan**, n. machover, E. Vargo

8:30 POLY 474. Biomimetic moisture responsive fabrics. **L. Lao**, Y. Wu, J. Fan

8:45 POLY 475. Designing liquid crystal elastomers as substrates for 3D electronics. **H. Kim**, J. Maeng, J. Gibson, Y. Shafiq, R. Rihani, B. Black, S. Georgakopoulos, T. Ware

9:00 POLY 476. Redox controlled unidirectional molecular transport. **Y. Qiu**, J.F. Stoddart

9:15 POLY 477. Sequence-defined redox-responsive polymers as artificial molecular muscles. **J.C. Barnes**

9:35 POLY 478. Smart nucleopolypeptide polymers. **C. Bonduelle**

9:50 Intermission.

10:00 POLY 479. Self-healing commodity copolymers. D. Davidovich, **M.W. Urban**

10:30 POLY 480. Soft lifters via layered liquid-crystal elastomers. **T. Guin**, T.J. White

10:45 POLY 481. Stimuli-responsive hydrogel/elastomer composites via fabric interphases. **A.M. Hubbard**, W. Cui, Y. Huang, R. Takahashi, M.D. Dickey, J. Genzer, D. King, J.P. Gong

11:00 POLY 482. Bioinspired toughening mechanism of elastomers. **K. Ahn**

11:25 POLY 483. Biomimetic polymer-based polymersomes as functional biomaterials. **S. Lecommandoux**

11:40 POLY 484. Elucidation of the design rules for polymer mimics antifreeze(glyco) proteins. **M.I. Gibson**, B. Graham, C. Stubbs, M. Hasan, A. Fayter, L. Wilkins

Section E

Rosen Centre Hotel
Salon 20

New Frontiers in Aerospace Polymers: Advances & Challenges in Experiments & Simulations

Thermoplastics & New Generation of Polymers for Aerospace Applications

Cosponsored by PMSE

Financially supported by Air Force Research Laboratory; Bruker Instruments; Anasys Instruments; Boeing

M. A. Meador, D. Nepal, J. S. Wiggins, *Organizers*

E. Barjasteh, S. Hawkins, *Presiding*



TECHNICAL PROGRAM

10:00 POLY 485. Sustainable, environmentally green polyurethanes as erosion-resistant coatings for aerospace applications. **P. Zarras**, B.G. Harvey, A.M. Hughes, J.D. Stenger-Smith, A. Chafin, A. Baca, R. Quintana, L. Cambrea, L. Baldwin, T. Dames, G.S. Ostrom, J. Letcher, M.J. Watrous, J. Amato

10:20 POLY 486. Rheology, melt processing, and crystallization modification of high performance polymers for thermoplastic composite applications. **S.E. Morgan**, K.M. Knauer, R. Shankar, M. Woellner, L. Kemp

10:50 POLY 487. *In situ* polymerisation on the carbon fiber surface for enhanced interfacial adhesion. **L.C. Henderson**, C.L. Arnold

11:20 POLY 488. Fastener free assembly of high performance composite structures. **M. van Tooren**

Section F

Rosen Centre Hotel
Salon 21

Poly(2-oxazoline)s & Polypeptoids

R. Hoogenboom, H. Schlaad, *Organizers*
R. N. Zuckermann, *Organizer, Presiding*
D. Zhang, *Presiding*

8:30 POLY 489. Universality of peptoid polymer chain conformation. S. Xuan, N. Luo, **R.N. Zuckermann**

9:00 POLY 490. 3D structure of achiral and chiral polypeptoids by means of molecular dynamics simulations and density functional theory calculations of spectroscopic data. **F. Jolibois**, L. Perrin, N. Bhattacharjee¹

9:20 POLY 491. Beyond classical hydrophilic-hydrophobic amphiphiles: Triblock poly(2-oxazoline)s with a fluorinated block as a new platform for advanced self-assembly. **S. Filippov**, L.K. B. Verbraeken, A. Riabtseva, R. Hoogenboom

9:50 Intermission.

10:05 POLY 492. Investigating the effect of charge-charge interaction on the solution self-assembly of sequence-defined ionic peptoid block copolymers. G.L. Sternhagen, S. Gupta, P. Du, Y. Zhang, V.T. John, G.J. Schneider, R. Kumar, S.W. Rick, **D. Zhang**

10:35 POLY 493. Polypropylen-based blends and compounds with antimicrobial activity. **M.S. Windberger**, A. Kelly, I. Mühlbacher, F. Wiesbrock

10:55 POLY 494. Poly(2-oxazoline)s as matrix excipient for sustained release formulations. **A. Tigrine**, A. Samaro, V. Van Hoorne, V. R de la Rosa, M. Vergaelen, M. Purino, B. Monnery, C. Vervaet, R. Hoogenboom

11:15 POLY 495. Poly(2-oxazolines) in the design of mucus-penetrating and mucoadhesive dosage forms for drug delivery. **V.V. Khutoryanskiy**, A.S. Victorova, R.I. Moustafine, G.K. Abilova, D.B. Kaldybekov, G.S. Irmukhametova, T.M. Ways, W. Lau, E.D. Mansfield, L. Ruiz-Rubio

Section G



TECHNICAL PROGRAM

Rosen Centre Hotel
Salon 22

General Topics: New Synthesis & Characterization of Polymers

D. Garcia, *Organizer*
J. Cole, J. Imbrogno, *Presiding*

8:00 POLY 496. Step-growth polymerization of fluoroalkenes toward polyaromatic hydrocarbon enchaind semi-fluorinated polymers. **K. Shelar**, B. Farajidizaji, G. Narayanan, K. Mukeba, A. Sygula, C.U. Pittman, D.W. Smith

8:20 POLY 497. Synthesis of (meth)acrylate copolymers from poly[phenyl (meth)acrylate] by transesterification using zinc art complex. **M. Oshimura**, T. Hirata, T. Hirano, K. Ute

8:40 POLY 498. Radical polymerization of vinylcyclopropanes through electron or energy transfer photocatalysis. **D. Chen**, G. Miyake

9:00 POLY 499. Organocatalyzed atom transfer radical polymerization of methacrylates at low PPM levels of catalyst. **J. COLE**, C. Federico, G. Miyake

9:20 POLY 500. Design and synthesis of functional polyethers using the N-Al adduct catalysts. **J. Imbrogno**, N.A. Lynd

9:40 POLY 501. Facile synthesis of medium- and long-chain aliphatic polyethers using organocatalysts. **A. Basterrechea**, E. Gabirondo, O.R. Coulembier, H. Sardon

10:00 POLY 502. Application of core-modified phenoxazine photoredox catalysts in organocatalyzed atom-transfer radical polymerization. **B. McCarthy**, G. Miyake

10:20 POLY 503. ADMET polymerization via microwave irradiation. T.W. Gaines, K.R. Williams, K.B. Wagener, **G. Rojas**

10:40 POLY 504. Organocatalyzed atom transfer radical polymerization of acrylonitrile using phenoxazine and dihydrophenazine-based photoredox catalysts. **D. Corbin**, B. McCarthy, G. Miyake

11:00 POLY 505. Radical ring-opening copolymerization of cyclic ketene acetals with vinyl monomers. **C. Lefay**

11:20 POLY 506. Chemically extended radical photopolymerization beyond temporal irradiation limitations: Radical dark curing photoinitiator. **K. Kim**, J. Sinha, K. Childress, C. Musgrave, J.W. Stansbury

11:40 POLY 507. Gold catalyzed polymerization reactions of unsaturated substrates: Toward new macromolecular chemistries. **E.R. King**, J. Tropp, N. Eedugurala, L.E. Gonce, S. Stanciu, J.D. Azoulay

WEDNESDAY AFTERNOON

Section A

Rosen Centre Hotel
Signature 2



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

Dispersivity in Block Copolymers: Synthesis, Characterization, Modeling & the Effects on Self-Assembly

Dispersivity in Block Polymer Amphiphiles

Cosponsored by PMSE

W. Gao, M. K. Mahanthappa, *Organizers*

P. D. Hustad, M. L. Robertson, *Organizers, Presiding*

1:00 POLY 508. Quantification of homopolymers and tri-block copolymers in polyoxyalkylene di-block copolymers. **W. Gao**, P. Yang, T. Zhang, J. Defelippis, L. Bai, E. Wasserman, E. Daus, S. Klamo

1:30 POLY 509. PEO-PPO-PEO pluronic block copolymers: Non-micellizable impurity effects on micellar packing and solution phase behavior in water. **C.Y. Ryu**

2:00 POLY 510. HPLC characterization of block copolymers. **T. Chang**

2:40 Intermission.

3:00 POLY 511. Molecular exchange kinetics of near-monodisperse polymeric micelles with crystalline cores. N. Koenig, L. Willner, **R. Lund**

3:30 POLY 512. Tailored cationic PISA-latexes for strong adhesion to anionic surfaces: Importance of purity and chain-extension as shown by adsorption. **J. Engstrom**, T. Bensefelt, L. Wagberg, F. D'Agosto, M. Lansalot, A. Carlmark, E.E. Malmstrom

Section B

Rosen Centre Hotel
Salon 12

Polymer Bioconjugates for a Changing World

Cosponsored by BIOT

J. Kaar, R. C. Page, J. K. Pokorski, *Organizers*

D. Konkolewicz, *Organizer, Presiding*

J. J. Gassensmith, *Presiding*

1:00 POLY 513. Poly(2-oxazoline) conjugates with antibiotics. A. Romanovska, M. Schmidt, C. Krumm, **J.C. Tiller**

1:20 POLY 514. Immunomodulatory polymeric NLRP3 activators as vaccine adjuvants. **S. Manna**, S. Maiti, W. Du, Z. Guan, A. Esser-Kahn

1:40 POLY 515. Intracellular delivery via noncharged sequence-defined cell-penetrating polymer conjugates. **N.N. Phan**, C.A. Alabi

2:00 POLY 516. Slow-release and extended shelf-life of coordination polymer encapsulated vaccines. **J.J. Gassensmith**

2:30 POLY 517. Zwitterion-modified dendrimer-entrapped gold nanoparticles loaded with gadolinium for enhanced CT/MR imaging of lung cancer metastasis. J. Liu, Z. Xiong, J. Zhang, C. Peng, M. Shen, **X. Shi**



TECHNICAL PROGRAM

2:50 Intermission.

3:20 **POLY 518.** Cyclic peptide / polymer conjugates for therapeutic applications. **S. Perrier**

3:50 **POLY 519.** Bio-conjugate approaches to mAb manufacturing. A. Palapuravan, Y. Gong, H. Soleymani, Y. Zhao, A. Greschner, T.R. Congdon, H.W. de Haan, N. Cottenye, A. Niederquell, M. Kuentz, J. Leroux, **M. Gauthier**

4:20 **POLY 520.** Increasing the stability of oxytocin by exploiting different polymer architectures and conjugation approaches. **D.M. Haddleton**

Section C

Rosen Centre Hotel
Salon 19

Transport in Polymer Membranes

Experiments & Simulations

M. D. Dadmun, T. Saito, C. M. Stafford, *Organizers*
A. Asatekin, Y. Ding, *Presiding*

1:00 **POLY 521.** Salt permeation mechanisms through charge-patterned mosaic membranes. **W.A. Phillip**

1:30 **POLY 522.** Influence of relative permittivity properties on ion transport in hydrated polymer membranes. **G.M. Geise**

1:50 **POLY 523.** Incorporating membrane deformation into the boundary layer equation to model water and reverse salt flux in engineered osmosis. **J.A. Idarraga-Mora**, M. Fulton, D. Ladner, S.M. Husson

2:10 **POLY 524.** Preparation of fabrics with directional water-transport property. **L. Lao**, D. Shou, Y. Wu, J. Fan

2:30 Intermission.

3:00 **POLY 525.** Molecular transport in amorphous polymeric materials: An *in silico* view. **C.M. Colina**

3:30 **POLY 526.** Theory of multi-ion transport in solvent-filled membranes. **A.R. Crothers**, C.J. Radke, A.Z. Weber

3:50 **POLY 527.** How membrane chemistry influences transport mechanisms in various separation processes. **A. Roy**, M. Brayden, M. Martinez, J. Liu, M. Paul, S. Rosenberg, M. Peery

4:10 **POLY 528.** Electron tomography reveals details of the internal microstructure of desalination membranes. T. Culp, Y. Shen, M. Paul, A. Roy, M. Kumar, **E. Gomez**

4:30 **POLY 529.** Molecular structure of commercial reverse osmosis polyamide barrier layers. **B. Ocko**, Q. Fu, N. Verma, R. Li, M. Fukuto, C.M. Stafford, B.S. Hsiao

Section D



TECHNICAL PROGRAM

Rosen Centre Hotel
Salon 7

Polymers & Biomimicry

Concepts in Biomimicry

T. Williams, *Organizer*

A. N. Dhinojwala, *Organizer, Presiding*

1:00 POLY 530. Biomimetic mineralization of collagen: Effects of polymer process-directing agent on matrix mineralization and osteoclast-mediated bone resorption. **A.M. Compaan**, Y. Zhang, J. Elias, L. Holliday, L. Gower

1:30 POLY 531. Bio-inspired cell cryopreservation using synthetic analogues. **K. Murray**, C. Stubbs, T. Bailey, M.I. Gibson

1:45 POLY 532. Bio-inspired peptide-polymer hybrid mucin analogues: Applications in osteoarthritis and kidney stone disease. **D. French**, L. Navarro, S. Zauscher

2:00 POLY 533. Fast synthesis of biodegradable elastomers with tunable mechanical and surface properties via thiol-ene click chemistry for skeletal muscle regeneration. **M. Mohamed**, A. Shahini, J. Caserto, A. El-Sokkary, M. Akl, S. Andreadis, C. Cheng

2:15 POLY 534. Development of a polymer-based delivery system for the treatment of *Clostridium difficile* using a Gallium-antigen analogue. **B. Hall**, C. Malley, M.D. Schulz

2:30 POLY 535. Biomimetic graft-copolymers for restoring the lubrication properties of damaged cartilage. G. Morgese, L. Trachsel, M. Zenobi-Wong, **E. Benetti**

2:50 Intermission.

3:00 POLY 536. Synthesis and assembly of Vinyl Sulfonamide Click Nucleic Acids (VS-CNAs). **B.P. Sutherland**, D.J. Bischoff, C.J. Kloxin

3:20 POLY 537. Complex DNA nanostructure assembly via hybridization chain reaction. **L. Lanier**, H. Bermudez

3:35 POLY 538. Biomimetic glycopolymer models for determination of interaction modes with amyloid β peptides. **A.N. Bristol**, P.K. Das, S.E. Morgan

3:50 POLY 539. Macromolecular engineering of electrocatalytic metallopolymers via ATRP: Artificial enzymes for water splitting. **M. Karayilan**, W.P. Brezinski, K. Clary, K.C. McCleary-Petersen, D.L. Lichtenberger, R.S. Glass, J. Pyun

4:05 POLY 540. Sequence-controlled glycopolymers by RAFT polymerization: Synthesis of prototypes of glycosaminoglycan mimics. **M. Minoda**

4:20 POLY 541. Synthesis of modular brush polymer-protein hybrids using diazotransfer and copper click chemistry. **L. Navarro**, D. French, S. Zauscher

Section E



TECHNICAL PROGRAM

Rosen Centre Hotel
Salon 20

New Frontiers in Aerospace Polymers: Advances & Challenges in Experiments & Simulations

Stimuli-Responsive Composites

Cosponsored by PMSE

Financially supported by Air Force Research Laboratory; Bruker Instruments; Anasys Instruments; Boeing

M. A. Meador, D. Nepal, J. S. Wiggins, *Organizers*

V. A. Davis, L. C. Henderson, *Presiding*

1:30 POLY 542. Recent development of stimuli-responsive polymers for adaptive applications at Air Force Research Laboratory: Polyimide-based origami, photomobility and hygromorphicity. **L. Tan**

2:00 POLY 543. Furan and maleimide-containing polyimides for reversibly assembling feedstocks. **C. Wohl**, S. Applin, C. Morales-Cruz, M. Swift, B. Horvath, H.C. Schniepp

2:30 POLY 544. New approaches to scaling the production of liquid crystal elastomers. **T. Guin**, L. Kearney, H. Humphrey, E. Burgeson, N.A. Nguyen, C. Bowland, A.K. Naskar

2:50 POLY 545. Tuning the viscoelastic properties and creep-recovery behavior of smart polymers using ionic liquids. **S. Ravula**, S. Sterling, I.M. Warner

3:10 Intermission.

3:30 POLY 546. High-performance polymers: Function follows form. **T.J. Dingemans**

4:00 POLY 547. Intrinsically self-healing isocyanurate-oxazolidone polymers with high service temperatures. **L. Zhang**, H. Sodano

Section F

Rosen Centre Hotel
Salon 21

Poly(2-oxazoline)s & Polypeptoids

R. Hoogenboom, H. Schlaad, R. N. Zuckermann, *Organizers*

T. Dargaville, W. Jang, *Presiding*

1:20 POLY 548. Conjugation and release of drugs from poly(2-oxazoline) hydrogels. **T. Dargaville**, J. Park, N. Bock, M. de Laat, R. Hoogenboom

1:50 POLY 549. Anionic ring-opening polymerization of activated aziridines to produce linear polyethylenimine. **P. Rupar**, L. Reisman, C.P. Mbarushimana, E.A. Rowe

2:20 POLY 550. Mimicking nucleopore by track-etched polycarbonate membranes modified by poly(2-alkyloxazoline). **P. Guegan**, D. Benaoudia, P. Kolbeck, S. Li, V. Bennevault, J. Mathé, F. Montel, J. Lacroix



TECHNICAL PROGRAM

2:50 Intermission.

3:05 POLY 551. Polyoxazoline-based polymers as multifunctional platform. **W. Jang**, J. Joe, J. Lee

3:35 POLY 552. From polymer to application: solvent electrospinning of poly(2-oxazoline)s. E. Schoolaert, R. Hoogenboom, **K. De Clerck**

4:05 POLY 553. Synthesis and application of molecularly imprinted poly(2-oxazoline)s based on cross-linking by direct amidation. **M. Ceglowski**, S. Smeets, R. Hoogenboom

4:25 POLY 554. Synthesis of linear poly(trimethylenimine) by living anionic ring-opening polymerization. **L. Reisman**, E.A. Rowe, P. Rupar

Section G

Rosen Centre Hotel
Salon 22

General Topics: New Synthesis & Characterization of Polymers

D. Garcia, *Organizer*
D. Love, H. J. Schanz, *Presiding*

1:00 POLY 555. Design, synthesis, and application of highly reducing organic photocatalysts. **R.M. Pearson**, G. Miyake

1:20 POLY 556. poly(*N*-Acetylguanidine)s as reactive handle or reactive intermediate for post-polymerization modification of pendant ester groups. **J. Van Guyse**, X. Xu, R. Hoogenboom

1:40 POLY 557. Alkyne-enabled methods for metathesis polymer synthesis. **W. Gutekunst**

2:00 POLY 558. Synthesis and thermal properties of linear poly-dicyclopentadiene and linear polybrominated polydicyclopentadiene. M.A. Blead, N.D. Steese, D. Barvaliya, X. Poole, **H.J. Schanz**

2:20 POLY 559. Highly tailorable polymers via the aza-Michael polymerization of hydrazides. **D. Love**, D. Domaille, B. Fairbanks, K. Kim, O. Williams, C. Bowman

2:40 POLY 560. Ring-opening reactions to functional polyamides and polyurethanes. **K. Odelius**

3:00 POLY 561. Polycyclic aromatic core—enchained perfluorocyclobutyl (PFCB) aryl ether polymers derived from phenanthrenequinone. **B. Farajidizaji**, G. Narayanan, K. Shelar, K. Mukeba, A. Sygula, C.U. Pittman, D.W. Smith

3:20 POLY 562. Melt-processable telechelic poly(ether imide)s end-capped with zinc sulfonate salts. **K. Cao**, Z. Zhou, G. Liu

3:40 POLY 563. Living anionic polymerization of aziridines tolerates water and gives fast access to amphiphilic multi-block copolymers. **T. Gleede**, T. Kuckhoff, E. Rieger, M. Wagner, F. Wurm

4:00 POLY 564. Halide rebound polymerization of twisted amides. **M. Xu**, L. Fu, A.M. Nicely, J. Yu, W. Gutekunst



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

4:20 POLY 565. Relay conjugation and chain-end functionalization of ROMP. **L. Fu**, T. ZHANG, W. Gutekunst

4:40 POLY 566. New isosorbide derived monomers for chain growth polymerizations. **R.J. Kieber**, C. Ozkardes, J.G. Kennemur

THURSDAY MORNING

Section A

Rosen Centre Hotel
Signature 2

Dispersity in Block Copolymers: Synthesis, Characterization, Modeling & the Effects on Self-Assembly

Discrete vs. Broad Block Polymer Dispersity

Cosponsored by PMSE
W. Gao, M. L. Robertson, *Organizers*
P. D. Hustad, M. K. Mahanthappa, *Organizers, Presiding*

8:30 POLY 567. Regulating the phase behaviour of block copolymers via polydispersity. **A. Shi**

9:00 POLY 568. Effects of polydispersity on microphase separation in thin films of diblock copolymers: Theories, simulations, and experiments. **R. Kumar**

9:30 POLY 569. Amplifying (im)perfection: Consequences of dispersity on the assembly of block co-oligomers. **E.W. Meijer**

10:10 Intermission.

10:30 POLY 570. Influence of laminar flow on dispersity in continuous-flow polymer synthesis. **F.A. Leibfarth**, M.H. Reis

11:00 POLY 571. Unexpected morphologies in discrete end-functionalized oligomers. **B. Lamers**, A. Palmans, E.W. Meijer

Section B

Rosen Centre Hotel
Salon 12

Polymer Bioconjugates for a Changing World

Cosponsored by BIOT
J. Kaar, D. Konkolewicz, R. C. Page, J. K. Pokorski, *Organizers*
S. Averick, D. A. Savin, *Presiding*

8:00 POLY 572. Functional enzyme-microgel bioconjugates. **A. Pich**, E. Gau



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

8:20 POLY 573. Polymer conjugation to enhance cellulase activity and preserve stability. **T. Wright**, M. Lucius, B. Schmitz, K. Makaroff, J. Stewart, H. Fischesser, J. Shepherd, J. Berberich, D. Konkolewicz, R.C. Page

8:40 POLY 574. Biocombinatorially selected peptide-polymer conjugates as polypropylene binders. **C. Juds**, T. Conrad, M. Weller, H. Börner

9:00 POLY 575. Site-specific polymerization techniques *via* genetic incorporation of synthetic handles. D. Rucco, A. Pritzlaff, **D.A. Savin**

9:30 POLY 576. Site-selective antibody drug conjugates enabled by cysteine arylation and native conjugation. **B.L. Pentelute**

10:00 Intermission.

10:30 POLY 577. Repurposing enzymes: Investigating the mechanism of horseradish peroxidase as a RAFT-initiase. **D. Konkolewicz**, R.C. Page, J. Berberich, A. Danielson, C. Kozuszek, D. Bailey Van Kuren, J. Bornstein

11:00 POLY 578. Lipase-polymer biohybrids. M. Kovaliov, **S. Averick**

11:30 POLY 579. Controlling biocatalysis by transiently switchable polymersome nanoreactors. **N. Bruns**, O. Rifaie-Graham, S. Ulrich, N.F. Galensowske, S. Balog, M. Chami, D. Rentsch, J.R. Hemmer, J. Read De Alaniz, L. Boesel

Section C

Rosen Centre Hotel
Salon 19

Transport in Polymer Membranes

Molecular Transport & Fouling

Cosponsored by PMSE[‡]
M. D. Dadmun, T. Saito, C. M. Stafford, *Organizers*
D. Hallinan, W. A. Phillip, *Presiding*

8:00 POLY 580. Facile fluorination of UF membranes by direct coating of perfluoropolymers to enhance antifouling properties for water purification. **T. Tran**, Y. Tu, S. Hall-Laureano, C. Lin, M. Kawy, H. Lin

8:20 POLY 581. Robust underwater anti-oil fouling coatings from spray assemblies of polyelectrolyte grafted silica nanochains. **Z. Liao**, G. Wu, S. Yang, D. Lee

8:40 POLY 582. Fouling mechanisms in constant flux crossflow ultrafiltration. **Y. Cheng**, A.Y. Kirschner, D.R. Paul, R.W. Field, B.D. Freeman

9:00 POLY 583. Exploring and modifying ionic lyotropic liquid crystal-based nanoporous polymer membranes for different water purification applications. **D.L. Gin**, S. Dischinger, J. Rosenblum, K. Linden, R.D. Noble

9:30 POLY 584. Concentration-dependent mechanical properties of polyurethane and polyurethane-based composites during chemical permeation. **D. Boyne**, M. Varady, T. Pearl, B.A. Mantooth



TECHNICAL PROGRAM

9:50 POLY 585. Highly selective organic solvent nanofiltration membranes based on polyepoxies to separate fatty acids and more. **N.B. Bowden**, C.M. Gilmer

10:10 Intermission.

10:40 POLY 586. Membranes for charge- and aromaticity-based separation of small molecules. I. Sadeghi, **A. Asatekin**

11:10 POLY 587. Equilibrium water uptake and transport in thin polymer films measured via Polarization-Modulated Infrared Reflection Absorption Spectroscopy (PM-IRRAS). A. Balwani, H. Ro, E.M. Davis, d.d. bendejacq, **C.M. Stafford**

11:30 POLY 588. Transport properties of water and salt ions in confined geometries of block copolymers. **D. Aryal**, R. Samanta, V. Ganesan

11:50 POLY 589. Fundamental investigation of the transport of water in epoxy/amine crosslinked polymers. **J. Vergara**, S.K. Yadav, J. La Scala, G.R. Palmese

Section D

Rosen Centre Hotel
Salon 7

Polymers & Biomimicry

Concepts in Biomimicry

A. N. Dhinojwala, *Organizer*
T. Williams, *Organizer, Presiding*

8:15 POLY 590. Biologically-inspired supramolecular systems: architecture and mechanics. **L. Korley**, C.B. Thompson

8:45 POLY 591. Snaking/twisting fibers formation of cyanobacterial supra-polysaccharides in drying process. **K. Budpu**, K. Okeyoshi, M. Okajima, T. Kaneko

9:05 POLY 592. From bio-inspired functional film to reactive nano-patterned honeycomb as a clickable platform. **L. Billon**, P. Marcasuzaa, S. Pearson

9:25 POLY 593. Thin films and nanoparticles with nanoscale reactive patches. D. Varadharajan, H. Turgut, H. Yabu, **G. Delaittre**

9:45 POLY 594. Synthetic melanin nanoparticles in 2D and 3D cell culture models: Mimicking human melanosomes. **N. Collins-McCallum**, Z. Wang, X. Zhou, B. Perez-White, N.C. Gianneschi

10:05 Intermission.

10:15 POLY 595. Sustainable packaging inspired by cellulose and chitin. **J.C. Meredith**

10:45 POLY 596. Self-assembled benzene tri-carboxamide hydrogels for tissue engineering. **M.B. Baker**



TECHNICAL PROGRAM

11:05 POLY 597. Super-oriented hydrogels of cyanobacterial mega-saccharide, sacran, and its biological functions. **M. Okajima**, S. Sornkamnerd, K. Amornwachirabodee, T. Kaneko

11:25 POLY 598. Bio-based amino acid polymers and their self-assembly phenomenon. **T. Kongprathet**, K. Takada, T. Kaneko

Section E

Rosen Centre Hotel
Salon 9

New Frontiers in Aerospace Polymers: Advances & Challenges in Experiments & Simulations

Multiscale Modeling of Aerospace Composite

Cosponsored by PMSE

Financially supported by Anasys Instruments; Bruker Instruments; Boeing; Air Force Research Laboratory

M. A. Meador, D. Nepal, *Organizers*

J. S. Wiggins, *Organizer, Presiding*

D. Bernhardt, *Presiding*

8:00 POLY 599. Multiscale computational modeling of polymer materials and composites. M.S. Radue, W. Pisani, H. Al Mahmud, **G. Odegard**

8:30 POLY 600. Property predictions and analysis for aerospace polymers using molecular simulation. **A. Browning**, J. Sanders, M. Halls, J. Gavartin, C. Krauter

9:00 POLY 601. Quantifying the impact of process pathway on the development of thermoset resin properties and morphology during cure: From experiment to simulation. **C. Estridge**

9:30 POLY 602. Hierarchical multiscale simulations approach for modeling failure in polymer matrix composites. X. Wu, A. Aramoon, **J.A. El-Awady**

10:00 Intermission.

10:20 POLY 603. Molecular dynamics simulations of MoS₂-dispersed epoxy nanocomposites. **R.J. Berry**, I. Barrett, G.S. Kedziora, J. Moller, T. Nguyen-Beck, N. Pestian, J. Ryan, D. Nepal

10:40 POLY 604. Coupling modeling with experimentation for aerospace materials development. **E. Siochi**

11:10 POLY 605. Modeling the role of bulk and surface characteristics of carbon fiber on thermal conductance across the carbon-fiber/matrix interface. **V. Varshney**, A. Roy, J. Baur

Section F

Rosen Centre Hotel
Salon 10

Poly(2-oxazoline)s & Polypeptoids



TECHNICAL PROGRAM

H. Schlaad, R. N. Zuckermann, *Organizers*
R. Hoogenboom, *Organizer, Presiding*
C. Weber, *Presiding*

8:30 POLY 606. Poly(cyclic imino ether)s beyond 2-oxazolines. **R. Hoogenboom**

9:00 POLY 607. Self-assembled multiresponsive polymer nanogels as contrast agents for ^{19}F magnetic resonance imaging. **K. Kolouchová**, O. Sedlacek, D. Jirak, D. Babuka, J. Kotek, M. Vit, J. Trousil, R. Konefal, O. Janouskova, B. Podhorska, M. Slouf, M. Hruby

9:20 POLY 608. Atomic-scale imaging of polypeptoid crystals. X. Jiang, D.R. Greer, D. Prendergast, R.N. Zuckermann, **N.P. Balsara**

9:50 Intermission.

10:05 POLY 609. End-functional poly(2-ethyl-2-oxazoline)s as versatile building blocks to combine CROP and RAFT. **C. Weber**, A. Trüttschler, M. Sahn, U.S. Schubert

10:35 POLY 610. Fluorine containing poly-2-oxazolines as contrast agents for ^{19}F MRI: Quest for the structure. **L. Kaberov**, Z. Sadakbayeva, A. Murmiliuk, E. Pavlova, J. Brus, R. Hoogenboom, S. Filippov

10:55 POLY 611. Antimicrobial telechelic partially hydrolyzed poly(2-oxazoline)s with two modes of action. **L. Benski**, M. Hijazi, F. Arfeen, C. Krumm, J.C. Tiller

11:15 POLY 612. Assembly of poly(2-alkyl-2-oxazoline)-block-poly(lactides) in water. **F.M. Winnik**, F. Pooch, H. Tenhu

11:45 Concluding Remarks.

THURSDAY AFTERNOON

Section A

Rosen Centre Hotel
Signature 2

Dispersivity in Block Copolymers: Synthesis, Characterization, Modeling & the Effects on Self-Assembly

Architectural Dispersivity in Block Polymers

Cosponsored by PMSE
P. D. Hustad, M. L. Robertson, *Organizers*
W. Gao, M. K. Mahanthappa, *Organizers, Presiding*

1:00 POLY 613. Multiblock copolymers and their self-assembly properties. **S. Perrier**

1:30 POLY 614. Crystallizable comb block polyolefins with broad polydispersity in molecular weight and composition. **P. Brant**



TECHNICAL PROGRAM

2:00 POLY 615. Partitioning of molecules in olefin block copolymer (OBC) morphologies: Effect on the size of ordered domains and the phase diagrams of disordered OBC/random copolymer blends. **J. Weinhold**, P.D. Hustad

2:40 Intermission.

3:00 POLY 616. Blockiness and sequence polydispersity effects on the self-assembly and interfacial properties of gradient copolymers. **V. Ganesan**

3:30 POLY 617. Facile synthesis and self-assembly of semi-dispersed miktoarm star polymers. **A.E. Levi**, J. Lequeieu, J. Horne, C.M. Bates, G.H. Fredrickson

Section B

Rosen Centre Hotel
Salon 12

Polymer Bioconjugates for a Changing World

Cosponsored by BIOT
J. Kaar, D. Konkolewicz, J. K. Pokorski, *Organizers*
R. C. Page, *Organizer, Presiding*
J. L. Price, *Presiding*

1:00 POLY 618. Structure-function-dynamics relationships in next generation protein-polymer conjugates. **S. Baker**, A. Munasinghe, H. Murata, K. Matyjaszewski, P. Lin, C.M. Colina, A.J. Russell

1:20 POLY 619. Polymer bioconjugates: An *in silico* perspective. **C.M. Colina**

1:50 POLY 620. Mimicking protein structure and function with peptide-polymer conjugates. **A. Knight**

2:20 POLY 621. Modeling of nanoparticles nanomedicines and molecular sliders on biopolymers. **P. Kral**

2:40 POLY 622. Molecular sieving through dendronization of enzymes. **A. Adronov**, S. McNelles

3:00 Intermission.

3:30 POLY 623. Biophysical assays for rapid assessment of protein-polymer bioconjugate stability. **R.C. Page**, D. Konkolewicz, T.A. Wright

4:00 POLY 624. PEG-based increases to protein conformational and proteolytic stability. **J.L. Price**

4:30 POLY 625. Manipulating hierarchy, mechanics, and function in polyurea-peptide hybrids. **L. Korley**, L.E. Matolyak, D. Jang, S. Chatterjee

Section C

Rosen Centre Hotel
Salon 6



TECHNICAL PROGRAM

Transport in Polymer Membranes

Nanocomposites & Characterization

M. D. Dadmun, T. Saito, *Organizers*
C. M. Stafford, *Organizer, Presiding*
E. Gomez, *Presiding*

1:00 POLY 626. Self-assembly of polymer-grafted nanoparticles for membrane separations. **D. Hallinan**

1:30 POLY 627. Understanding water and ion transport properties through MOF/polymer nanocomposite membranes. **T. LEE**, J. Oh, H. Park

1:50 POLY 628. Graphene oxide embedded polyamide thin films for water desalination. M. Abbaszadeh, D. Krizak, **S. Kundu**

2:10 POLY 629. High flux nanocellulose-embedded mixed matrix membranes. **J. Zheng**, N. Li, P. Hadi Myavagh, B.S. Hsiao

2:30 Intermission.

3:00 POLY 630. Membranes with spatially varying permeability. A. Blevins, L. Cox, J. Killgore, **Y. Ding**

3:30 POLY 631. Molecular structure of aromatic reverse osmosis polyamide barrier layers prepared at the oil/water interface. **Q. Fu**, N. Verma, H. Ma, F. Medellin-Rodriguez, R. Li, M. Fukuto, B.S. Hsiao, B. Ocko

3:50 POLY 632. Reactivity at the solid/liquid interface of a desalination model system. **C. Buechner**, S. Gericke, H. Bluhm

4:10 POLY 633. Overcoming the permeability-rejection trade-off of RO membranes via activation with a novel organic solvent. **M. Shin**, J. Lee

4:30 POLY 634. Extrinsic water content in polyelectrolyte multilayers. **R.L. Abbett**, J.B. Schlenoff

Section D

Rosen Centre Hotel
Salon 7

Polymers & Biomimicry

Concepts in Biomimicry

T. Williams, *Organizer*
A. N. Dhinojwala, *Organizer, Presiding*

1:00 POLY 635. Controlled functionalization of carbon nanomaterials for multifunctional applications. **L. Dai**



TECHNICAL PROGRAM

1:30 POLY 636. Micro-nanofibrillar polycaprolactone scaffolds as translatable osteoconductive grafts: An exploration of osteoblast viability, osteogenic phenotype, and innate antibacterial efficacy. **J.W. Moxley**, P. Ghannadian, T. Webster

1:50 POLY 637. Laser pulse heating of nanocomposites to create self-cleaning superhydrophobic surfaces. **S.F. Bartolucci**, J.A. Maurer

2:10 POLY 638. Plant-based polyphenol coatings for preparing highly active protein surfaces. A.M. Sousa, T. Li, S. Varghese, P.J. Halling, **K. Lau**

2:30 Intermission.

2:40 POLY 639. Mussel-inspired polyesters with aliphatic pendant groups demonstrate the importance of hydrophobicity in wet adhesion. A. Narayanan, S. Kaur, A.N. Dhinojwala, **A. Joy**

3:10 POLY 640. Synthesis of bioinspired polymeric adhesives for precise control of properties via well-defined crosslinking chemistry. **H. Chung**, I. Pramudya, C. Kim

3:30 POLY 641. Fully degradable polycarbonate/polypeptide hybrid copolymer bioadhesives for soft tissue repair. **J. Wilson**, A. Heise

3:50 POLY 642. Synthetic biology enables production of repetitive mussel foot proteins with enhanced underwater adhesion. **E. Kim**, F. Zhang

4:10 POLY 643. Understanding the bioadhesion of chitosan-catechol polymers. **A. Narkar**, K. Ahn

Section E

Rosen Centre Hotel
Salon 9

General Topics: New Synthesis & Characterization of Polymers

D. Garcia, *Organizer*
M. Carter, B. S. Lokitz, *Presiding*

1:00 POLY 644. Closing the gap between metal binding and polymer architecture. **W.R. Archer**, S. Winn, M. Sawyer, M.D. Schulz

1:20 POLY 645. Synthesis and viscoelastic properties of physically crosslinked linear and branched copolymer hydrogels. **D. Debnath**, C.R. Pugh

1:40 POLY 646. Poly(ether imide)s oligomers with tailored yellowness. **K. Cao**, M. Zhang, G. Liu

2:00 POLY 647. Nanoscale resolution of electric-field induced motion in ionic copolymer films. **B.S. Lokitz**, J. Dugger, J.F. Browning

2:20 POLY 648. Design and fabrication of hybrid poly(olefin)-acrylic latex particles. **M. Carter**, P. Luo, L. Chen, R. Moglia, T. Ratani, S. Brown, M. Janco, J. Gu, W. Gao, J. Ngunjiri, J. Kohn, R. Even



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- 2:40 POLY 649.** Template synthesis of polyelectrolyte multilayer nanocapsules via layer-by-layer deposition on crystallized miniemulsion nanodroplets. **A. Jafari**, H. Sun, B. Sun, H. Cui, C. Cheng
- 3:00 POLY 650.** Insight into the effect of gamma radiation on graft polymerization of graphene oxide using simultaneous radiation grafting methodology. **A. Khurshid**
- 3:20 POLY 651.** Opportunities for electrochemistry in Reversible Addition-Fragmentation chain-Transfer (RAFT) polymerization systems. **F. Lorandi**, M. Fantin, S. Shanmugam, Y. Wang, K. Matyjaszewski
- 3:40 POLY 652.** Acyloxyimide derivatives as peroxides alternatives for the melt grafting of maleic anhydride onto polyethylene. **Y. Guillaneuf**
- 4:00 POLY 653.** Dynamic sulfur bonds initiate polymer modification. C. Westerman, **C. Jenkins**
- 4:20 POLY 654.** Synthesis and architectural control of isosorbide-based polyethers via ring-opening polymerization. **D. Saxon**, M. Nasiri, M. Mandal, S. Maduskar, C.J. Cramer, P.J. Dauenhauer, A. LaPointe, T.M. Reineke
- 4:40 POLY 655.** New macromonomer synthetic strategies for the modular synthesis of brush polymers. **M.D. Ryan**, G. Miyake

Section F

Rosen Centre Hotel
Salon 10

General Topics: New Synthesis & Characterization of Polymers

D. Garcia, *Organizer*
C. M. Bates, L. Leal, *Presiding*

- 1:00 POLY 656.** Synthesis, characterization, and cure chemistry of a bis(allylidene) functionalized multicyclic cage compound derived from norbornadiene. **K.E. Rosenkoetter**, M. Garrison, R. Quintana, B.G. Harvey
- 1:20 POLY 657.** Enyne functionalization of metathesis initiators. **T. ZHANG**, L. Fu, W. Gutekunst
- 1:40 POLY 658.** Taming the domino reaction for controlled radical polymerization. **J. Niu**, H. Huang
- 2:00 POLY 659.** Self-assembly, symmetry breaking, and block polymer architecture. **C.M. Bates**
- 2:20 POLY 660.** Fluorination of polyisoprene with fluorine-containing hypervalent iodine reagents. **Y. Cao**, N.V. Tsarevsky
- 2:40 POLY 661.** Determination of the chemical heterogeneity of ternary copolymers. **D. Lohmann**, T. Hofe, W. Radke
- 3:00 POLY 662.** Light-driven synthesis of bottlebrush polymers using organocatalyzed atom transfer radical polymerization. **O.N. Manahan**, B. Buss, G. Miyake
- 3:20 POLY 663.** High-mechanical-strength telechelic poly(ether imide)s end-capped with ureidopyrimidione. **K. Cao**, G. Liu



TECHNICAL PROGRAM

3:40 POLY 664. Effect of quench depth on crystallization in semicrystalline block copolymer/salt mixture studied by depolarized light scattering. X. Li, w.S. Loo, X. Jiang, X. Wang, M.D. Galluzzo, **K. Mongcopa**, **A. Wang**, N.P. Balsara, B.A. Garetz

4:00 POLY 665. Multi-functional and robust liquid crystalline brush-like copolymers: Synthesis, structure, and property analysis. **D. Ndaya**, R. Bosire, R. Kasi

4:20 POLY 666. Bioresorbable and biocompatible block copolymers: *In vitro* studies for targeted biomedical applications. **N.M. Mulchandani**, K. Masutani, S. Kumar, S. Sakurai, Y. Kimura, V. Katiyar

PMSE

Division of Polymeric Materials Science and Engineering

C. Snyder, E. Harth and J. Schaefer, *Program Chairs*

SUNDAY MORNING

Section A

Rosen Centre Hotel
Salon 17

Antimicrobial & Cell-Penetrating Polymers

Cosponsored by POLY†

Financially supported by Biomaterials Science (RSC journal); Polymer Chemistry (RSC journal); Polymers (MDPI journal); TOSOH Bioscience, LLC

A. Joy, *Organizer*

E. Palermo, *Organizer, Presiding*

8:55 Introductory Remarks.

9:00 PMSE 1. Antimicrobial polymer surfaces to fight bacterial biofilm formation: From basic concepts to applications. **K. Lienkamp**

9:20 PMSE 2. Highly tunable antimicrobial technology: Creating zwitterionic functional polymers from low T_g PSA to high T_g thermoplastics coating applications. **M.B. Ali**

9:40 PMSE 3. Antimicrobial and cell-penetrating conjugated oligo- and polyelectrolytes. **K.S. Schanze**

10:00 PMSE 4. Design of antimicrobial polymers: Effect of the polymer architecture and monomer sequence. P. Judzewitsch, R. Zangeneh, E. Wong, **C. Boyer**



TECHNICAL PROGRAM

10:20 PMSE 5. Controlling polymer backbones in ROMP using cycloalkene derivatives. **N.S. Sampson**

10:40 Intermission.

11:10 PMSE 6. Methacrylamide-based antimicrobial peptide mimics prepared via RAFT: effects of structure on activity. **S.E. Morgan**, L.C. Paslay, S. Goetz, B.A. Abel, G. Sahukhal, M.O. Elasri, C.L. McCormick

11:30 PMSE 7. Molecular design and activity of sequence-defined antimicrobial macromolecules. **C.A. Alabi**

11:50 PMSE 8. Antibacterial phosphonium polymers: Tuning surface and solution activity. **E.R. Gillies**, P.J. Ragogna, T.J. Cuthbert

12:10 PMSE 9. Photo-chemical discovery of anti(myco)bacterial polymers. **M.I. Gibson**, S. Richards, C. Guy, R. Tomás, E.C. Fullam

Section B

Rosen Centre Hotel
Salon 16

ACS Award for Team Innovation: Symposium in Honor of Vivek M. Prabhu, Christopher L. Soles, Eric K. Lin & Wen-Li Wu

Q. Lin, *Organizer*

C. R. Snyder, *Organizer, Presiding*

9:00 Introductory Remarks.

9:10 PMSE 10. Industry-government partnership for the development of supramolecular hydrogels as therapeutics and therapeutic delivery agents. **J. Hedrick**

9:40 PMSE 11. Impact behavior of crosslinked polymer networks. **J. Lenhart**

10:10 Intermission.

10:25 PMSE 12. Current and future opportunities for user science at the NIST Center for Neutron Research. **R.M. Dimeo**

10:55 PMSE 13. Integrated simulation and experimental platforms for molecular characterization of complex materials. **J.J. De Pablo**

11:25 PMSE 14. Rheo-Raman microscope: Probing physical and chemical processes in soft matter. A.K. anthony.kotula@nist.gov, M. Meyer, J. Plog, **K. Migler**

Section C

Rosen Centre Hotel
Salon 15



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

Hybrid Functional Materials from Controlled Assembly of Polymer & Inorganic Nanoparticles

Polymer-Nano Hybrids in Solution

Financially supported by Huazhong University
J. He, Y. Lin, Z. Nie, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 PMSE 15. Polymer-directed, reversible nanoparticle self-assembly. **L. Liz Marzan**

9:05 PMSE 16. Solvation-induced self-assembly in aqueous solutions of ions, nanoparticles, and polyelectrolytes. **J. Douglas**

9:35 PMSE 17. Polymer-enabled colloidal synthesis and self-assembly of functional nanostructures. Q. Xiong, S. Hou, Y. Chen, **H. Duan**

10:05 Intermission.

10:20 PMSE 18. Intimate and permanent tethering of thermal-responsive polymer on plasmonic nanoparticle enables switchable optical properties and dual-functional catalytic activities. **Z. Lin**

10:50 PMSE 19. Dynamic nanostructures fabricated by the self-assembly of functional polymers and nanoparticles. **S. Park**

11:20 PMSE 20. Self-assembly of inorganic-organic hybrid macromolecules containing well-defined molecular clusters. **T. Liu**

11:50 PMSE 21. Functional polymers for perovskite nanoparticle synthesis. **T. Emrick**, H. Kim

Section D

Rosen Centre Hotel
Salon 24

General Papers-New Concepts in Polymeric Materials

E. Harth, *Organizer*
A. Warren, Y. Zhou, *Presiding*

8:30 PMSE 22. Advance in the development of carbon dots. **Y. Zhou**, R.M. Leblanc

8:50 PMSE 23. Fabrication and characterization of poly (lactic acid)/hydroxyapatite biofilms for bone graft harvest site fixations. A. Prasad, R. Sankar, **V. Katiyar**

9:10 PMSE 24. Thin-film stable glasses of ultra monodisperse polystyrene. **A. Raegen**, J. Forrest



TECHNICAL PROGRAM

9:30 PMSE 25. Strain-promoted cycloadditions for the synthesis and functionalization of polymers and nanocomposites. **A. Adronov**, V. Kardelis, K. Li

9:50 Intermission.

10:10 PMSE 26. Interfacial viscoelasticity and electroconvective flow in liquid electrolytes above the diffusion limit. **A. Warren**, L.A. Archer

10:30 PMSE 27. Crystallinity and morphology studies in blends of biodegradable poly (lactic acid)/poly (butylene succinate) and effect of modified nanoamphiphilic chitosan as studied by DSC and synchrotron x-ray scattering. P. Boruah, S. Sakurai, R. Gupta, **V. Katiyar**

10:50 PMSE 28. Macroporous carbon based thermoset derived from industrial side stream humins. **A. Mija**, P. Tosi

Section E

Rosen Centre Hotel
Salon 8

Multicomponent Block Polymer Systems

K. Mineart, R. Riggleman, *Organizers, Presiding*

8:30 PMSE 29. Resolving the kinetic pathways for polyelectrolyte coacervates formation using time-resolved SAXS. M. Amann, J. Stensgaard Diget, **R. Lund**

8:50 PMSE 30. Characterization of single- vs. dual-dorona thermoresponsive polyelectrolyte complex micelles. **S. Shah**, A. Alli, L. Leon

9:10 PMSE 31. Competition of solvation and entropic effects in ion-containing block polymers. **J. Qin**

9:50 Intermission.

10:00 PMSE 32. Transport-morphology relationships in polymerized ionic liquid multiblock polymers. **Y.A. Elabd**

10:40 PMSE 33. Gyroids with an organosilicon block for membrane applications. **Q. Zhu**, P. Meyer, N.A. Lynd, C.G. Willson

11:00 PMSE 34. Synthesis of charged mosaics from self-assembled block polymers for dual metal patterning. **B.A. Fultz**, B. Dunoyer de Segonzac, J.G. Kennemur

Section F

Rosen Centre Hotel
Salon 14

Molecular Engineering of Interphases in Polymeric Materials: Advances in Experiments & Simulations



TECHNICAL PROGRAM

Surfaces & Interfaces

Financially supported by Carbon Nexus
L. C. Henderson, R. Jayan, *Organizers*
H. Heinz, D. Nepal, *Organizers, Presiding*

8:30 PMSE 35. Organized assembly of biopolymer components at interfaces. **V.V. Tsukruk**

9:10 PMSE 36. Polymer conformation and hydration at interfaces with solids. **E. Dormidontova**

9:30 PMSE 37. Smart polymers in miscible solvent mixtures in bulk and at interfaces. **K. Kremer**

10:10 Intermission.

10:30 PMSE 38. Rule-defying hedgehog particles. **N. Kotov**, D. Montjoy, J. Bang, H. Hou

11:10 PMSE 39. Smart windows with heat-shielding and self-cleaning: Near-infrared reflective photonic crystals via layer-by-layer self-assembly. **S. Shiratori**, C. Nakamura

11:30 PMSE 40. Modeling dynamics of shape changes and spreading of hydrogels in oil-water mixtures. **C. Choudhury**, O. Kuksenok

Section G

Rosen Centre Hotel
Salon 11

General Papers-New Concepts in Polymeric Materials

E. Harth, *Organizer*
B. Baldwin, A. Sathyan, *Presiding*

8:30 PMSE 41. Ring-opening polymerization of functional lactams. **A. Sathyan**, R.C. Hayward, T. Emrick

8:50 PMSE 42. Preparation and characterization of acid-base blend anion exchange membrane. **B. Motealleh**, T. Senathiraja, W. Khan, C.J. Cornelius

9:10 PMSE 43. Polymeric memristors from *n*-alkyl methacrylate to model neuromorphic dynamics. **B.T. Grant**, T. McFarlane, S.H. Foulger, I. Bandera

9:30 PMSE 44. Polymerization of new monomers in organocatalyzed atom transfer radical polymerization enabled by rational photocatalyst design. **B. Buss**, G. Miyake

9:50 Intermission.

10:10 PMSE 45. Incorporation of traditional and ionic liquid-based plasticizers into components produced by stereolithography. **B. Baldwin**, A.W. Etheredge, M.T. Harden, M.W. Reichert, **G.M. Poole**



TECHNICAL PROGRAM

10:30 PMSE 46. Nanoporous polymer microspheres with nitrile and amidoxime functionalities for gas capture and precious metal recovery from e-waste. **C.T. Yavuz**, N.A. Dogan, Y. Hong, E. Ozdemir

10:50 PMSE 47. Simulation of the degradation of cyclic ketene acetal and vinyl-based copolymers synthesized via a radical process. **C. Lefay**

Section H

Rosen Centre Hotel
Salon 13

General Papers-New Concepts in Polymeric Materials

E. Harth, *Organizer*
E. J. Price, C. Shen, *Presiding*

8:30 PMSE 48. Precise network polymerized ionic liquids for low-voltage, dopant-free soft actuators. **C. Shen**, C.M. Evans

8:50 PMSE 49. Tetracene-based conjugated polymers for amplified fluorescent detection of singlet oxygen. **C. Wang**, E.E. Nesterov

9:10 PMSE 50. Conjugated polymer hierarchical nano- and mesoscale assemblies prepared by externally initiated controlled chain-growth polymerization. **C. Kei**, J.C. Mai, E.E. Nesterov

9:30 PMSE 51. Tailoring the properties of Sylgard 184: Room-temperature curing time, adhesion energy, and water affinity. **E. Murphy**, J.H. Dumont

9:50 Intermission.

10:10 PMSE 52. Large particle electrospinning for increased functionality. **E. Ewaldz**, I. Campbell, J. Randrup, R. Patel, B. Brettmann

10:30 PMSE 53. Novel intumescent, epoxy-based flame retardant coatings based on partially neutralized poly(acrylic acid) blends. **E.J. Price**, J. Covello, A. Tuchler, G.E. Wnek

10:50 PMSE 54. Sustainable terpene-based polymeric materials. **E.E. Malmstrom**, L. Fogelstrom, A. Stamm, M. Tengdelius, A. Biundo, P. Syrén

11:10 PMSE 55. Zwitterionic patchy polymer microparticles for a controlled self-assembly. **F. Naderi Mehr**, D. Grigoriev, N. Pureskiy, A. Boker

Innovative Chemistry & Materials for Electrochemical Energy Storage

Li-Ion & Na-Ion

Sponsored by ENFL, Cosponsored by CATL, INOR and PMSE



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

Interdisciplinary Chemistry for New Frontiers in Biology and Medicine

NanoBio

Sponsored by ANYL, Cosponsored by BIOL, COLL‡, MPPG, PHYS‡ and PMSE‡

New Frontiers in Aerospace Polymers: Advances & Challenges in Experiments & Simulations

Advances in Thermoset Polymers & Composites

Sponsored by POLY, Cosponsored by PMSE

SUNDAY AFTERNOON

Section A

Rosen Centre Hotel
Salon 17

Antimicrobial & Cell-Penetrating Polymers

Cosponsored by POLY‡
Financially supported by Biomaterials Science (RSC journal); Polymer Chemistry (RSC journal); Polymers (MDPI journal); TOSOH Bioscience, LLC
A. Joy, *Organizer*
E. Palermo, *Organizer, Presiding*

1:55 Introductory Remarks.

2:00 **PMSE 56.** Designing simple polymers for membrane activity. **G.N. Tew**

2:20 **PMSE 57.** Polymer-based lipid nanodiscs. **T. Ravula**, N. Hardin, B. Sahoo, **A. Ramamoorthy**

2:40 **PMSE 58.** Mimicry of sequence-specific biopolymer functions with sequence-random polymers. **S.H. Gellman**

3:00 **PMSE 59.** Machine learning antimicrobial and cell penetrating peptides. **G. Wong**

3:20 Intermission.

3:50 **PMSE 60.** Sequence and dispersity as determinants of photodynamic antibacterial activity exerted by peptidomimetic oligo(thiophene)s. **E. Palermo**, Z. Zhou

4:10 **PMSE 61.** Broad-spectrum, biodegradable macromolecular antimicrobials with high selectivity. **J. Hedrick**, Y. Yang

4:30 **PMSE 62.** Use of polymers to repurpose drugs, synergize with antibiotics, and mitigate antibiotic resistance. **Y. Yang**



TECHNICAL PROGRAM

4:50 PMSE 63. Daylight-driven rechargeable antibacterial and antiviral nanofibrous membranes for bioprotective applications. **Y. Si**, G. Sun

5:10 PMSE 64. Constructing facial amphiphilic antimicrobials from multicyclic natural products. **C. Tang**

Section B

Rosen Centre Hotel
Salon 16

ACS Award for Team Innovation: Symposium in Honor of Vivek M. Prabhu, Christopher L. Soles, Eric K. Lin & Wen-Li Wu

C. R. Snyder, *Organizer*
Q. Lin, *Organizer, Presiding*

1:30 PMSE 65. New efforts in software, modeling, and machine-learning in the NIST *nSoft* Consortium. **T. Martin**, R.L. Jones

2:00 PMSE 66. Quantifying tie-molecules in semicrystalline polymers. **C.R. Snyder**

2:30 PMSE 67. Use of big instruments in industry/academia collaborations: The impact of neutrons techniques on applied problems. **D.D. Bendejacq**

3:00 Intermission.

3:15 PMSE 68. Understanding gelatin structures through technology collaborations. **E. Maziarz**, J. Bachert, B. Crawshaw, X.M. Liu

3:45 PMSE 69. Validation of a surfactant micelle rheology model using SANS and other analytical techniques. K. Vogtt, H. Jiang, G. Beaucage, W. Zou, G. Tan, R.G. Larson, G. Smith, T. Martin, R.L. Jones, P. Koenig, S. Sealschott, **M.R. Weaver**

4:15 PMSE 70. Award Address (ACS Award for Team Innovation sponsored by the ACS Corporation Associates). Characterization of photoresist fundamentals by scattering and spectroscopic methods. **V. Prabhu**

Section C

Rosen Centre Hotel
Salon 15

Hybrid Functional Materials from Controlled Assembly of Polymer & Inorganic Nanoparticles

Polymer-Nano Hybrids in Solid States

Financially supported by Huazhong University
J. He, Z. Nie, *Organizers*
Y. Lin, *Organizer, Presiding*



TECHNICAL PROGRAM

- 1:30 **PMSE 71.** Assembly of polymer-grafted gold nanoparticles into superlattice for memory devices. **J. Zhu**, K. Wang
- 2:00 **PMSE 72.** Topological engineering of giant molecules: Structures and functions. **S.Z. Cheng**
- 2:30 **PMSE 73.** Hybrid functional nanomaterials from controlled assembly of block copolymer and inorganic nanoparticles. **U.B. Wiesner**
- 3:00 Intermission.
- 3:15 **PMSE 74.** Large-area fabrication of functional hybrid materials for optical, electronic and energy applications using brush block copolymers as templates. **J.J. Watkins**
- 3:45 **PMSE 75.** Programming nanoparticle assembly via polymer crystallization. **C. Li**
- 4:15 **PMSE 76.** Toward designer nanocomposites. **T. Xu**
- 4:45 **PMSE 77.** Alignment of nanoplates in lamellar diblock copolymer domains and the effect of particle volume fraction on phase behavior. **R.J. Composto**, N.M. Krook, M. Marechal, P. Rannou, J.S. Meth, C.B. Murray

Section D

Rosen Centre Hotel
Salon 24

General Papers-New Concepts in Polymeric Materials

E. Harth, *Organizer*
G. Dianat, G. Narayanan, *Presiding*

- 1:30 **PMSE 78.** Effect of dispersion of graphene on thermal stability and dynamic mechanical properties of melt processed PLA. G. Chakraborty, G. Pugazhenthii, **V. Katiyar**
- 1:50 **PMSE 79.** Synthesis and characterization of Perfluorocyclohexenyl Aryl Ether (PFCH) polymers with divergent glass transition temperatures. **G. Narayanan**, B. Farajidizaji, K. Shelar, K. Mukeba, A. Sygula, C.U. Pittman, D.W. Smith
- 2:10 **PMSE 80.** 3D-printed, electrically-driven soft actuators based on hydrogel-elastomer hybrids. **G. Haghighashtiani**, E. Habtour, M.C. McAlpine
- 2:30 Intermission.
- 2:50 **PMSE 81.** Solventless fabrication of shaped asymmetric polymer membranes. **G. Dianat**, N. Movsesian, M. Gupta
- 3:10 **PMSE 82.** Triggered disassembly of cross-linked polyurethanes through cascading bond cleavage. **G.C. Daniels**, E. Camerino, J.H. Wynne, E.B. Iezzi
- 3:30 **PMSE 83.** Incorporation of phosphate-based flame retardants into components produced by stereolithography. A.W. Etheredge, A. Dada, **G.M. Poole**, M.W. Reichert



TECHNICAL PROGRAM

3:50 PMSE 84. Preliminary analysis of the influence of synthesis parameters and curing conditions in the fabrication of clay brick-based geopolymers. **G. Silva**, S. Kim, A. Castañeda, B. Bertolotti, J. Nakamatsu, R. Aguilar

Section E

Rosen Centre Hotel
Salon 8

Multicomponent Block Polymer Systems

K. Mineart, R. Riggleman, *Organizers, Presiding*

1:00 PMSE 85. Using theory and simulations to predict assembly in amphiphilic block polymer solutions for non-linear polymer architectures. **A. Jayaraman**

1:40 PMSE 86. Molecular modeling of shape transformations of polystyrene vesicles. **K. Chakraborty**, S. Loverde

2:00 PMSE 87. UV-light-induced reversible shape transformation of polymersomes. **Y.C. Simon**, T. Chidanguro, E. Ghimire

2:20 PMSE 88. Triphasic pentalock copolymers with a perfluoroalkyl middle block. **J. Kressler**, D. Heinz

2:40 Intermission.

2:50 PMSE 89. Co-assembly behavior of linear amphiphilic triblock copolymers in the fabrication of polymer vesicles. **E. Ghimire**, F. O'dowd, T. Chidanguro, Y.C. Simon

3:10 PMSE 90. Morphology transitions and mechanical response of multicomponent block copolymer systems. **K.R. Shull**, S. Chen

3:50 PMSE 91. Investigating the impacts of microdomain geometry on reverse micelle mobility within organogels. **W.W. Walker**, K. Mineart

4:10 PMSE 92. Rapid self-assembly in ternary “wet brush” block copolymer/homopolymer blend thin films. **G. Doerk**, R. Li, M. Fukuto, K. Toth, A. Rodriguez, C. Osuji, K. Yager

Section F

Rosen Centre Hotel
Salon 14

Molecular Engineering of Interphases in Polymeric Materials: Advances in Experiments & Simulations

Functional & Hairy Nanoparticles

Financially supported by Carbon Nexus
L. C. Henderson, R. Jayan, *Organizers*
H. Heinz, D. Nepal, *Organizers, Presiding*



TECHNICAL PROGRAM

1:30 PMSE 93. Covalent functionalization of redox-exfoliated layered transition metal dichalcogenides (group IV – VII). A. Jawaid, A. Ritter, **R.A. Vaia**

2:10 PMSE 94. Effect of size asymmetry on morphology and dynamics of ionomers. **B. Ma**, M. Olvera De La Cruz

2:30 PMSE 95. Applications of surface-initiated polymerization for tailoring particle surfaces and interactions and the design of functional materials. **M.R. Bockstaller**

3:10 Intermission.

3:30 PMSE 96. Unraveling the conformations of backbone and side-chains in bottlebrush polymers. K. Bejagam, S. Singh, **S.A. Deshmukh**

3:50 PMSE 97. Light-enabled reversible self-assembly and tunable optical properties of stable hairy nanoparticles. **Z. Lin**

4:30 PMSE 98. Surface chemistry and electronic properties of functionalized MXenes. **G.R. Neher**, J. Heckler, D.B. Lioi, F. Mehmood, A.R. Sharits, D. Nepal, R. Pachter, R.A. Vaia, W. Kennedy

Section G

Rosen Centre Hotel
Salon 11

Molecular Engineering of Peptide Assemblies

Assemblies & Coacervates

H. Acar, S. Lecommandoux, *Organizers*
H. Cui, M. V. Tirrell, *Organizers, Presiding*

1:15 Introductory Remarks.

1:20 PMSE 99. Controlled self-assembly of peptide nanotubes via sequence modification and kinetic control. **Y. Tian**, F. Polzer, H. Zhang, J.G. Saven, K.L. Kiick, D.J. Pochan

1:35 PMSE 100. Controlled fabrication of peptide-based nanosheets. **V.P. Conticello**

2:00 PMSE 101. Self-assembly of biomimetic surfactants and peptide amphiphiles in nonpolar solvents. **J.W. Schneider**

2:25 PMSE 102. Tubular assemblies of peptide-drug conjugates. **H. Cui**

2:50 PMSE 103. Transient programmable peptide self-assembly. **P. Thordarson**, J.P. Wojciechowski

3:05 Intermission.

3:25 PMSE 104. Aggregation and coacervation of the tau peptide. **J.E. Shea**



TECHNICAL PROGRAM

3:50 PMSE 105. Structure-property relationships of oligonucleotide polyelectrolyte complexes and complex micelles. **M.V. Tirrell**, J. Viereg, M.J. Lueckheide

4:15 PMSE 106. Biomolecules for non-biological things: Materials construction through computational peptide design and hierarchical solution assembly. **D.J. Pochan**

4:40 PMSE 107. Understanding charge-complementary peptide co-assembly using a computational-experimental framework. D.T. Seroski, K.M. Wong, Q. Shao, C.K. Hall, A. Paravastu, **G. Hudalla**

4:55 PMSE 108. Probing the role of hydrophobicity in complex coacervation. **S. Tabandeh**, R. Valmonte, L. Leon

Section H

Rosen Centre Hotel
Salon 13

Recent Trends in Polymer Photochemistry: From Molecular Design to Future Applications

Photo-Responsive Polymers

Financially supported by Polymer Competence Center Leoben
C. Bowman, T. Griesser, S. Marco, S. Schlögl, *Organizers*
A. Guymon, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 PMSE 109. Programming functionality in liquid crystalline polymer networks and elastomers. **T.J. White**

2:05 PMSE 110. Heavy lifting with soft materials: Layered liquid crystal elastomer actuators. **T. Guin**, T.J. White

2:25 PMSE 111. Photo-induced motion of water on tailored polymer surfaces. **E. Rossegger**, D. Hennen, T. Griesser, W. Kern, S. Schlögl

2:45 PMSE 112. Shape-responsive main chain liquid crystalline epoxy elastomers. **J.M. McCracken**, J.D. Berrigan, T.J. White

3:05 Intermission.

3:20 PMSE 113. Using light to actuate polymer sheets. **M.D. Dickey**, J. Genzer, A. Hubbard, R. Mailen, Y. Liu, M. Zikry, D. Davis

3:50 PMSE 114. Photo-switchable polymer networks. **S. Schlögl**

4:10 PMSE 115. Influence of photopolymerized polymer network development on the electro-optic responses of polymer stabilized cholesteric liquid crystals. **K. Lee**, V.P. Tondiglia, T.J. White, T.J. Bunning, M. McConney

4:30 PMSE 116. Photo-cleaving and photo-linking: Applications for networks and self-assemblies. C. Machado, S. Arencibia, **D.A. Savin**



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

Innovative Chemistry & Materials for Electrochemical Energy Storage

Li-Ion & Na-Ion

Sponsored by ENFL, Cosponsored by CATL, INOR and PMSE

Interdisciplinary Chemistry for New Frontiers in Biology and Medicine

Microbia

Sponsored by ANYL, Cosponsored by BIOL, COLL[‡], MPPG, PHYS[‡] and PMSE[‡]

New Frontiers in Aerospace Polymers: Advances & Challenges in Experiments & Simulations

Additive Manufacturing for Aerospace Application

Sponsored by POLY, Cosponsored by PMSE

MONDAY MORNING

Section A

Rosen Centre Hotel
Salon 17

Antimicrobial & Cell-Penetrating Polymers

Cosponsored by POLY[‡]

Financially supported by Biomaterials Science (RSC journal); Polymer Chemistry (RSC journal); Polymers (MDPI journal); TOSOH Bioscience, LLC

E. Palermo, *Organizer*

A. Joy, *Organizer, Presiding*

8:55 Introductory Remarks.

9:00 PMSE 117. Hydrogel effects rapid biofilm debridement with *ex-situ* contact-kill to eliminate multidrug resistant bacteria *in vivo*. **M. Chan Park**, C. Yeo

9:20 PMSE 118. Quantifying the electrostatics of polycation-lipid bilayer interactions. **F. Geiger**

9:40 PMSE 119. Fast acting antimicrobial polyionens: Activity-structure relationships, self-deactivation, and hydrogels. **J.C. Tiller**, A. Strassburg, C. Krumm



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

10:00 PMSE 120. Antifouling coating strategies for antimicrobial applications. **Z. Cao**

10:20 PMSE 121. Developing antibacterial polyurethanes and poly(ester urethane)s: A balancing act of bacterial toxicity and mammalian cell compatibility. C. Peng, S. Mankoci, A. Vishwakarma, C. Tantisuwanno, H.A. Barton, **A. Joy**

10:40 Intermission.

11:10 PMSE 122. Role of cationic groups in antimicrobial peptide activity: Toward switchable antimicrobials. **G.A. Caputo**

11:30 PMSE 123. Antimicrobial polymers containing thiazole groups. A. Muñoz-Bonilla, D. López, R. Cuervo-Rodríguez, **M. Fernández-García**

11:50 PMSE 124. Exploiting the redox chemistry of catechol for antipathogenic application. **B.P. Lee**

12:10 PMSE 125. Importance of sequence, degree of polymerization, and defects in antimicrobial polymers. **S. Barbon**, N.P. Truong, A. Anastasaki, M. Whittaker, C.J. Hawker

Section B

Rosen Centre Hotel
Salon 16

Biomimetic Materials

Financially supported by National Science Foundation Materials Research Science and Engineering Center (NSF MRSEC)

J. K. Montclare, R. S. Tu, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 PMSE 126. Protein-based biomaterial designs for tissue regeneration. **D.L. Kaplan**

8:45 PMSE 127. Processing effects on conformational transformation of *Nephila pilipes* spider silk fibroins. P. Ni, L. Chang, G. Wu, N. Teng, S. Hung, H. Wu, T. yang, **J. Yang**

9:10 PMSE 128. Adhesion control of human umbilical vein endothelial cells using clickable poly(2-oxazoline)-grafted biosynthesized extracellular matrix protein. **A. Takasu**

9:35 PMSE 129. Peptide-triggered growth factor gene transfer in bone repair. **M.O. Sullivan**

10:00 PMSE 130. Biomimetic tooth repair: Amelogenin-derived peptide enables *in vitro* remineralization of human enamel and dentin. **D.T. Yuceso**y, H. Fong, S. Dogan, M. Sarikaya

10:25 PMSE 131. Synthetic-recombinant hybrid presentation of adhesive domains to cells in 3D biomaterials. **J. Champion**

10:50 PMSE 132. Injectable supramolecular hydrogel formed from gelatin and cyclodextrin-grafted chitosan nanoparticles for pH-responsive drug release. **L. Xiao**, L. Huang, L. Liu, G. Yang



TECHNICAL PROGRAM

11:15 PMSE 133. Collagen-peptide conjugates for biomimetic delivery strategies. J. Qin, L. Dunshee, R. Thapa, M. Sullivan, **K.L. Kiick**

Section C

Rosen Centre Hotel
Salon 15

Hybrid Functional Materials from Controlled Assembly of Polymer & Inorganic Nanoparticles

Poly-Nano in Bio

Financially supported by Huazhong University

J. He, Y. Lin, *Organizers*

Z. Nie, *Organizer, Presiding*

8:30 PMSE 134. Programming nanoparticle structures. **O. Gang**

9:00 PMSE 135. Controlling filler organization with tailored interfaces and the impact on dielectric properties. **L. Schadler**, A. Prasad, X. Ning, J. Pribyl, S. Kumar, B.C. Benicewicz

9:30 PMSE 136. Engineering cross-linkable plasmonic vesicles for synergistic chemo-photothermal therapy using orthogonal light irradiation. K. Zhu, J. Hu, **S. Liu**

10:00 Intermission.

10:15 PMSE 137. Nanoparticle-mediated assembly of engineered proteins: New structures with unique cellular delivery capabilities. **V.M. Rotello**

10:45 PMSE 138. Localization of nanoparticles controlled by amphiphilic block copolymer. **R. Wang**

11:15 PMSE 139. Hybrid lipid-nanoparticle nanostructures: computer simulation insights. H. Sharma, **E. Dormidontova**

Section D

Rosen Centre Hotel
Salon 10

ACS Award in Applied Polymer Science: Symposium in Honor of Shanti Swarup

Financially supported by PPG Industries

D. C. Webster, *Organizer, Presiding*

8:30 Introductory Remarks.

8:40 PMSE 140. Super oxygen barrier for food packaging and flame retardancy for textiles from polyelectrolyte-based nanocoatings. **J.C. Grunlan**, R.J. Smith, M. Leistner



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

9:10 PMSE 141. Recent developments in cashew nut shell liquid technology. **A. Natesh, F. Tavares**

9:40 PMSE 142. Combinatorial and high-throughput methods to accelerate the development of coatings systems. **D.C. Webster**

10:10 Intermission.

10:40 PMSE 143. New cure chemistries for energy savings in industrial coatings. **C. Harris**

11:10 PMSE 144. Ionic materials: Applications and future prospects. **M.A. Hickner**

Section E

Rosen Centre Hotel
Salon 24

Multicomponent Block Polymer Systems

K. Mineart, R. Riggleman, *Organizers, Presiding*

8:30 PMSE 145. Block copolymer nanocomposites. **U.B. Wiesner**

9:10 PMSE 146. Micellar structure in the PMMA-b-PnBA-b-PMMA / polycarbosilane system and mechanical behavior of the corresponding block copolymer-templated ceramics. L. Rueschhoff, L. Baldwin, R. Wheeler, M.J. Dalton, H. Koerner, m. cinibulk, **M.B. Dickerson**

9:30 PMSE 147. 3D printing structural color with block copolymer based photonic crystals. **B. Boyle, G. Miyake**

9:50 PMSE 148. Segmented block copolymers made via cyclic carbonate aminolysis and thiol-norbornene and thiol-maleimide click reactions: Potential substitutes for thermoplastic polyurethane elastomers. E. Leitsch, G. Beniah, K. Jin, **J.M. Torkelson**

10:10 Intermission.

10:20 PMSE 149. Novel thermoplastic elastomers from renewable terpene (meth)acrylates. **R.L. Atkinson, O.R. Monaghan, S.M. Howdle**

10:40 PMSE 150. Synthesis, self-assembly, and characterization of multicomponent polyether-based materials. **N.A. Lynd**

11:00 PMSE 151. Combining synthesis with self-assembly in block copolymers. **M. Wang, Z. Qiang, S.A. Akolawala**

11:40 PMSE 152. Multicomponent block copolymers consisting of soft and hard segments: Effect of copolymer architecture on the thermal, mechanical, and crystallization properties. **N.M. Mulchandani, K. Masutani, S. Sakurai, Y. Kimura, V. Katiyar**

Section F



TECHNICAL PROGRAM

Rosen Centre Hotel
Salon 14

Molecular Engineering of Interphases in Polymeric Materials: Advances in Experiments & Simulations

Functional & Hairy Nanoparticles

Financially supported by Carbon Nexus
R. Jayan, D. Nepal, *Organizers*
H. Heinz, L. C. Henderson, *Organizers, Presiding*

8:30 PMSE 153. Mechanics of hairy nanoparticle assemblies and catch-bond inspired interfaces. **S. Keten**

9:10 PMSE 154. Decorating cellulose nanocrystals with carbon quantum dots for flexible chiral luminescent materials. **R. Xiong**, S. Yu, J. Zhou, M. Kreckler, L. Zhang, V.V. Tsukruk

9:30 PMSE 155. From quantum to continuum: Multi-scale modelling of nanocomposites. **P.V. Coveney**

10:10 Intermission.

10:30 PMSE 156. Optoelectronic properties versus bridge interfaces of a series DBpfA type block copolymers. **M. Hasib**, S.S. Sun

10:50 PMSE 157. Single chain nanoparticles and microcapsules formed by copolymers: Mechanistic insight and applications. **A. Ghobadi**, A. Bartolini, P. Tempesti, M. Mamsusa, D. Berti, J. Smets, Y. Aouad, P. Baglioni

11:30 PMSE 158. Interplay of nanointerface curvature and calcium binding in weak, polyelectrolyte-coated nanoparticles. **E. Gonzalez Solveyra**, R.J. Nap, I. Szleifer

Section G

Rosen Centre Hotel
Salon 11

Molecular Engineering of Peptide Assemblies

Minimalism in Peptide Assembly

H. Cui, M. V. Tirrell, *Organizers*
H. Acar, S. Lecommandoux, *Organizers, Presiding*

8:00 PMSE 159. Using cavitation rheology to understand dipeptide-based gels. **A. Fuentes**, **L. Thomson**, C. Chauveau, B. Dietrich, D.J. Adams

8:15 PMSE 160. Self-assembly of short peptides and peptide-aromatic conjugates. **M.J. Webber**

8:40 PMSE 161. Metabolite-responsive peptide nanostructures. **R. Ulijn**



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- 9:05 **PMSE 162.** β -sheet forming peptide hydrogels: from self-assembly to functional biomaterials. **A. Saiani**
- 9:30 **PMSE 163.** Peptide-based materials and applications in biomedical engineering. **H. Acar**
- 9:55 Intermission.
- 10:15 **PMSE 164.** Controlling the properties of dipeptide-based gels by chirality. K. McAuly, B. Dietrich, H. Su, H. Cui, S. Rogers, A. Seddon, E.R. Draper, **D.J. Adams**
- 10:40 **PMSE 165.** Molecular self-assembly of metabolites and peptides: Physiology, pathology, and nanotechnology. **E. Gazit**
- 11:05 **PMSE 166.** Instructed-assembly of isopeptides. H. He, D. Yang, **B. Xu**
- 11:30 **PMSE 167.** Localized peptide self-assembly on nanoparticles and surfaces. M.P. Conte, R. Ulijn, **K. Lau**
- 11:45 **PMSE 168.** Amino acid-encoded biocatalytic self-assembly enables the formation of transient functional nanostructures. **M. Kumar**

Section H

Rosen Centre Hotel
Salon 13

Recent Trends in Polymer Photochemistry: From Molecular Design to Future Applications

Photolithography & Functional Biomaterials

Financially supported by Polymer Competence Center Leoben
C. Bowman, T. Griesser, A. Guymon, S. Schlögl, *Organizers*
S. Marco, *Organizer, Presiding*

- 8:30 **PMSE 169.** Designing materials for high-resolution imaging applications. **C.G. Willson**
- 9:00 **PMSE 170.** Multiplexed polymer brush nanopatterning. **A.B. Braunschweig**, C. Carbonell, D. Valles, A. Wong
- 9:20 **PMSE 171.** Pitch-division photolithography at 365 nm. **P. Meyer**, J. Kim, N.A. Lynd, C.G. Willson
- 9:40 **PMSE 172.** Photopatterning conjugated polymers with cleavable solubilizing alkyl chains. **S.W. Thomas**
- 10:00 Intermission.
- 10:15 **PMSE 173.** Controlled and localized photopolymerization of molecularly imprinted polymer nanocomposites as synthetic antibodies for biomedicine. **K. Haupt**, C. Gonzato, B. Tse Sum Bui, E. Paruli III
- 10:45 **PMSE 174.** Using photochemistry to improve cochlear implant materials. **A. Guymon**, B. Leigh, M. Hansen



TECHNICAL PROGRAM

11:05 PMSE 175. Versatile thiol-based reactions for micrometer- and nanometer-scale photopatterning of polymers and biomolecules. **T. Griesser**, F. Mostegel, G.J. Leggett

11:25 PMSE 176. UV-cured acrylic hydrogels as delivery materials for photosensitizers for use in photodynamic therapy. S. Glass, T. Pelras, B. Trinklein, B. Abel, C. Elsner, A. Schulze, **T. Scherzer**

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Sponsored by PROF, Cosponsored by AGFD, ANYL, BIOL, BIOT, CARB, CELL, CHED, CMA, COLL, COMP, ENVR, GEOC, I&EC, MEDI, MPPG, NUCL, ORGN, PHYS, PMSE, POLY, PRES, WCC and YCC

Innovative Chemistry & Materials for Electrochemical Energy Storage

Solid & Polymer Electrolytes

Sponsored by ENFL, Cosponsored by CATL, INOR and PMSE

Interdisciplinary Chemistry for New Frontiers in Biology and Medicine

Biomarker Discovery

Sponsored by ANYL, Cosponsored by BIOL, COLL[‡], MPPG, PHYS[‡] and PMSE[‡]

Transport in Polymer Membranes

Morphology, Solid State & Physical Properties of Membranes

Sponsored by POLY, Cosponsored by PMSE[‡]

MONDAY AFTERNOON

Section A

Rosen Centre Hotel
Salon 17

Antimicrobial & Cell-Penetrating Polymers

Cosponsored by POLY[‡]
Financially supported by Biomaterials Science (RSC journal); Polymer Chemistry (RSC journal); Polymers (MDPI journal); TOSOH Bioscience, LLC



TECHNICAL PROGRAM

E. Palermo, *Organizer*
A. Joy, *Organizer, Presiding*

1:55 Introductory Remarks.

2:00 **PMSE 177.** Antimicrobial polymers: Key structural parameters in their performance. **L. Yang**

2:20 **PMSE 178.** Cationic calixarene derivative as a membrane-active antimicrobial agent. **K. Yasuhara**, T. Nakano, H. Kibata, J. Kikuchi

2:40 **PMSE 179.** Molecular engineering of antimicrobial polymers to target biofilms. **H. Takahashi**, K. Kuroda

3:00 **PMSE 180.** Biofilm busting RAFT antimicrobials: Maximizing therapeutic window through controlling length, polarity and sequence. **K. Locock**

3:20 **PMSE 181.** Solid antibacterial polymeric materials elaboration by dispersion of amphiphilic methacrylic SG1-based copolymers. **C. Lefay**

3:40 Intermission.

4:10 **PMSE 182.** Dextran-derived block copolymers as biofilm dispersing agents. **M. Chan Park**

4:30 **PMSE 183.** Nanothin silk-based antimicrobial coatings. **R.H. Zha**, P. Delparastan, T.D. Fink, T. Scheibel, P.B. Messersmith

4:50 **PMSE 184.** Engineering polymeric biomaterials in the era of antimicrobial resistance. **J. Haldar**

5:10 **PMSE 185.** Using aldehyde synergism to direct the design of degradable pro-antimicrobial polymer networks. D. Amato, D. Amato, Y. Adewunmi, O. Mavrodi, K. Parsons, S. Swilley, D. Braasch, D. Mavrodi, **D.L. Patton**

Section B

Rosen Centre Hotel
Salon 16

Biomimetic Materials

Financially supported by National Science Foundation Materials Research Science and Engineering Center (NSF MRSEC)

R. S. Tu, *Organizer*
J. K. Montclare, *Organizer, Presiding*
S. Khare, *Presiding*

1:00 Introductory Remarks.

1:05 **PMSE 186.** Epoxy resins from trehalose, cyclodextrin, and soybean oil yield tunable mechanical performance, cell adhesion, and degradation. **T.M. Reineke**



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

1:45 PMSE 187. Bio-inspired metal-coordination crosslinking: Easy access to broad dynamics when engineering polymer gel mechanics. **N. Holten-Andersen**

2:10 PMSE 188. Recapitulating tissue dynamics *in vitro* through bioorthogonal photochemistry. J.A. Shadish, L. Liu, **C.A. DeForest**

2:35 PMSE 189. Electrostatically driven bioinspired materials. **L. Leon Gibbons**

3:00 PMSE 190. Engineering intelligent protein biomaterials. **J.K. Montclare**

3:25 PMSE 191. Emergent behavior of multicompartments capsules activated by a thermal trigger. **S.R. Raghavan**, K.C. DeMella

3:50 PMSE 192. Protein hydrogels from marine invertebrates: A platform for tunable functionality. **M. Gupta**, P. Dennis, R.R. Naik

Section C

Rosen Centre Hotel
Salon 15

Hybrid Functional Materials from Controlled Assembly of Polymer & Inorganic Nanoparticles

New Synthesis in Poly-Nano

Financially supported by Huazhong University
Y. Lin, Z. Nie, *Organizers*
J. He, *Organizer, Presiding*

1:30 PMSE 193. Colloidal polymerization of dipolar heterostructured nanoparticles. **J. Pyun**

2:00 PMSE 194. New ligand designs for hybrid polymer-inorganic materials. M. Macleod, H. Nguyen, Y. Gu, J. Zhao, N. Oldenhuis, J. Wang, **J.A. Johnson**

2:30 PMSE 195. Fabricating precisely structured polymeric assemblies through structural preorganization and energy optimization. **D. Chen**

3:00 Intermission.

3:15 PMSE 196. Functional hybrid inorganic-organic nanomaterials (HIONs) designed for advanced applications and sustainability. **K.L. Wooley**

3:45 PMSE 197. Near-infrared light-responsive polymer nanovectors containing a single upconversion nanoparticle. J. Xiang, **Y. Zhao**

4:15 PMSE 198. Layered plasmonic nanocomposites. **A.R. Tao**

4:45 PMSE 199. External field-controlled self-assembly and disassembly of block copolymers and its application. **W. Jiang**, M. Wu



TECHNICAL PROGRAM

Section D

Rosen Centre Hotel
Salon 10

ACS Award in Applied Polymer Science: Symposium in Honor of Shanti Swarup

Financially supported by PPG Industries
D. C. Webster, *Organizer, Presiding*

1:30 PMSE 200. Photoactivation for polymerization, end-group functionalization, and bioconjugation. R.N. Carmean, M.B. Sims, C.A. Figg, G. Scheutz, T. Kubo, T. Becker, **B.S. Sumerlin**

2:00 PMSE 201. Fundamental understanding of low energy bake automotive coating technologies. **H. Ro**, E. Puodziukynaite, B. Okerberg, R. Rock, C.A. Wilson, P. Votrubařzal

2:30 PMSE 202. High-performance emulsion polymers and coatings by *in-situ* (one pot) post functionalization. **J. Klier**, J.D. Schiffman, M. Huang

3:00 Intermission.

3:30 PMSE 203. Smarter corrosion management solutions via self-healing coatings. **G.O. Wilson**

4:00 PMSE 204. Award Address (ACS Award in Applied Polymer Science sponsored by the Eastman Chemical Company). Polymers for automotive compact process painting. **S. Swarup**

Section E

Rosen Centre Hotel
Salon 24

Materials for High-Performance Impact Mitigation: Design, Synthesis, Characterization & Validation

Biomimetic Impact Materials & Ballistic Rate Impact Testing

E. Arruda, J. J. De Pablo, J. Lenhart, *Organizers*
C. L. Soles, *Organizer, Presiding*

1:00 PMSE 205. Biomimetic nanocomposites. **N. Kotov**

1:40 PMSE 206. Crystalline silk nanodisc-based polylactide bionanocomposite. R. Patwa, **V. Katiyar**

2:00 PMSE 207. Impact resistance of nanocellulose films with bioinspired Bouligand microstructures. **S. Keten**

2:40 Intermission.



TECHNICAL PROGRAM

3:00 PMSE 208. High-rate deformation behavior and extraordinary energy absorption of carbon nanotubes mats and thin glassy polymer films. **E.L. Thomas**, J. Hyon, O. Lawal, O. Fried, J. Streit, R.A. Vaia

3:40 PMSE 209. Impact energy delocalization properties of carbon-based nanomaterials and nanocomposites. **J. Lee**, W. Xie

4:20 PMSE 210. Response of cellular materials to impact: Characterization and visualization. **O. Petel**

Section F

Rosen Centre Hotel
Salon 14

Molecular Engineering of Interphases in Polymeric Materials: Advances in Experiments & Simulations

Nanocomposites & Nanomechanics

Financially supported by Carbon Nexus
H. Heinz, D. Nepal, *Organizers*
L. C. Henderson, R. Jayan, *Organizers, Presiding*

1:30 PMSE 211. Design of interfaces of polymer nanocomposites to advance thermomechanical performance via predictive modeling. **W. Xia**

1:50 PMSE 212. Switchable polymer properties: Computational modeling. **G.C. Schatz**

2:30 PMSE 213. Effect of surface treatment on viscoelastic behavior of epoxy nanocomposites. **S. Ahuja**

2:50 PMSE 214. Dynamic scanning indentation for polymer interphases: Unlocking nanoscale viscoelastic measurements across time and space. **C. Brinson**

3:30 Intermission.

3:50 PMSE 215. Ghost particles: Effect of constrained space on glassy polymer network formation and mechanics. **J. Winetrou**, T. Palmer, J.S. Wiggins

4:10 PMSE 216. Molecular design and engineering of hybrids at the extreme limits of molecular-scale confinement. **R. Dauskardt**

4:50 PMSE 217. Trap state distribution in polymer nanocomposite interphases from first principles. **A. Shandilya**, R. Sundararaman

Section G

Rosen Centre Hotel
Salon 11

Molecular Engineering of Peptide Assemblies



TECHNICAL PROGRAM

Peptides for Medicine

H. Cui, S. Lecommandoux, *Organizers*
H. Acar, M. V. Tirrell, *Organizers, Presiding*

1:15 PMSE 218. Intra-mitochondrial peptide assembly for new cancer therapy. **J. Ryu**

1:30 PMSE 219. Mitochondrial targeting of therapeutics. **S.O. Kelley**

1:55 PMSE 220. Multicompartment self-assembled gel that facilitates time-resolved delivery of combination therapy and synergized killing of cancer. **J.P. Schneider**

2:20 PMSE 221. Peptide hydrogels for sustained release of analgesics. **R. Hoogenboom**

2:45 PMSE 222. Anti-angiogenic self-assembled hydrogel for treatment of neovascular ocular diseases. **B. Sarkar, P. Nguyen, Z. Siddiqui, V. Kumar**

3:00 Intermission.

3:20 PMSE 223. Peptide-modulated self-assembly of photosensitive drugs for antitumor phototherapy. **X. Yan**

3:45 PMSE 224. New peptide based approaches for regenerative medicine. **M. Stevens**

4:10 PMSE 225. Targeting glioblastoma multiforme with ssDNA nanotubes *in vitro* and *in vivo*. **E. Kokkoli**

4:35 PMSE 226. Multicomponent supramolecular polymers as a platform for the design of glycopeptide antitumor vaccines. D. Strassburger, N. Stergiou, E. Schmitt, **P. Besenius**

5:00 PMSE 227. Peptide-polymer nanostructures and hydrogels to control cellular growth. **T. Weil**

Section H

Rosen Centre Hotel
Salon 13

Recent Trends in Polymer Photochemistry: From Molecular Design to Future Applications

Light-Based 3D Printing

Financially supported by Polymer Competence Center Leoben
C. Bowman, A. Guymon, S. Marco, S. Schlögl, *Organizers*
T. Griesser, *Organizer, Presiding*

1:30 PMSE 228. Dyes in DLP formulations: Beyond the precision. **A. Chiappone, I. Roppolo, F. Pirri**

2:00 PMSE 229. Toughening multi-material additive manufacturing through selective photochemistry. **N. Dolinski, E.B. Callaway, R.C. Chavez, Z.A. Page, F. Eisenreich, S. Hecht PhD, C.J. Hawker**



TECHNICAL PROGRAM

2:20 PMSE 230. 3D printing of multifunctional metal oxides via a novel photopolymer system. **D. Yee**, M.L. Lifson, J.R. Greer

2:40 PMSE 231. Low-cytotoxic thiol/yne formulations for the 3D printing of tailor made medical devices. **D. Hartmann**, A.B. Oesterreicher, T. Rockenbauer, M. Ast, T. Griesser

3:00 Intermission.

3:15 PMSE 232. UV-initiated reactive processing in extrusion-based 3D printing. **N. Levenhagen**, M.D. Dadmun

3:35 PMSE 233. 3D printing of highly stretchable, shape-memory and self-healing elastomer toward novel 4d printing. **X. Kuang**, H.J. Qi

3:55 PMSE 234. Constructing tough, stain-tolerant microlattices from one-pot, low-viscosity resins in aerobic conditions. **W. Voit**, B. Lund

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Sponsored by PROF, Cosponsored by AGFD, ANYL, BIOL, BIOT, CARB, CELL, CHED, CMA, COLL, COMP, ENVR, GEOC, I&EC, MEDI, MPPG, NUCL, ORGN, PHYS, PMSE, POLY, PRES, WCC and YCC

Innovative Chemistry & Materials for Electrochemical Energy Storage

Supercapacitors

Sponsored by ENFL, Cosponsored by CATL, INOR and PMSE

Interdisciplinary Chemistry for New Frontiers in Biology and Medicine

DNA/RNA & Disease Diagnosis

Sponsored by ANYL, Cosponsored by BIOL, COLL, PHYS and PMSE

Transport in Polymer Membranes

Block Copolymers, Morphology Control & Poly(ionic Liquids)

Sponsored by POLY, Cosponsored by PMSE‡



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

Undergraduate Research Posters

Polymer Chemistry

Sponsored by CHED, Cosponsored by PMSE, POLY and SOCED

MONDAY EVENING

Section A

Orange County Convention Center
West Hall C

Sci-Mix

E. Harth, *Organizer*

8:00 - 10:00

33, 49, 80, 158. See previous listings.

236, 268, 353, 356, 359-360, 362, 364, 366, 372-374, 380-387, 389-390, 394, 399-400, 402, 408, 411-412, 416-420, 422, 425, 432-433, 436, 438, 440, 443, 448-449, 451-452, 454-456, 458, 461, 468, 470, 475, 477-479, 515, 552, 583, 610, 642, 676. See subsequent listings.

Revamping Practical Chemistry Teaching for the New Frontier

Sponsored by CHED, Cosponsored by PMSE, POLY and RUBB

TUESDAY MORNING

Section A

Rosen Centre Hotel
Salon 9

Innovations in Polymer Crosslinking Technology

Bio-Based Networks

S. Swarup, *Organizer*
S. Caillol, D. C. Webster, *Organizers, Presiding*

8:20 Introductory Remarks.



TECHNICAL PROGRAM

8:30 PMSE 235. New vinyl ether monomers via lipase catalysis towards cationically crosslinkable thermosets. **M.K. Johansson**

9:00 PMSE 236. Plant oil-derived emulsion polymers with post-polymerization induced mechanical enhancement. **M. Lamm, P. Li, C. Tang**

9:20 PMSE 237. Biobased non isocyanate polyurethanes: Mechanistic investigation of reaction between dialdehydes and carbamates. A. Renner, **E.M. Serum**, D.C. Webster, **M.P. Sibi**

9:40 PMSE 238. Ambiently cured, bio-based, non-isocyanate polyurethane produced from polycarbamate-dialdehyde crosslinking. **S.D. Silbert**, E.M. Serum, M.P. Sibi, D.C. Webster

10:00 Intermission.

10:30 PMSE 239. Bio-based epoxy thermosets from fatty acid derivatives. **S. Nameer**, D. Larsen, M.K. Johansson

10:50 PMSE 240. Novel bio-based methacrylate resins based on flavones. **A. Clay**, J. Mitchell, J.F. Stanzione, J. La Scala

11:10 PMSE 241. Ionically cross-linked silk microfibers/alginate tough composite hydrogels with hierarchical structures. **L. Meng**, J. Yang

Section B

Rosen Centre Hotel
Salon 16

Biomimetic Materials

Financially supported by National Science Foundation Materials Research Science and Engineering Center (NSF MRSEC)

J. K. Montclare, R. S. Tu, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 PMSE 242. Utilization of the inherent stereochemical and functional diversities of peptide or carbohydrate natural products to produce unique biomimetic materials. **K.L. Wooley**

8:45 PMSE 243. Facile synthesis of sequence-defined glycomimetic polymers. **J. Niu**, C. Yang, J. Flynn

9:10 PMSE 244. Controlled synthesis of multiblock copolymers composed of sequential peptides and vinyl polymers for functional biomaterials. **T. Koga**, S. Nishimura, N. Higashi

9:35 PMSE 245. Model-driven molecular engineering of polypeptide-based complex macromolecules. **Y. Lin**

10:00 PMSE 246. Capturing protein activity in simple synthetic polymers. **G.N. Tew**

10:25 PMSE 247. Foldamer materials: Biomimetic assemblies encoded by sequence-specific peptoid oligomers. **K. Kirshenbaum**, R.N. Zuckermann, C. Dehigaspitiya, R. Quddus, D.M. Nalband



TECHNICAL PROGRAM

10:50 PMSE 248. Periodically sequenced polypeptides as biomimetic surface-active molecules at liquid-gas interfaces. **R.S. Tu**

11:15 PMSE 249. Computational design of stimulus-responsive protein-based mesoscale assemblies. **S. Khare**

Section C

Rosen Centre Hotel
Salon 15

Hybrid Functional Materials from Controlled Assembly of Polymer & Inorganic Nanoparticles

Self-Assembly & Application of Poly-Nano

Financially supported by Huazhong University
J. He, Y. Lin, Z. Nie, *Organizers*
J. Zhu, *Presiding*

8:00 PMSE 250. Programmable soft matter: From active membranes to self-replication. **A. Boker**

8:30 PMSE 251. Surface co-assemblies of polymer brushes. **H. Zhao**

9:00 PMSE 252. Bottom-up approaches for precisely nanostructuring hybrid organic/inorganic multi-component composites. **Y. Qin**

9:30 Intermission.

9:45 PMSE 253. Supramolecular recognition in dynamic and responsive polymeric hydrogels. **M.J. Webber**

10:15 PMSE 254. Colloidal particle arrays: Patterned lithographic and virus assemblies. **R.C. Advincula**

10:45 PMSE 255. DNA biotemplated 3-dimensional copper nanowire composite films. **F. Burpo**, S. Lowell, E.A. Nagelli, F. Zhang, E. Onuomadonkeng

11:15 PMSE 256. Tailor the architecture and composition of block copolymers for unconventional nanostructures. **W. Li**

Section D

Rosen Centre Hotel
Salon 10

Autonomous Processes, Chemomechanics & Active Matter Using Polymers & Soft Materials

Financially supported by PPG Industries
T. Emrick, *Organizer*
A. Balazs, *Organizer, Presiding*



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

8:30 PMSE 257. Folding and expanding bilayer and multilayered particles. **R.C. Advincula**

9:00 PMSE 258. Chemotactic droplet interactions. C. Meredith, P. Moerman, Y. Chiu, J. Groenewold, W. Kegel, A. van Blaaderen, **L.D. Zarzar**

9:30 PMSE 259. Driving reconfiguration, assembly, and motion of hydrogel sheets with light. **R.C. Hayward**

10:00 Intermission.

10:15 PMSE 260. Enzyme-powered protocells as dual-direction self-propulsive motors. **A. Sen**

10:45 PMSE 261. Capsules that exhibit spontaneous inflation, core ejection, and pulsed release of solute. **S.R. Raghavan**, K.C. DeMella

11:15 PMSE 262. Competition and cooperation among chemically active sheets and particles. A. Laskar, O.E. Shklyaev, **A. Balazs**

Section E

Rosen Centre Hotel
Salon 8

Materials for High-Performance Impact Mitigation: Design, Synthesis, Characterization & Validation

Impact in Novel Gels, Networks & Glasses

E. Arruda, J. Lenhart, C. L. Soles, *Organizers*
J. J. De Pablo, *Organizer, Presiding*

8:00 PMSE 263. Mitigating post-impact energy release from liquid fuels. **J.A. Kornfield**

8:40 PMSE 264. Design of two-dimensional polymers with high stiffness, strength and toughness from monolayer to bulk high-performance films. **E. Sandoz-Rosado**, J. Andzelm, E. Wetzel

9:20 PMSE 265. Materials mechanics for high-acceleration systems. **A. Crosby**

10:00 Intermission.

10:40 PMSE 266. Visualizing damage: Mechanoresponsive materials for quantifying force in glassy polymer networks. **C.S. Davis**, J. Woodcock, M. Wang, R. Beams, S. Stranick, A.M. Forster, J.W. Gilman

11:20 PMSE 267. Energy dissipation mechanisms in multiple network elastomers. **C. Creton**, Y. Chen, P. Millereau

Section F

Rosen Centre Hotel
Salon 14



TECHNICAL PROGRAM

Molecular Engineering of Interphases in Polymeric Materials: Advances in Experiments & Simulations

Nanocomposites & Nanomechanics

Financially supported by Carbon Nexus
H. Heinz, L. C. Henderson, *Organizers*
R. Jayan, D. Nepal, *Organizers, Presiding*

8:30 PMSE 268. Pre-cured epoxy amine microspheres with tailored reactivity for the study of glassy polymer network formation and mechanics. **T. Palmer**, J. Winetrou, J.S. Wiggins

8:50 PMSE 269. Reduced graphene oxide: Aramid nanofiber capacitors for structural energy and power. **J.L. Lutkenhaus**, M. Green, D. Lagoudas, J. Boyd, H. Ardebili

9:30 PMSE 270. Molecular-continuum model for elasticity of thermoplastic polyurethane nanocomposites at large deformations. **A. Sarvestani**, S. Hawkins, D. Nepal

9:50 PMSE 271. Fundamental insight into strain-induced crystallization of polyurethane and its composites *via in situ* AFM. **S. Hawkins**, E. Sullivan, A. Sarvestani, K. Dayal, H. Heinz, D. Nepal

10:10 Intermission.

10:30 PMSE 272. Hyper-strained PMMA crystals by fast quenching with entropy diluents. **Y. Kang**

11:10 PMSE 273. Hybrid ionogels by complexation of poly(ionic liquid)s with nanocellulose. **H. Lee**, A. Erwin, L. Pittner, V. Korolovych, O. Strytsky, V. Shevchenko, V.V. Tsukruk

11:30 PMSE 274. Rapid and highly efficient synthesis of a scalable two-dimensional covalent organic framework (COF) by photon-assisted imine condensation reaction on the water surface. **K. Soyoung**, H.C. Choi, L. Hyunseob, J. Lee

Section G

Rosen Centre Hotel
Salon 11

Molecular Engineering of Peptide Assemblies

Polypeptide-Based Assemblies

H. Acar, H. Cui, M. V. Tirrell, *Organizers*
S. Lecommandoux, *Organizer, Presiding*
T. J. Deming, *Presiding*

8:00 PMSE 275. Metal coordination: An efficient structuring switch for polypeptide polymers. **C. Bonduelle**, S. Lecommandoux

8:15 PMSE 276. Peptide and polypeptide hybrid nanomaterials. **N.R. Cameron**



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- 8:40 PMSE 277.** Backbone engineering of informational polypeptides. **S.H. Gellman**
- 9:05 PMSE 278.** New methods to introduce diverse functionality into synthetic polypeptides. **T.J. Deming**
- 9:30 PMSE 279.** Biomimetic membranes based on peptides and polymers. **W. Meier**, C. Palivan
- 9:55** Intermission.
- 10:05 PMSE 280.** Sequence-controlled polypeptides: Understanding biology via coacervation. **S.L. Perry**
- 10:30 PMSE 281.** Designer polypeptides for enhanced RNA and helper protein co-delivery. **P.T. Hammond**
- 10:55 PMSE 282.** Synthesis of brush polypeptides. **J. Cheng**
- 11:20 PMSE 283.** Peptide-mediated surface deposition of polymers and polymer nanoparticles. **H.A. Klok**
- 11:45 PMSE 284.** Chemoselective post-modifications of thermosensitive polypeptides towards bioactive self-assembled materials. **E.B. Garanger**, M. Rosselin, Y. Xiao, S. Lecommandoux

Section H

Rosen Centre Hotel
Salon 13

Recent Trends in Polymer Photochemistry: From Molecular Design to Future Applications

New Trends in Thiol-ene Chemistry & Photopolymerization

Financially supported by Polymer Competence Center Leoben
T. Griesser, A. Guymon, S. Marco, S. Schlögl, *Organizers*
C. Bowman, *Organizer, Presiding*

- 8:30 PMSE 285.** Photoinitiated heterogeneous radical-mediated thiol-ene polymerizations. **D.A. Shipp**
- 9:00 PMSE 286.** Degradable thiol-ene thermosets: Incorporating hydrolysable crosslinks to achieve tunable network dissolution in aqueous solutions at low pH. **B.M. Alameda**, C. Sarantes, N. Pierini, D.L. Patton
- 9:20 PMSE 287.** Phosphate-based crosslinked polymers from iodo-ene photopolymerization. **J. Sinha**, B.D. Fairbanks, M. Chen, H. Song, C. Bowman
- 9:40 PMSE 288.** Photocatalyzed thiol-alkyne chemistry: An efficient and oxygen accelerated coupling. **M. Allegranza**, A. Thompson, A. Kloster, D. Konkolewicz
- 10:00** Intermission.

10:15 PMSE 289. Exploiting step-growth thiol-ene photopolymerizations for design of degradable poly(thioether acetal) networks. **D.L. Patton**, B. Alameda, W. Walker, R. Sloan, M. Sandoz, S. Roland, C. Sarantes



TECHNICAL PROGRAM

10:45 PMSE 290. Photoredox copolymerization to synthesize gradient polyesters. **R. Tong**

11:05 PMSE 291. Photo-Induced phase separation in dimethacrylate/diepoxy systems using different reaction temperatures and curing methods. **E. Hasa, A. Guymon**

11:25 PMSE 292. Graphene-polymer nanocomposite mediated photopolymerizations. **R.C. Advincula**

11:45 PMSE 293. *In-situ* rheology of photopolymerizing ionic liquids. **R.D. Corder, J.E. Bara, S. Khan**

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TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

Transport in Polymer Membranes

Flow Batteries & Alkaline Fuel Cells

Sponsored by POLY, Cosponsored by PMSE[‡]

New Frontiers in Aerospace Polymers: Advances & Challenges in Experiments & Simulations

Bioinspired Materials for Aerospace Composite

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TUESDAY AFTERNOON

Section A

Rosen Centre Hotel
Salon 9

Innovations in Polymer Crosslinking Technology

Recyclable, Reversible & Dynamic Networks

D. C. Webster, *Organizer*
S. Caillol, S. Swarup, *Organizers, Presiding*

1:30 PMSE 294. Recyclable networks and network composites with dynamic cross-links for improved sustainability and high-value applications: Robust property recovery after reprocessing via alkoxyamine, hydroxyurethane, and thiourethane chemistries. L. Li, X. Chen, S. Hu, K. Jin, **J.M. Torkelson**

2:00 PMSE 295. Reprocessable polymer networks bearing hydroxyurethane dynamic linkages: Effect of backbone structure on reprocessability and network conformation. **X. Chen**, L. Li, T. Wei, J.M. Torkelson

2:20 PMSE 296. Reversible crosslinking of polydienes: A new approach toward recyclability of elastomers. P. Berto, S. Grelier, **F. Peruch**

2:40 PMSE 297. Versatile approach to polyester vitrimers. **J.L. Self**

3:00 Intermission.

3:30 PMSE 298. Recoverable intrinsic self-healable polymer elastomer. **P. Cao**, B. Li, K. Xing, A.P. Sokolov, T. Saito

3:50 PMSE 299. Mild thermally induce reversible exchange of anilinium salts for mechanically stable dynamic polymeric materials. **P. Chakma**, Z. Digby, D. Konkolewicz, M.P. Shulman, L. Kuhn, J. Sparks



TECHNICAL PROGRAM

4:10 PMSE 300. Foaming and crosslinking of polybutadiene with s-tetrazine. **D.A. Loy**, W. Sun, R. Bagge

4:30 PMSE 301. Acceleration of the thermal ring opening polymerization and crosslinking of benzoxazine monomers by telechelic polymers. A. Nadeem, S. Keefe, E.A. Brown, **D.A. Rider**

Section B

Rosen Centre Hotel
Salon 16

Biomimetic Materials

Financially supported by National Science Foundation Materials Research Science and Engineering Center (NSF MRSEC)

J. K. Montclare, *Organizer*

R. S. Tu, *Organizer, Presiding*

L. Leon, *Presiding*

1:00 Introductory Remarks.

1:05 PMSE 302. Biomimetic polymer models for natural and synthetic soft matter assemblies. **M.V. Tirrell**

1:45 PMSE 303. Finding secondary structure motifs among DNA aptamers selected via CompELS screening. **V.T. Milam**, R. Sullivan, M. Adams, R.R. Naik

2:10 PMSE 304. Solid–state biomimetic crystallization of biomembrane–like high–mobility organic semiconductors. **H. Chen**

2:35 PMSE 305. Molecular biomimetics: Genetically designed peptides for technology and medicine. **M. Sarikaya**

3:00 PMSE 306. Biomimetic polymers as custom bioinks for 3D printing. **S.C. Heilshorn**

3:25 PMSE 307. Rational design of helical nanotubes. **V.P. Conticello**

3:50 PMSE 308. Polymer-regulated growth of hybrid semiconductor nanostructures with applications as ‘electronic noses’. **R.C. Hayward**

4:15 PMSE 309. Multifunctional diblock copolypeptide hydrogels for biological studies. **T.J. Deming**

Section C

Rosen Centre Hotel
Salon 15

Hybrid Functional Materials from Controlled Assembly of Polymer & Inorganic Nanoparticles

Polymer & Energy Application



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

Financially supported by Huazhong University

J. He, Y. Lin, Z. Nie, *Organizers*

W. Li, *Presiding*

1:00 PMSE 310. Nanoengineering of complex polymeric nanoparticles towards diverse applications. I. Pijpers, J. Shao, A. Wauters, P. Welzen, T. de Martino, D. Williams, J. van Hest, **L. Abdelmohsen**

1:30 PMSE 311. Nanoparticle-modified microgels: Towards adaptive hybrid catalysts. **A. Pich**, D. Kleinschmidt

2:00 PMSE 312. Crystallization of poly(3-hexylthiophene) on graphitic surfaces with different curvatures. **L. Zhai**, C. Shen

2:30 PMSE 313. Silica-conjugated polymer hybrid fluorescent nanoparticles preparation by surface-initiated polymerization. S. Chatterjee, C. Wang, S. Youm, **E.E. Nesterov**

3:00 Intermission.

3:15 PMSE 314. Morphology control of thermoplastic polyurethane-olefin block copolymer-carbon black blends for enhanced piezoresistive sensing at both low and high strains. L. Duan, M. Spoerk, T. Wieme, P. Cornillie, H. Xia, J. Zhang, L. Cardon, **D.R. D'hooge**

3:45 PMSE 315. Sulfonated hybrid mesoporous silica-polymer particles as solid-acid catalysts for cellulose hydrolysis and as solid electrolytes for lithium ion batteries. Y. Yang, W. Nason, L. Smith, **S. Granados Focil**

4:15 PMSE 316. Thermally conductive graphene-based polymer nanocomposites: Nanoparticles quality and controlled assembly to enhance heat transfer efficiency. **A. Fina**, M. Bernal, s. colonna, G. Ferraro, M. Eleuteri, A. Di Piero, G. Saracco

4:45 PMSE 317. Nanostructured biodegradable multilayered films for cell isolation and recovery. **W. Li**

Section D

Rosen Centre Hotel

Salon 10

Autonomous Processes, Chemomechanics & Active Matter Using Polymers & Soft Materials

Financially supported by PPG Industries

A. Balazs, T. Emrick, *Organizers*

L. C. Bradley, *Presiding*

1:30 PMSE 318. How variations in minimally adhesive hydrogels and brushes impact near-surface swimming of motile bacteria. **M.M. Santore**, M. Shave

2:00 PMSE 319. Propulsion of colloids in chemically active systems. **B. Rallabandi**, **F. Yang**, H.A. Stone

2:30 PMSE 320. Modeling the Brownian hydrodynamics of intracellular motion. **R.N. Zia**

3:00 Intermission.



TECHNICAL PROGRAM

3:15 PMSE 321. Characterizing the dynamic pathways to self-assembly of DNA-coated colloids. **W.B. Rogers**, A. Hensley

3:45 PMSE 322. Topological defects in active nematics. **Z. Dogic**

4:15 PMSE 323. Responsive swelling of anisotropic colloids to control active motion. **L.C. Bradley**, H.S. Hamilton, R. Enright

Section E

Rosen Centre Hotel
Salon 8

Materials for High-Performance Impact Mitigation: Design, Synthesis, Characterization & Validation

Fundamentals of Impact in Cross-Linked Epoxy Networks

J. J. De Pablo, J. Lenhart, C. L. Soles, *Organizers*
E. Arruda, *Organizer, Presiding*

1:00 PMSE 324. Polymer networks for impact mitigation. **K. Masser**, J. Lenhart, E. Bain, D. Knorr, T. Long

1:40 PMSE 325. Role of fast polymer dynamics as quantified by inelastic neutron scattering on the mechanical toughness of polymeric materials. **C.L. Soles**, K. Ito, A. Burns, M. Tyagi, K. Masser, J. Lenhart, A.F. Yee

2:20 Intermission.

3:00 PMSE 326. Toughness, tack, and high-frequency viscoelastic properties of model epoxies. **K.R. Shull**, Q. Wang, M. Eaton

3:40 PMSE 327. Data-driven approach for high performance polymer nanocomposite characterization and design using NanoMine. **C. Brinson**, L. Schadler, W. Chen, A. Lin, B. Hu, Y. Wang

4:20 PMSE 328. Thermal response epoxy under high rate impact loading via incorporation of Diels-Alder substructures. **J. Gao**, G.R. Palmese

Section F

Rosen Centre Hotel
Salon 14

Molecular Engineering of Interphases in Polymeric Materials: Advances in Experiments & Simulations

Graphitic & Polymeric Interphases

Financially supported by Carbon Nexus
R. Jayan, D. Nepal, *Organizers*
H. Heinz, L. C. Henderson, *Organizers, Presiding*



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

1:30 PMSE 329. Structure and behavior of carbon interfaces from multiscale modeling. **B.I. Jakobson**

2:10 PMSE 330. Interphase study polymer-CNT system. M.H. Kirmani, P.J. Monje, P. Wang, A. Davijani, P. Gulgunje, **S. Kumar**

2:50 PMSE 331. Nanophase-separated polymers with extraordinarily broad interphase composition ranges: Gradient copolymer blends, block-gradient copolymers, and segmented multiblock polymers with interblock hydrogen bonding. L. Li, S. Marrou, L. Brunel, G. Beniah, E. Leitsch, **J.M. Torkelson**

3:10 Intermission.

3:30 PMSE 332. Interface zone and functionalization effect study of CNT/polymeric nanocomposites via Transmission Electron Microscopy (TEM) and Electron Energy Loss Spectroscopy (EELS). **R. Liang**, J. Park

4:10 PMSE 333. Using SuFEx chemistry to modify carbon fiber interfaces. **L.C. Henderson**, D.J. Eyckens, J.D. Randall

4:30 PMSE 334. Plasma-modified graphene for improved interfacial bonding of epoxy adhesives for the aerospace and automotive structures. **S. Rahatekar**, W. Li, H. Yazdani, K. Koziol

Section G

Rosen Centre Hotel
Salon 11

Molecular Engineering of Peptide Assemblies

Protein-Inspired Engineering

H. Acar, H. Cui, *Organizers*
S. Lecommandoux, M. V. Tirrell, *Organizers, Presiding*

1:15 PMSE 335. Design of peptide nanotubes from tandem repeat protein modules. **S.A. Hughes**, F. Wang, S. Wang, M. Kreutzberger, T. Osinski, A. Orlova, J. Wall, X. Zuo, E. Egelman, V.P. Conticello

1:30 PMSE 336. Unlocking the mysteries of amyloid diseases with macrocyclic β -sheet peptides. **J.S. Nowick**

1:55 PMSE 337. Guiding functionality through peptide engineered biomimetic interfaces. **C. Tamerler**

2:20 PMSE 338. Design of polypeptide-based bioconjugates and their self-assembly into functional biomaterials. **S. Lecommandoux**, E. garanger, C.V. Bonduelle

2:45 PMSE 339. Cellular expression of temperature-dependent ELP microdomains modulates clathrin, caveolin, flotillin, and dynamin-dependent endocytosis. **J.A. MacKay**, D. Tyrpak, A. Truong, H. Avila, Z. Li, Y. Wang, S. Hamm-Alvarez, C. Okamoto

3:10 Intermission.

3:20 PMSE 340. Templated silk fibril growth of artificial capsid polypeptides. L. Willems, M. Marchetti, W. Roos, P. van der Schoot, G. Wuite, **R. de Vries**



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- 3:45 PMSE 341.** Genetically encoded biomaterials that self-assemble across multiple length scales. **A. Chikoti**
- 4:10 PMSE 342.** Engineering physical and chemical properties of self-assembled globular protein vesicles. **J. Champion**
- 4:35 PMSE 343.** Pathway-dependent supramolecular assembly of engineered proteins and polypeptides. **J. Pille**, S. Timmermans, M. Abdelghani, D. Vervoort, C. Pretto, J. van Hest
- 5:00 PMSE 344.** Yolk-shell assembly formation based on polyion complex of proteins. **Y. Liu**, T. Mori, Y. Katayama, A. Kishimura

Section H

Rosen Centre Hotel
Salon 13

Recent Trends in Polymer Photochemistry: From Molecular Design to Future Applications

Photoinitiators, Photocatalysis & Emerging Applications

Financially supported by Polymer Competence Center Leoben
C. Bowman, T. Griesser, A. Guymon, S. Marco, *Organizers*
S. Schlögl, *Organizer, Presiding*

- 1:30 PMSE 345.** Photobase generators: Polyvalent tools for polymerization under irradiation. **C. Croutxe-Barghorn**, D. Perrot, A. Ibrahim, X. Allonas
- 2:00 PMSE 346.** $^1\text{O}_2$ Generation in supramolecular polymer hydrogel for asymmetric photocatalysis. **S. Biswas**, M. Kumar, A. Levine, R. Ulijn, A.B. Braunschweig
- 2:20 PMSE 347.** Singlet fission in combinatorial diketopyrrolopyrrole—rylene supramolecular films. **A. Levine**, C. Schierl, B. Basel, M. Ahmed, B. Camargo, D. Guldj, A.B. Braunschweig
- 2:40 PMSE 348.** UV-grafting and the impacts of monomer structure on ion-exchange membrane performance. **J.K. Rasmussen**, C.A. Bothof, S. Colak Atan, R.T. Fitzsimons, G.W. Griesgraber, A. Vail, E.P. Narveson
- 3:00** Intermission.
- 3:15 PMSE 349.** Photoinitiators: Reactivity, efficiency, and wavelength dependence. **G. Gescheidt**
- 3:45 PMSE 350.** Dynamic PEG–peptide hydrogels via visible light and FMN-induced tyrosine dimerization. **H. Liu**, H. Nguyen, C. Lin
- 4:05 PMSE 351.** Initiation of radical photopolymerization with photoactive silica particles. **K. Krawczyk**, P. Roszkowski, **W. Kern**, M. Sahin, S. Schlögl, S. Kaiser, J. Wang, H. Grützmaier
- 4:25 PMSE 352.** Janus heterogeneity at the surface of nanoparticles by light irradiation. **S. Marco**, N. Razza, G. Rizza



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

Applied Materials for New Frontiers: Ten Years of ACS Applied Materials & Interfaces

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Carl S. Marvel Award for Creative Polymer Chemistry Award in Honor of Matt Becker

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LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

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Innovative Chemistry & Materials for Electrochemical Energy Storage

Beyond Li-Ion

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Transport in Polymer Membranes

Gas Separation

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New Frontiers in Aerospace Polymers: Advances & Challenges in Experiments & Simulations



TECHNICAL PROGRAM

Multifunctional Composite for Aerospace

Sponsored by POLY, Cosponsored by PMSE

Undergraduate Research in Polymer Science

Sponsored by POLY, Cosponsored by PMSE

TUESDAY EVENING

Section A

Orange County Convention Center
West Hall C

PMSE-POLY Poster Session

Antimicrobial & Cell-Penetrating Polymers

E. Harth, *Organizer*

5:00 - 7:00

PMSE 353. Controlled antibiotic-loaded, drug-eluting implants for osteomyelitis. **D. Li**, Y. Huang, H. Shen, Y. Ma

PMSE 354. Antimicrobial peptide mimetic functional polyethers. **M. Kim**, W. Mun, G. Cho, J. Kwon, R.J. Mitchell, B. Kim

PMSE 355. *In vivo* anti-biofilm and anti-bacterial non-leachable coating thermally polymerized on the cylindrical catheter. M. Chan Park, **Y. Wu**

PMSE 356. Rechargeable antibacterial N-halamine films with antifouling function for food packaging applications. **Y. Ma**, J. Li, K. Huang, N. Nitin, Y. Si, G. Sun

PMSE 357. Nanoparticles of short cationic peptidopolysaccharide self-assembled by hydrogen bonding with antibacterial effect against multi-drug resistant bacteria. M. Chan Park, **Z. Hou**

Section A

Orange County Convention Center
West Hall C

PMSE-POLY Poster Session

General Posters/New Concepts in Polymeric Materials



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

E. Harth, *Organizer*

5:00 - 7:00

PMSE 358. Continuous detoxification of CWAs by MOF and polymer composite with electrospinning and electrospray. **J. Seo**, K. Cho, M. Lee, K. Baek

PMSE 359. Engineered polymer nanoparticles with unprecedented antimicrobial efficacy and therapeutic indices against multidrug-resistant bacteria and biofilms. **A. Gupta**, R.F. Landis, V.M. Rotello

PMSE 360. Direct mechanochemical synthesis of the piezoelectric phase of PVDF. **A. Joaquim**, O. Paul, A. Thai, A. Ueda, A. Zavalin, L. Ouyang, Y. Barnakov, F. Williams

PMSE 361. Exploring polypeptide secondary structure and local interactions with magnetic resonance. **A.H. Charlier**, I.R. Smith, G.F. Fanucci, D.A. Savin

PMSE 362. Polymer chain interaction to improve the properties of flexible polyimides. **A. Rivera Nicholls**, M. Pellissier, Y. Perez, J. Allan Stock, J. Harmon

PMSE 363. Enlarging a synthetic route to furan-maleimide based thermally remendable materials. **A.V. Polezhaev**, V. Kabantseva, N. Karelina, A. Kireynov, T. Petrova, E. Platonova, V. Solodilov, E. Vlasov, D. Zakharova

PMSE 364. Modifying dextran with stable boronic ester groups to produce an oxidation-sensitive, biocompatible polymer. **A. Manaster**, C. Batty, P. Tiet, E.M. Bachelder, K. Ainslie, K.E. Broaders

PMSE 365. Self-healing of chloroprene rubber based on ionic interaction and hydrogen bonding. **A. Cheng**, S. Lai

PMSE 366. Reactive layer functionalization of UV curable coatings. S. Neuhaus, M. Wink, V. Petry, C. Peter, **A. Moeck**

PMSE 367. Coarse-grained molecular dynamics simulation of supramolecular anticancer nanotubes. **A. Manandhar**, M. Kang, S. Loverde

PMSE 368. Exploring the potential use of zinc oxide surface as seed layer to grow orientated piezoelectric polyvinylidene fluoride layers. **A. Thai**, O. Paul, A. Joaquim, M. Ridley, S.A. Jones, A. Falconer, A. Smith, A. Ueda, R.R. Mu, F. Williams

PMSE 369. Increased thermal properties of benzoxazine polymers cured with end-group tosylated polymers. **A. Nadeem**, E.A. Brown, D.A. Rider

PMSE 370. Wetting and transport on swellable, surface-immobilized polymer brush-network systems. **B.A. Fickel**, M.A. Biesalski

PMSE 371. Enhancement of quaternary ammonium poly(arylene ether sulfone) anion exchange membrane properties by blending with sulfonated comb-shaped poly(phenyl sulfone)-base polymer. **B. Motealleh**, T. Senathiraja, W. Khan, C.J. Cornelius

PMSE 372. Novel composite polymer electrolytes with superior ionic conductivity with nanodomain of ILs in polymer matrix for highly reversible solid-state Lithium Metal Batteries (LMBs). **B. Prasad Thapaliya**, C. Do-Thanh, C.J. Jafta, R. Tao, X. Sun, S. Dai



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- PMSE 373.** Self-immolative polymers with potent and selective antibacterial activity by hydrophilic side chain grafting. **C. Ergene**, E. Palermo
- PMSE 374.** Synthesis of thiolactone polymer brushes: Sequential and one-pot reactions to design multifunctional and patterned brush surfaces. **C. Reese**, B.J. Thompson, C.M. Stafford, D.L. Patton
- PMSE 375.** Freshness indicator for monitoring changes in quality of packaged food products during storage. S. Baek, S. Thanakkasaranee, **C. Huh**, M. Kwon, D. Min, J. Seo
- PMSE 376.** Designing nanoporous carbon microstructure for electrode materials in supercapacitors. **C. Yoksiri**, S. Wongkasemjit, T. Chaisuwan
- PMSE 377.** Synthesis of organotin polyesters from camphoric acid and their ability to inhibit the Zika virus. **C.E. Carraher**, F. Mosca, P. Slawek, M. Roner, L. Miller, J. Haky, A. Campbell
- PMSE 378.** Synthesis and characterization of metal-containing polymers: Polymers from chloramphenicol. **C.E. Carraher**, Z.M. Rabinowitz, M. Roner, J. Frank, S. Jafri, A.H. Patel, F. Mosca, P. Slawek, P. Thaker, A. Zamora, F. Fox IV, F. Russell
- PMSE 379.** Delivery of antimicrobial polymers through coacervation to mitigate toxicity. Z. Voo, **C. Alexander**, J. Hedrick, Y. Yang
- PMSE 380.** Self-assembly and characterization of a novel conjugated polyelectrolyte multilayer film. **C.L. Rooney**, **D.B. Berkinsky**, M.S. Johal, J. Beardslee
- PMSE 381.** Synthesis and characterization of PA-6 films containing reinforcing nanocarbon materials. **D.N. Wedgeworth**, J.W. Rawlins, T.S. Rushing, J. Jefcoat, M.K. Shukla
- PMSE 382.** Application of plasticized PEMA/PMMA sensing film for sorption of BTEX compounds in vapor phase using a Quartz Crystal Microbalance (QCM) at 298.15 K. **D. Adapa**, V. Bhethanabotla, S. Campbell, A. Iyer
- PMSE 383.** NOESY and COSY ¹H NMR spectroscopy of self-healing acrylic copolymers. **D. Davydovich**, M.W. Urban
- PMSE 384.** Poly(ethylene glycol)-peptide based ideal hydrogels: An atomistic molecular dynamics study. **D. Anstine**, S. Jayaraman Rukmani, A. Munasinghe, P. Lin, C.M. Colina
- PMSE 385.** Silica polypeptide composite Janus particles. **E. Samantaray**, A.M. Blake, J.P. Wooding, M. Losego, **P.S. Russo**
- PMSE 386.** Using multiwall carbon nanotubes to reinforce dynamically crosslinked polymers. **E. Stopler**, K. Weaver, P. Chakma, D. Konkolewicz
- PMSE 387.** Strategies towards controlled surface decoration of Au-NRs. **E. Gonzalez Solveyra**, I. Szleifer
- PMSE 388.** Cross-linked networks that disassemble in fluoride salt solutions. **E. Camerino**, G.C. Daniels, J.H. Wynne, E.B. Iezzi
- PMSE 389.** Gelatin-cellulose nanofiber biotemplated platinum nanowire porous fibers. **F. Burpo**, M.Y. Ryu, E.A. Nagelli, F. Zhang, E. Onuomadonkeng



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- PMSE 390.** Rational design and assembly of macroporous nanotubes derived from collagen-mimetic peptides. **G. Touponse**, A. Merg, V. Conticello
- PMSE 391.** Reactive amphiphilic conjugated polymers for inhibiting amyloid β assembly. **H. Sun**, S. Wang
- PMSE 392.** Rheology and characterization of high-solids slurries for direct ink writing. **H.K. Woods**, Z. Adams, E. Sinner, B. Brettmann
- PMSE 393.** Estimation of chemical changes of actual XLPE cable insulator thermally aged by conductor current. **H. Misaka**, T. Takahashi
- PMSE 394.** Molecular mobility and charge transport in Polymers of Intrinsic Microporosity (PIMs) as revealed by dielectric spectroscopy. **H. Yin**, A. Schönhals, M. Boehning
- PMSE 395.** Development of highly conductive silk fibroin electrochromic nanofibers. **H. Wan**, C. Chen, T. Yang
- PMSE 396.** Environmentally friendly preparation of size-controlled poly(vinylidene fluoride) nanoparticle dispersion. **H. Heo**, D. Han, I. Park, J. Ha, H. Kang, S. Lee, S. Lee, E. Sohn
- PMSE 397.** Effect of molecular weight on the structure and properties of silk sericins. **I. Um**, C. Park
- PMSE 398.** Simple synthesis of multifunctional polymer dots through the irradiation of accelerated electron beams on polysaccharides. **I. In**, J. Ryu, S. Park
- PMSE 399.** Effects of polymer conjugation site on the functionality of an antimicrobial protein-polymer hybrid. **J. Farmakes**, S. Neupane, H. Li, Y. Pan, Z. Yang
- PMSE 400.** Porous electrospun polymer/titanium oxide nanofibers hybrid composites for antibacterial photocatalytic activity. **J. Orlando**, x. dong, T. Limbu, L. Yang, F. Yan
- PMSE 401.** Upcycling PET refuse to advanced therapeutics for the treatment of nosocomial and mycobacterial infections. J.P. Tan, **J. Tse How Jason**, N. Park, V.A. Piunova, Y. Yang, J. Hedrick
- PMSE 402.** Development of conductive and fire-retardant polymer-derived ceramics (PDCs) composite nanofibers. **J.E. Calderon-Flores**, L. Zhai
- PMSE 403.** Confinement of lyotropic liquid crystals in polymer fibers via coaxial electrospinning. M.J. Bertocchi, D.C. Ratchford, R. Casalini, J.H. Wynne, **J. Lundin**
- PMSE 404.** Mechanistic insights into self-decontaminating polyHIPE foams for force protection applications using *in-situ* DRIFTS. R.B. Balow, C.L. McGann, G.C. Daniels, S.L. Giles, **J. Lundin**, P.E. Pehrsson, **J.H. Wynne**
- PMSE 405.** Resorcinarene-based hierarchically porous polymer networks utilized for water purification. **J. Willman**, D. Bozdog, H. Zhou
- PMSE 406.** Light-responsive helical foldamer. **J.L. Bocanegra**
- PMSE 407.** Designing polymeric biomaterials for medical adhesives and sealants. **J. Ryu**, I. In, S. Park



TECHNICAL PROGRAM

- PMSE 408.** Controlled topology toughening epoxy via incorporation of partially reacted substructures. **J. Gao**, G.R. Palmese
- PMSE 409.** Plasma-assisted mechanochemistry to form covalent bonds between polymers and fillers in polymer composites. **J. Park**
- PMSE 410.** Sensing chemical warfare agent simulants via natural and synthetic photonic crystals. B.P. Fisher, A.N. Abel, B.D. Evans, J.S. Gofus, **J. Kittle**
- PMSE 411.** Photocurable resins for additive manufacturing. **J. Mitchell**, A. Clay, D. Lastovickova, D. VanOosten, F. Toulan, E.J. Robinette, J.F. Stanzione, G.R. Palmese, J. La Scala
- PMSE 412.** Biochromatic sensors for food safety. **J.B. Parker**, W.T. Pennington, T.W. Hanks
- PMSE 413.** Conjugated oligomer/polymer nanowires assembled via both halogen and chalcogen bondings. D. Koo, **J. Park**
- PMSE 414.** Chiroptical heterojunction thin-films prepared by controlled self-organization of conjugated polymer/enantiomer small molecule blends. **J. Lim**, N. Kim, J. Kim, H. Han, H. Lim
- PMSE 415.** Pore-engineered silica nanoreactors for chemical interaction-guided confined synthesis of porous platinum-nanodendrites. **J. Koo**, A. Kumar, I. Lee
- PMSE 416.** Surface enhancement of luminescent solar concentrator. **J. Wang**
- PMSE 417.** Rubber-to-liquid transition in iron(II) tris(2,2'-bipyridine) crosslinked poly(dimethylsiloxane) networks. **K.N. Fink**, D.R. Eason, Z.H. Williams, M.S. Hamburger, A.D. Schwab
- PMSE 418.** Cellulose nanocrystals combined with natural polymers for controllable iridescence and improved mechanical properties. **K.M. Adstedt**, R. Xiong, E. Popenov, V. Cherpak, R. Geryak, V.V. Tsukruk
- PMSE 419.** Benzoquinone-derived porous hydrophenazine framework for efficient and reversible iodine capture. **K. Jie**, S. Dai
- PMSE 420.** Optimization of the mechanical and physical properties of a polymer fuel cell membrane. **K.Y. Wanzi**
- PMSE 421.** Bio-inspired anisotropically wetting hydrophobic surface from snake ventral skin. **K. Kawamura**, M. Tenjimbayashi, D. Watanabe, D. Citterio, S. Shiratori
- PMSE 422.** Synthesis and evaluation of jet-printable polymer-coated carbon nanotube inks as calcium ion sensitive electrodes. A. Osumah, G.E. Larson, H.M. Kabir, **K.V. Waynant**
- PMSE 423.** Interplay of structure, dynamics and viscoelastic properties in supramolecular networks of telechelic polymers. **K. Xing**, M. Tress, A. Genix, P. Cao, H.J. Martin, B. Li, S. Cheng, M.D. Dadmun, T. Saito, A.P. Sokolov
- PMSE 424.** Hierarchical open porous black PDMS membrane toward efficient solar to steam generation. **K. Go**, M. Gil, S. Moon, K. Lee
- PMSE 425.** Synthesis of dendronized gold nanoparticles with acid-labile bonds for controlled delivery of cancer therapeutics. **L. Dockery**, M. Daniel



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- PMSE 426.** Self-assembly behavior of drugs and proteins based on amphiphilic block copolymers. **L. Jia**, R. Wang
- PMSE 427.** Glycosaminoglycans-mimicking polymers conjugated gold nanoparticles for promoting neural differentiation of embryonic stem cells. S. Zhang, **L. Wang**, H. Chen
- PMSE 428.** Design of temperature-responsive hydrogels used for vaccine storage and transportation. **L. Tang, L. Gong, G. Zhou, J. Tang, J. Zheng**
- PMSE 429.** Crystal structures of triphenylamine-based donor acceptor molecules for solar cell applications. P.T. Pham, W.W. Dahhan, **M. Bader**
- PMSE 430.** Assessing and improving machine learning model predictions of polymer glass transition temperatures. **M. Ramprasad**, C. Kim, A. Jha
- PMSE 431.** Preparation of anisotropically compartmentalized Janus particle with electrohydrodynamic jetting. **M. Gil**, K. Go, S. Moon, K. Lee
- PMSE 432.** Integration of antifouling and nitric oxide-releasing polymer for enhanced biocompatibility of insulin cannula. **M. Chug**, S. Hopkins, J. Pant, M. Douglass, C. Feit, H. Handa, E.J. Brisbois
- PMSE 433.** Enhanced electrical conductivity of immiscible blends filled with nickel particles. **M. Jurca**, M. Goralik, J. Vilcakova, K. Natalia, M. Masar, S.H. Foulger
- PMSE 434.** Tailoring poly(styrene-b-ethylene-co-butylene-b-styrene) (SEBS) for high-fidelity nanoimprint lithography molds. **M. Griep**, R. Mrozek
- PMSE 435.** Inverse liquid-solid chromatography to characterize adsorption isotherms of drugs to polymeric materials used in human-on-a-chip systems for drug discovery. **M. Schnepfer**, J. Roles, J.J. Hickman
- PMSE 436.** Ultrastiff and tough organic/inorganic double network hydrogels. **M. Milovanovic**, N. Rauner, M. Meuris, J.C. Tiller
- PMSE 437.** Preparation and characterization of starch-brea gum films. **M.A. Masuelli**
- PMSE 438.** Synthesis and aqueous self-assembly of amphiphilic gradient bottlebrush copolymers. **M. Mazloumi**, J. Rzayev
- PMSE 439.** Structure-property relationships for new brush polymers. **M.D. Ryan**, G. Miyake
- PMSE 440.** Reaction and reactor conditions: How vessel geometry and light source intensity affect photoinduced electron/energy transfer reversible addition-fragmentation transfer polymerization. **M. Allegranza**, P. Kurek, A. Kloster, K. Weaver, R. Manahan, W.T. De Alwis, J.A. Reeves, C. Boyer, D. Konkolewicz
- PMSE 441.** Dual-responsive polydimethylsiloxane networks. **M. Giebler**, S.V. Radl, M. Ast, S. Kaiser, S. Schlögl, T. Griesser, W. Kern
- PMSE 442.** Towards precise molecular shape control. **M. Sharafi**, S.T. Schneebeli
- PMSE 443.** Low crystallite phase ordering in semi-crystalline polymer filaments: A low-cost, translational route to reduce warp in fused deposition modeling 3D printing applications. **N. Aboutalebi Anaraki**, K. Crawford



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

- PMSE 444.** Association of nano-cellulosic materials with polyelectrolyte complex coacervates. **N. Khan**, C. Travis, N. Zaragoza, B. Brettmann
- PMSE 445.** Porous, graphene-based 3-D aerogel for attenuation & absorption of EM waves. **N. Chadha**
- PMSE 446.** Biodegradable triblock copolymers: Tailoring the block length to control the physical properties. **N.M. Mulchandani**, K. Masutani, S. Sakurai, Y. Kimura, V. Katiyar
- PMSE 447.** Evaluation of fluoroethylene vinyl ether polyurethane films for improved durability to weathering. **N. Weise**, I. Long, A.E. Mera, J.H. Wynne
- PMSE 448.** Developing adhesives from elemental sulfur, garlic extracts, and divinylbenzene through inverse vulcanization. **N. Anderson**, C. Jenkins
- PMSE 449.** Water-resistant gas sensor fabrication by integration of superhydrophobic nanofibers with Ag-NP functionalized P3HT-CNT electrodes. **N. Azim**, Y. Li Sip, L. Zhai
- PMSE 450.** Fabrication, optimization, and analysis of graphene oxides doped polyvinylidene fluoride nanocomposite for surface acoustic wave sensor application. **O. Paul**, A. Thai, A. Joaquim, M. Ridley, S.A. Jones, A. Falconer, A. Smith, A. Ueda, R.R. Mu, F. Williams
- PMSE 451.** Hydrogen peroxide-triggered payload release from polycaprolactone-based nanoparticles. **P. Hsu**, C. Arboleda, J. Olejniczak, A. Almutairi
- PMSE 452.** Stimuli-responsive foams for the energy efficient building enclosure systems. **P. Mishra**, M. Tao, S.V. Dessel, S. Granados Focil
- PMSE 453.** Utilizing RAFT polymerization and dynamic thiol-Michael chemistry for tunable thermoresponsive dynamic polymer networks. **P. Chakma**, Z. Digby, J. Via, M.P. Shulman, J. Sparks, D. Konkolewicz
- PMSE 454.** Photosensitizing antimicrobial polymer solid-state composites for water treatment. **R. Wodzinski**, J.D. Mizvesky, M.R. Elshaer
- PMSE 455.** Design of degradable thermoplastic poly(thioether acetals) via thiol-Michael polyaddition. **R.K. Sloan**, D.L. Patton
- PMSE 456.** Harnessing properties of thermotropic and lyotropic liquid crystalline polymers and molecules soluble in both aqueous and organic solvents. **R. Bosire**, D. Ndaya, R. Kasi
- PMSE 457.** Exploring photo-curable thiol-yne resins for the 3D printing of orthodontic clear aligners. **R. Schwarz**, H. Griesser, D. Hartmann, A.B. Oesterreicher, M. Pichelmayer, T. Griesser
- PMSE 458.** Hydrophobic driven self-assembling polyacrylic acid-gemcitabine nanoparticles for targeted therapy of pancreatic cancer. **R. Catarata**, N. Azim, E. Oriol, L. Zhai
- PMSE 459.** $\text{LiCo}_{0.8}\text{Fe}_{0.2}\text{PO}_4$ /carbon nanofiber self-standing cathodes for 5 V-class lithium ion batteries. Y. Kobayashi, **R. Kurihara**, N. Tachikawa, W. Weng, Y. Katayama, S. Shiratori
- PMSE 460.** Superhydrophobic, self-cleaning and UV resistant coating with mechanochemical robustness. **S. Afrin**, D. Fox, L. Zhai



TECHNICAL PROGRAM

- PMSE 461.** Importance of substrate rigidity on the depth profile and interfacial structure of sputtered dielectric films. **S.J. Rinehart**, M.D. Dadmun
- PMSE 462.** Stimuli responsive conductive organogels from P3HT and Fmoc. R. Wijayapala, M. Lakdusinghe, **S. Kundu**
- PMSE 463.** Effect of halloysite nanotubes on shape stabilities of polyethylene glycol-based composite phase change materials. **S. Thanakkasaranee**, C. Huh, J. Seo
- PMSE 464.** Polycaprolactone-based coatings to enhance controlled drug release from ultra-long gastric residence dosage forms. **S. Singh-Moorthy**, **M. Schwarz**, R. Kanasty, J. Yang, I. Gunniss, T. Tai, B. Carter, B. Debenedictis, D. Dufour, H. Sun, L. Siddiqui, J. Fisher, A. Bellinger, D. Altreuter
- PMSE 465.** Polypropylene glycol/silver nanoparticles composite: *In-situ* preparation, characterization, and anticorrosion property for carbon steel in acid solution. **S.A. Umoren**
- PMSE 466.** Molecular scale modifications of thiol-ene networks for enhanced macroscopic properties. **S. Arencibia**, A. Hernandez, D.A. Savin
- PMSE 467.** Study of surface charge on gelatin-graphene oxide aerogels. **S. Guajardo**, T. Figueroa, M. Meléndrez, **K. Fernandez**
- PMSE 468.** Molecular modeling of complex cross-linked networks of PEGDA nanogels. **S. Jayaraman Rukmani**, P. Lin, C.M. Colina
- PMSE 469.** Multiple responsive reversible shape memory OBC/PCL blends. **S. Fan Jiang**, S. Lai
- PMSE 470.** Crosslinkable, chitosan-enabled, moisture-resistant multilayer gas barrier thin film. **S. Lazar**, O. Garcia-Valdez, E. Kennedy, P. Champagne, M. Cunningham, J.C. Grunlan
- PMSE 471.** Solution-processable, thin and high dielectric polyurea gate insulator with strong hydrogen bonding for low-voltage operation of organic thin-film transistors. **S. Yoo**, D. Kim, T. Ha, J. Won, K. Jang, Y. Kim
- PMSE 472.** Self-assembly of lipidated α -AA peptides into nanostructures. **S. Singh**, T. Peng, N. Khadka, **J. Cai**
- PMSE 473.** *In situ* monitoring of proteins adsorption and desorption on smart surface using quartz crystal microbalance. **T. Kaku**, J. Li, T. Nishimoto, K. Homma, K. Sawada, Y. Tokura, Y. Hiruta, A.M. Akimoto, K. Nagase, H. Kanazawa, S. Shiratori
- PMSE 474.** Synthesis of PEG-PLGA diblock with high PEG/PLGA block ratio for the PEG-PLGA/laponite hydrogels with thermoresponsive sol-gel transitions. **T. Maeda**, M. Kitagawa, A. Hotta, S. Koizumi
- PMSE 475.** Influence of the method of crosslinking on the properties of polyisobutylene-based networks. **T. Holbrook**
- PMSE 476.** Enzyme triggered rapid disassembly of polymeric nanoassemblies. **V. Kumar**, Y. Bae, O. Munkhbat, M. Franc, S. Peddolla, S. Thayumanavan
- PMSE 477.** Chemiluminescence driven polymerization of acrylamide. **W.T. De Alwis**, M. Allegrezza, M. Dolan, A. Kloster, D. Konkolewicz



TECHNICAL PROGRAM

- PMSE 478.** Multi-block anion exchange membranes with long flexible alkyl side chains. **W. Khan**, A. Herrera, T. Tran, C.J. Cornelius
- PMSE 479.** Establishing substituent effects on hydrolytic degradation behavior of poly(thioether acetal) networks from thiol-ene photopolymerization. **W. Walker**, M. Sandoz, S. Roland, D.L. Patton
- PMSE 480.** Preparation and characterization of lotus powder/PDMS mixed matrix membranes for enhanced ethanol recovery. **X. He**, T. Wang, J. Chen, J. Li
- PMSE 481.** Determining number-average molecular weight for polyelectrolytes using NMR diffusometry. **X. Li**, A. Han, R.H. Colby, L.A. Madsen
- PMSE 482.** Preparation and characterization of hydrophobically modified polyacrylamide and its drag reduction performance by hybridizing with exfoliated nanolayered montmorillonite. L. Xing, **Y. Ke**
- PMSE 483.** Rational structural-based design of polyacrylate/acrylamide as ultralow fouling materials. **Y. Zhang**, B. REN, T. Wang, Z. Feng, L. Tang, S. Xie, J. Zheng
- PMSE 484.** PEO-based composite electrolytes incorporating lignocellulosic nanofibrils and PEGDME for solid-state lithium-ion batteries. X. Li, R. Wang, Y. Min, **Y. Liu**
- PMSE 485.** Supramolecular DNA assembly for surface functionalization of live cells. **Y. Wang**, P. Shi
- PMSE 486.** Nano-patterning of solvent between apposing planar brushes under pressure. C. Pastorino, **Y. kim**, S. Minko, M. Mueller
- PMSE 487.** Fabrication of the ultrafast adsorption nanofibrous membrane for water treatment by hydrophilic group surface migration. **Y. Xu**
- PMSE 488.** Athero-inflammatory nanotherapeutics: Ferulic acid-based poly(anhydride-ester) nanoparticles with targeting amphiphilic macromolecules shells. **Y. Cao**, **S. Song**, K.E. Uhrich
- PMSE 489.** Nanocomposites of electrospun polyelectrolyte hydrogel nanofibers and loaded metal nanoparticles for catalytic reduction of organic dyes. **Y. Li Sip**, L. Zhai
- PMSE 490.** Shape memory assisted self-healing behavior of biobased NR/PCL blends. **Y. Huang**, S. Lai
- PMSE 491.** Preparation and mechanical properties of non-stoichiometric PSS/PDADMA polyelectrolyte complexes. **Y. Chen**
- PMSE 492.** Elucidation of the degradation mechanism for a novel self-degradation adhesive. **W. HYON**, S. Shibata, S. HYON, K. Matsumura
- PMSE 493.** Versatile azoheteroarene molecular photoswitches: Governing site-selectivity in synthesis and incorporation in novel organic photovoltaic and biomaterials. **Z. Chimponda**, **M. Bajaj**, **C.A. Chapusha**, Y.K. Jones, **S.M. Cooper**
- PMSE 494.** Impact of multi-stage biaxial stretching on thermal conductivity of GNP/UHMWPE membrane. **Z. Qi**, H. Wu, S. Guo
- PMSE 495.** Synthesis of cyclic unimolecular polyolefins via Templated Ring-Opening Metathesis (TROM). **Z. Zhou**



TECHNICAL PROGRAM

PMSE 496. Design and fabrication of advanced polybenzimidazole fibrous membranes for fuel cells. **Z. Zhou**, X. Wu, T.R. Aulich, J. Hurley, J. Thakare

PMSE 497. UV-A organic photodetectors based on poly[bis(4-phenyl)(2,4,6-trimethylphenyl)amine] with high detectivity, self-power, and spectral selectivity. **Z. Wang**

Section A

Orange County Convention Center
West Hall C

PMSE-POLY Poster Session

Innovations in Polymer Crosslinking Technology

E. Harth, *Organizer*

5:00 - 7:00

PMSE 498. Chemically fueled covalent crosslinking of polymer materials. **B. Zhang**, I. Jayalath, J. Ke, J. Sparks, D. Konkolewicz

PMSE 499. Electrofabrication of biomaterials: A bio-mimetic electrochemical approach to fabricate hydrogels and confer functions. **J. Li**, W.E. Bentley, G.F. Payne

PMSE 500. Dynamic control of hydrogel crosslinking through reversible sortase-mediated transpeptidation. **M. Arkenberg**, D. Moore, C. Lin

PMSE 501. Controlling the network dynamics of polyelectrolyte complexes. **M. Yang**, J. Shi, J.B. Schlenoff

PMSE 502. Sustainable route for reactive cross-linking of polylactic acid/cellulose nanocrystal films: investigations of processability and structure-property relationship. **P. Dhar**, A. Kumar, **V. Katiyar**

Section A

Orange County Convention Center
West Hall C

PMSE-POLY Poster Session

Materials for High-Performance Impact Mitigation: Design, Synthesis, Characterization & Validation

E. Harth, *Organizer*

5:00 - 7:00

PMSE 503. Multifunctional, hybrid silica coatings on mild steel. **R. Suleiman**, A. Sorour, M. Mizanur Rahman



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

PMSE 504. Facile design of multi-responsive liquid crystalline brush-like copolymers for color modulation. **D. Ndaya**, R. Bosire, R. Kasi

PMSE 505. Preparation and characterization of organic modified bentonite for the treatment of chromium and nitrate in groundwater. **Y. Gao**, S. Bao

PMSE 506. Inhibiting the atomic layer deposition of TiO₂ using brush polymers. **M. Mettry**, R. Wojtecki

PMSE 507. Characterization of novel biomimetic peptide-polymer conjugate using the properties of antimicrobial peptide Maximin H5. **E. Nicolau**

PMSE 508. Synergistic effects of boron nitride alignment and xylitol crystals in a thermally conductive composite. **M. Kashfipour**, J. Zhu, N. Mehra, R. Dent

PMSE 509. 3D characterization of polyamide reverse osmosis membranes in the transmission electron microscope. **T. Culp**, M. Kumar, E. Gomez

Section A

Orange County Convention Center
West Hall C

PMSE-POLY Poster Session

Molecular Engineering of Interphases in Polymeric Materials: Advances in Experiments & Simulations

E. Harth, *Organizer*

5:00 - 7:00

PMSE 510. Improvement in performance of SPEEK membranes by PSSA-g-PVDF proton conductive wire. **X. Zhou**, Q. Zhou, X. Sun

Section A

Orange County Convention Center
West Hall C

PMSE-POLY Poster Session

Multicomponent Block Polymer Systems

E. Harth, *Organizer*

5:00 - 7:00



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

PMSE 511. Poly(ester urethane) elastomer degradation characterization using thermal and mechanical analyses. **A.S. Edgar**, J.A. Torres, D. Yang

Section A

Orange County Convention Center
West Hall C

PMSE-POLY Poster Session

Recent Trends in Polymer Photochemistry: From Molecular Design to Future Applications

E. Harth, *Organizer*

5:00 - 7:00

PMSE 512. Grayscale digital light processing 3D printing for multifunctionally graded materials. **X. Kuang**, H.J. Qi

Dispersity in Block Copolymers: Synthesis, Characterization, Modeling & the Effects on Self-Assembly

Posters

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New Frontiers in Aerospace Polymers: Advances & Challenges in Experiments & Simulations

Posters

Sponsored by POLY, Cosponsored by PMSE

Poly(2-oxazoline)s & Polypeptoids

Posters

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Undergraduate Research in Polymer Science

Posters



TECHNICAL PROGRAM

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WEDNESDAY MORNING

Section A

Rosen Centre Hotel
Salon 9

Innovations in Polymer Crosslinking Technology

3D Printing & Crosslinking Chemistries

S. Caillol, *Organizer*
S. Swarup, D. C. Webster, *Organizers, Presiding*

8:30 PMSE 513. Nanostructuring and cross-linking in 3D printed polymer systems. **R.C. Advincula**

9:00 PMSE 514. 3D-printable, high-performance polyimide for additive manufacturing. **S. Hosseini**, M. Tajik Asl, W. Voit

9:20 PMSE 515. Metal-binding polysiloxane networks through borane-catalyzed vulcanization. **C. Sample**, M.W. Schulze, V. Lensch, L. Boonchaiphruak, C.M. Bates, C.J. Hawker

9:40 PMSE 516. Exploiting the hydrogen abstraction driven crosslinking of poly(α -pinene methacrylate) for the production of renewable polyHIPES. **O.R. Monaghan**, S.M. Howdle, D. Irvine

10:00 Intermission.

10:30 PMSE 517. Synthesis of cross-linkable polyethers and polyamides by anionic ring-opening polymerization. **S. Carlotti**

11:00 PMSE 518. Preparation of cross-linked polyesters by the radical copolymerization of cyclic ketene acetals and divinyl ether derivatives. **Y. Guillaneuf**

11:20 PMSE 519. Aza Michael addition for additive manufacturing of rigid and rubbery polymers. **A. Clay**, J. Mitchell, G.R. Palmese, E.J. Robinette, J. La Scala

11:40 PMSE 520. Glycidyl carbamate functional polymers: A non-isocyanate polyurethane. **D.C. Webster**

12:00 PMSE 521. Pt-cured silicone elastomers: Toward understanding hydrosilylation, Si-H autoxidation to Si-OH and Si-OH condensation to a secondary Si-O-Si network. **K.J. Wynne**, A. Kayesh, C. Wang

Section B

Rosen Centre Hotel
Salon 3



TECHNICAL PROGRAM

Cooperative Research Award: Symposium in Honor of Christopher Stafford, Edwin Chan, Michael Hickner, Coray Colina, James Sturnfield, Steven Rosenberg & Abhishek Roy

S. C. Jana, *Organizer*
C. L. Soles, *Organizer, Presiding*

8:00 Introductory Remarks.

8:10 PMSE 522. How membrane technology contributes to sustainability and life sciences. **A. Roy**, S. Rosenberg, M. Paul, S. Jons, M. Peery

8:45 PMSE 523. Advanced membrane characterization enabled by molecular layer-by-layer deposition of polyamides. P.M. Johnson, E. Chan, K.E. Feldman, D. Sunday, D. Shaffer, T.J. Zimudzi, M.A. Hickner, A. Roy, S. Rosenberg, **C.M. Stafford**

9:20 PMSE 524. New platform for the fabrication and tailoring of ultrathin polyamide films for desalination membranes. M. Shin, S. Park, **J. Lee**

9:55 Intermission.

10:15 PMSE 525. Understanding the next generation reverse osmosis membranes from atomistic simulations. **C.M. Colina**

10:50 PMSE 526. Using quantitative IR spectroscopy to probe thin polymer films. T.J. Zimudzi, **M.A. Hickner**

11:25 PMSE 527. Next-generation nanofiltration membranes based on aligned and bicontinuous self-assembled systems. **C.O. Osuji**, X. Feng, Q. Imran, K. Kawabata, X. Lu, L. Sixdenier, G. Kaufman, U. Gabinet, M. Elimelech

Section C

Rosen Centre Hotel
Salon 15

Hybrid Functional Materials from Controlled Assembly of Polymer & Inorganic Nanoparticles

Poly-Nano Synthesis & its Application

Financially supported by Huazhong University
Y. Lin, Z. Nie, *Organizers*
J. He, *Organizer, Presiding*

8:00 PMSE 528. Functionalized transition metal carbides (MXenes) for improved interface and mechanical properties of polymer nanocomposites. **C.B. Hatter**, B. Anasori, Y. Gogotsi

8:20 PMSE 529. Additive manufacturing of dye-sensitized solar cells with nanowires for increased stability, performance, and conductivity. **S. Jackson**, M. Roy, P. Tran, T. Dickens



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

8:40 PMSE 530. Electrically and ionically conductive microstructures of Metal Organic Frameworks (MOFs). **H.P. Rathnayake**, S. Dawood, A. Letfullina

9:00 PMSE 531. Preparation of positively charged membranes by blending polyvinylidene fluoride (PVDF) with the synthesized cationic poly (ionic liquid). **S. Shen**, R. Bai

9:20 Intermission.

9:35 PMSE 532. Designing polymer nanocomposites for membrane gas separation: An integrated experimental and modeling approach. **H. Lin**

9:55 PMSE 533. Affinity of functionalized graphene and linker molecules to industrial carbon fibers. **R. Sarder**

10:15 PMSE 534. Morphology transition in block copolymer/quantum dot hybrids *via* ligand displacement and formation of photoluminescent nano-objects. **S. Singh**, B. Nandan

10:35 PMSE 535. Controlling the pore size of mesoporous carbon thin films. **Z. Zhou**, G. Liu

10:55 PMSE 536. Graphene-multiwalled carbon nanotubes-polyurethane nanocomposite for electromagnetic interference shielding. **V. Choudhary**

11:15 PMSE 537. Extreme heat shielding by clay/chitosan nanobrick wall assembled on flexible foam. **S. Lazar**, F. Carosio, A. Davesne, M. Jimenez, S. Bourbigot, J.C. Grunlan

11:35 PMSE 538. Synthesis of novel cellulose based composite fibers by electrospinning technique. **R.N. Udangawa**, C. Willard, C. Mancinelli, C. Chapman, A. Pochiraju, L. Hou, T.J. Simmons, R.J. Linhardt

Section D

Rosen Centre Hotel
Salon 11

Autonomous Processes, Chemomechanics & Active Matter Using Polymers & Soft Materials

Financially supported by PPG Industries
A. Balazs, *Organizer*
T. Emrick, *Organizer, Presiding*

8:30 PMSE 539. Designing active membranes: Focus on feedback mechanisms in gel and composites. **O. Kuksenok**

9:00 PMSE 540. Microscale engineering of magnetically actuated, reconfigurable and motile soft polymeric architectures. **O.D. Velev**

9:30 PMSE 541. Self-reporting and self-regulating liquid crystals. **N.L. Abbott**

10:00 PMSE 542. Building supracolloidal objects with responsive interactions. **T. Emrick**

Section E



TECHNICAL PROGRAM

Rosen Centre Hotel
Salon 8

Materials for High-Performance Impact Mitigation: Design, Synthesis, Characterization & Validation

Impact & Jamming for Personal Protection

E. Arruda, J. J. De Pablo, C. L. Soles, *Organizers*
J. Lenhart, *Organizer, Presiding*

8:00 PMSE 543. Multi-layered structure approach for impact mitigation. **E. Nicoli**, M.F. Sonnenschein, L. Ma, B.L. Wendt

8:40 PMSE 544. Metrologies to address elastic and viscous contributions to energy dissipation in multi-axial impacts.
A.M. Forster, M. Riley, S. Mates

9:20 PMSE 545. High-rate deformation of auxetic disordered networks. **E. Chan**, E. Han, N. Pashine, K. Murphy, D. Reid, M. Shen, H. Jaeger, S. Nagel, C.L. Soles, J.J. De Pablo

10:00 Intermission.

10:20 PMSE 546. Design strategies for low-velocity impact absorbing materials. **H. Jaeger**

11:00 PMSE 547. Development of advanced environmental protection garments containing Shear Thickening Fluid enhanced textiles (STF-Armor™) for puncture, MMOD, and dust mitigation for improved astronaut protection. **N.J. Wagner**, R. Dombrowski, M. Katzarova, B. Peters

11:40 PMSE 548. Polymer-derived ceramic composites of graphene. **L. Zhai**, C. Shen

Section F

Rosen Centre Hotel
Salon 14

Molecular Engineering of Interphases in Polymeric Materials: Advances in Experiments & Simulations

Graphitic & Polymeric Interphases

Financially supported by Carbon Nexus
H. Heinz, L. C. Henderson, *Organizers*
R. Jayan, D. Nepal, *Organizers, Presiding*

8:30 PMSE 549. Bonding of dissimilar materials in advanced composites. **R.J. Varley**, J. Zhang, C. Creighton, M. deSouza

9:10 PMSE 550. Moving carbon fiber and composite materials research beyond the lab bench. **R.F. Hess**

9:30 PMSE 551. Insights into PMMA/CNT assembly and nanoscale structure-property relationships in polymer/CNT composites. **H. Heinz**



TECHNICAL PROGRAM

9:50 PMSE 552. Nanoscale characterization of epoxy nanocomposites: Connecting chemistry and morphology with local properties. **N. Pestian**, S. Hawkins, J. Bates, J. Ryan, I. Barrett, D. Nepal

10:10 PMSE 553. Bond breaking in epoxy systems. **T.S. Nguyen**, G.S. Kedziora, J. Moller, R.J. Berry, T. Breitzman

Section G

Rosen Centre Hotel
Salon 18

Molecular Engineering of Peptide Assemblies

Helical Peptides

H. Cui, S. Lecommandoux, M. V. Tirrell, *Organizers*
H. Acar, *Organizer, Presiding*
N. Stephanopoulos, *Presiding*

8:00 PMSE 554. Bundlers: Supramolecular assembly and functionalization of coiled coils using click chemistry. **B.P. Sutherland**, N.I. Halaszynski, J.Y. Lee, D.J. Pochan, C.J. Kloxin

8:15 PMSE 555. Design, synthesis, self-assembly, and covalent capture of heterotrimeric collagen helices. **J.D. Hartgerink**

8:40 PMSE 556. Next-generation collagen hybridizing peptides. **M.S. Yu**

9:05 PMSE 557. Self-organizable α -helix bundle assemblies. **J.G. Rudick**

9:30 PMSE 558. 2D multicomponent core-shell nanosheets fabricated from designed collagen-mimetic peptides. **A. Merg**, G. Touponse, H. Su, A. Bazrafshan, K. Salaita, V.P. Conticello

9:45 Intermission.

10:05 PMSE 559. Hybrid nanomaterials through the self-assembly of coiled-coil peptides and DNA nanostructures. **N. Stephanopoulos**

10:30 PMSE 560. Peptide stapling and oligomerization in coiled-coil based membrane fusion. **A. Kros**

10:55 PMSE 561. Understand kinetic pathway toward controlled hierarchical assembly. **T. Xu**

11:20 PMSE 562. α -Helical peptide membranes. **H.C. Fry**

11:45 PMSE 563. Post-assembly surface reactivity of 1,2-dithiolane modified self-assembling peptides. **J.E. Smith-Carpenter**

Section H



TECHNICAL PROGRAM

Rosen Centre Hotel
Salon 13

Recent Trends in Polymer Photochemistry: From Molecular Design to Future Applications

Photolithography & Emerging Applications

Financially supported by Polymer Competence Center Leoben
C. Bowman, T. Griesser, A. Guymon, S. Marco, S. Schlögl, *Organizers*
W. Kern, *Presiding*

8:30 PMSE 564. From STED nanoscopy via STED nanolithography to STED photochemistry. **T.A. Klar**

9:00 PMSE 565. UV-induced morphological changes in block polymer assemblies. **C. Machado**, R. Tran, T.A. Jenkins, M.B. Sims, B.S. Sumerlin, D.A. Savin

9:20 PMSE 566. Synthesis and characterization of photodegradable thermoplastic elastomers. **W.T. De Alwis**, J.A. Reeves, M.T. Dolan, D. Konkolewicz

9:40 Intermission.

9:55 PMSE 567. UV-mediated crosslinking of poly(2-oxazoline)s: Fabrication of polymers for biomedical applications. **F. Wiesbrock**, K.P. Luef, E. Rossegger

10:25 PMSE 568. Plastic scintillators with efficient light output and pulse shape discrimination produced via photo-initiated polymerization. **A. Lim**, A.C. Mahl, J. Latta, H. Yemam, U. Greife, A. Sellinger

10:45 PMSE 569. Plastic with highly soluble dopants for scintillators. **S. Sonawane**, K.F. Johnson, J.B. Schlenoff

11:05 Concluding Remarks.

Dispersity in Block Copolymers: Synthesis, Characterization, Modeling & the Effects on Self-Assembly

Disperse Block Polymer Self-Assembly

Sponsored by POLY, Cosponsored by PMSE

Producing Equilibrium Amorphous Packings

Vapor Deposited Glasses

Sponsored by PHYS, Cosponsored by COLL and PMSE[‡]



TECHNICAL PROGRAM

Innovative Chemistry & Materials for Electrochemical Energy Storage

Beyond Li-Ion

Sponsored by ENFL, Cosponsored by CATL, INOR and PMSE

Transport in Polymer Membranes

Gas Separation

Sponsored by POLY, Cosponsored by PMSE‡

New Frontiers in Aerospace Polymers: Advances & Challenges in Experiments & Simulations

Thermoplastics & New Generation of Polymers for Aerospace Applications

Sponsored by POLY, Cosponsored by PMSE

WEDNESDAY AFTERNOON

Section A

Rosen Centre Hotel
Salon 9

General Papers-New Concepts in Polymeric Materials

E. Harth, *Organizer*
J. Caffyn, G. Delaittre, *Presiding*

1:30 PMSE 570. Nitroxide radical nanoparticles by ultrafast tandem ROMP/ROMPISA. D. Le, **G. Delaittre**

1:50 PMSE 571. Recycling plastic bottle waste into novel aerogels for high-value engineering applications. **H.M. Duong**, D.K. Le, Q.B. Thai, R. Leung Hoe Inn, X. Zhang, K. Hong wei, N. Gek nian, N. Phan-Thien, T.P. Luu

2:10 PMSE 572. Polymeric semiconductors based on *meso*-substituted BODIPY for (opto)electronic applications. **H. Usta**, C. Kim, b.J. Kim

2:30 Intermission.

2:50 PMSE 573. Molecularly defined synthetic delivery systems for RNA. **P. Talukder**, O.F. Khan, J.S. Chahal, J.S. McPartlan, J. Huang



TECHNICAL PROGRAM

3:10 PMSE 574. Drug-loaded biodegradable scaffold for controlled release in regenerative medicine. **J.A. Santillán Mercado**, J.G. Padilla Zayas, J. Cheng, E. Nicolau, P.B. Messersmith

3:30 PMSE 575. Design and syntheses of bio-based exotic amino acid derived cationic polyamide. **J. Phanthuwongpakdee**, S. Dwivedi, K. Takada, S. Babel, T. Kaneko

3:50 PMSE 576. Characterization of novel reactively blended wheat gluten gels loaded with polyvinylidene fluoride and high molecular weight polyethylene oxide. **J. Caffyn**, R. Parnas

Section B

Rosen Centre Hotel
Salon 16

General Papers-New Concepts in Polymeric Materials

E. Harth, *Organizer*
K. Bullard, J. Jefcoat, *Presiding*

1:30 PMSE 577. Synthesis and characterization of biological nanomaterial/polyvinylidene fluoride composites. **J. Jefcoat**, E. Barnes, H. Peel, E. Alberts, C. Weiss, P. Buchanan

1:50 PMSE 578. Effects of composition on block-copolymer-derived carbon nanofibers: Porous structures and electrochemical properties. **J.M. Serrano**, G. Liu

2:10 PMSE 579. Design of emulsion-templated mesoporous-macroporous polyurea gels. **K. Mawhinney**, S.C. Jana

2:30 Intermission.

2:50 PMSE 580. Thermal vs. mechanical rejuvenation of a-PS: molecular dynamics reveal different microscopic scenarios. **K. Grigoriadi**, M. Wübbenhorst, L. van Breemen, P. Anderson, M. Hütter

3:10 PMSE 581. Semifluorinated poly(ether sulfones) and fluorinated arylene vinyl ether polymers: Synthesis and characterization. **K. Mukeba**, G. Narayanan, B. Farajidizaji, K. Shelar, A. Sygula, C.U. Pittman, **D.W. Smith**

3:30 PMSE 582. End-on orientation of semiconducting polymer chains and its applications to organic solar cells. **K. Tajima**

3:50 PMSE 583. Mild modification of cellulose nanocrystal surface chemistry with nucleophiles. **K. Bullard**, M. Srinivasarao, W. Gutekunst

Section C

Rosen Centre Hotel
Salon 15

Hybrid Functional Materials from Controlled Assembly of Polymer & Inorganic Nanoparticles

Polymer Film & its Applications



TECHNICAL PROGRAM

Financially supported by Huazhong University

J. He, Y. Lin, Z. Nie, *Organizers*

W. Li, *Presiding*

1:30 PMSE 584. Polymer brush-grafted nanoparticles as oil lubricant additives for friction and wear reduction: Effect of brush composition. **B. Seymour**, B. Zhao

1:50 PMSE 585. New scalable-up approach to non-iridescent structural blue films with relatively high tensile properties via RAFT emulsion polymerization. **Q. Xiang**

2:10 PMSE 586. Enhancing the thermal conductivity of crosslinked epoxy resins by the addition of bisphenyl units and silica nanoparticles. **M.S. Windberger**, E. Dimitriou, F. Wiesbrock

2:30 PMSE 587. Anisotropic self-assembly of spherical ligand grafted nanoparticles through polymer crystallization. **X. Ning**, L. Schadler, J. Pribyl, B.C. Benicewicz, A. Jimenez, S. Kumar

2:50 Intermission.

3:05 PMSE 588. Effect of a silane coupling agent on superhydrophobic SiC/CNTs coatings onto an aluminum substrate. **G. Jiang**, **H. Jinhuan**

3:25 PMSE 589. Self-assembly of supramolecular truncated cuboctahedron into double helical nanowires with non-natural parastichy pattern. **H. Wang**, K. Wang, Y. Xu, S. Chen, M. Hart, L. Wojtas, L. Zhou, L. Gan, X. Yan, Y. Li, J. Lee, X. Wang, C. Zhang, S. Zhou, T. Zhai, H. Yang, M. Wang, Q. Sun, B. Xu, Y. Jiao, P.J. Stang, J.L. Sessler, X. Li

3:45 PMSE 590. Metal-organic framework-based porous liquids with tunable pore functionality and sorption properties. **S. He**, L. Chen, T. Li

4:05 PMSE 591. Controlled multilayered vesicular assembly via polyoxometalate-oligofluorene (sphere-rod) conjugates. **J. Luo**, T. Liu, S.Z. Cheng, T. Liu

4:25 PMSE 592. Polymer coated lanthanide based nanoparticles as PARACEST MRI contrast agents. **P. Roy**, D.R. Talham

Section D

Rosen Centre Hotel
Salon 11

General Papers-New Concepts in Polymeric Materials

E. Harth, *Organizer*

M. Elsabahy, K. Lee, *Presiding*

1:30 PMSE 593. Development of PDMS-based inks for additive manufacturing. **K. Lee**, C. Park, E. Murphy, J.H. Dumont, A. Labouriau

1:50 PMSE 594. Novel self-healing CFRP composites with high glass transition temperatures. **L. Zhang**, H. Sodano



TECHNICAL PROGRAM

2:10 PMSE 595. Stimuli responsive microscale architectures: Two-photon lithography with shape memory polymers. **L. Navrazhnykh**, J.R. Greer

2:30 Intermission.

2:50 PMSE 596. Emulsion-based bioinks for 3D bioprinting of scaffold-supported composite hydrogels. **L. Wenger**, C. Radtke, J. Göpper, M. Wörner, J. Hubbuch

3:10 PMSE 597. Absorbable hemostatic hydrogels comprising sacrificial templates for the assembly of honeycomb-like nanofibrous mats of chitosan. **M. Elsabahy**, E.E. Leonhardt, N. Kang, M.A. Hamad, K.L. Wooley

3:30 PMSE 598. Conjugated polymers with embedded aggregation-induced emitters. **M.D. Cole**, R. Holley, R. Meyer, T. Emrick

3:50 PMSE 599. Electrically and magnetically active polymer composites for tailoring mammalian and bacterial cell response. **M.M. Fernandes**, E. Carvalho, J. Padrao, C. Ribeiro, A. Nicolau, M. Gama, S. Lanceros-Mendez

Section E

Rosen Centre Hotel
Salon 8

Materials for High-Performance Impact Mitigation: Design, Synthesis, Characterization & Validation

Impact in Semicrystalline Polymers & Composites

E. Arruda, J. J. De Pablo, C. L. Soles, *Organizers*
J. Lenhart, *Organizer, Presiding*

1:00 PMSE 600. Applications of synchrotron x-ray scattering to structure analyses of polymers under deformation. **A. Takahara**, K. Kojio, C. Cheng, N. Dechnarong

1:40 PMSE 601. Atomistic modeling of semicrystalline polyethylene fibers. **I. Yeh**, J. Lenhart, J. Andzelm

2:10 PMSE 602. Strain rate effects during ultra-high strain rate penetration of polymeric materials. M. Bowering, W. Heard, T. E. Lacy, Jr., C.U. Pittman, **S. Kundu**

2:40 Intermission.

3:00 PMSE 603. Dynamic strain localization and fragmentation in tubes influenced by polymer coating. **K. Ravi-Chandar**

3:40 PMSE 604. Thermo-mechanical characterization and constitutive modeling of polyurea variants. **A. Amirkhizi**

4:20 PMSE 605. Experimental studies on impact failure of soft body armors at micro to macro size scales. **W. Chen**, M. Hudspeth, Z. Guo, B.H. Lim, J. Gao

Section F



TECHNICAL PROGRAM

Rosen Centre Hotel
Salon 14

General Papers-New Concepts in Polymeric Materials

E. Harth, *Organizer*
N. Dasgupta, Z. Zhou, *Presiding*

1:30 PMSE 606. Electrospun PLA/CNC nanocomposite fiber as a controlled release vehicle for urea fertilizer. **N. S, P. Dhar, V. Katiyar**

1:50 PMSE 607. Understanding nanospheres interaction with biological environment. **M. Reis Nogueira de Lima, J. Kohn**

2:10 PMSE 608. Synthesis of polycarbosilane systems for the advanced manufacturing of polymer-derived ceramics. **L. Baldwin, L. Rueschhoff, M.J. Dalton, H. Koerner, m. cinibulk, K. Martin, M.B. Dickerson**

2:30 Intermission.

2:50 PMSE 609. Dilatancy-like behavior in electrospun polymer fibers with liquid cores: Applications to sound damping. **M.J. Bertocchi, P. Vang, R.B. Balow, J.H. Wynne, J. Lundin**

3:10 PMSE 610. Investigating the reactivity and mechanical properties of poly (1,6) hexane diol-co-citric acid via reactive molecular dynamics simulations. **N. Dasgupta, D. Yilmaz, A.C. Van Duin**

3:30 PMSE 611. Deposition of porous membranes with controlled morphology and chemical functionality for fabrication of giant vesicles. **N. Movsesian, G. Dianat, M. Tittensor, N. Malmstadt, M. Gupta**

3:50 PMSE 612. Using differential scanning calorimetry to characterize the crosslinking of polydimethylsiloxane. **M. Salamon, J. Timmerman**

Section G

Rosen Centre Hotel
Salon 18

Molecular Engineering of Peptide Assemblies

New Directions in Peptide Assembly

H. Acar, M. V. Tirrell, *Organizers*
H. Cui, S. Lecommandoux, *Organizers, Presiding*

1:15 PMSE 613. Fabrication of self-assembling antimicrobial nanofibers via peptide self-assembly. **H. Dong, D. Xu, W. Chen, W. Qiang**

1:30 PMSE 614. Towards control of energy migration within dynamic peptide-based supramolecular materials. **J.D. Tovar**



TECHNICAL PROGRAM

1:55 PMSE 615. System chemistry, dynamic chemical networks, and the emergence of functional peptide assemblies. **D.G. Lynn**

2:20 PMSE 616. Fast gels and slow gels: Understanding dynamics in a bioconjugated peptide network. **R.S. Tu**

2:45 PMSE 617. Ultra-robust supramolecular nanostructures with tunable surface chemistries from novel synthetic amphiphiles. **T. Christoff-Tempesta**, J. Tian, D. Kim, A. Lew, W. Lindemann, J. Ortony

3:00 Intermission.

3:20 PMSE 618. Self-assembled tetrapeptide nanocoils for delivery of hydrogen sulfide (H₂S). **J.B. Matson**, Y. Wang

3:45 PMSE 619. Coarse-grained modeling of peptide assembly in bulk and at interfaces. **M. Shell**

4:10 PMSE 620. Reversible self-assembly of peptide and peptide-DNA superstructures. **S.I. Stupp**

4:35 PMSE 621. Molecular modeling of peptide-drug amphiphiles. M. Kang, A. Manandhar, P.K. Tang, **S. Loverde**

5:00 PMSE 622. Secondary structure directed self-assembly and crosslinking of peptide based block copolymers. **M. Barz**

Section H

Rosen Centre Hotel
Salon 13

General Papers-New Concepts in Polymeric Materials

E. Harth, *Organizer*
Q. Liu, S. Stalin, *Presiding*

1:30 PMSE 623. Enhancement of shape fidelity for 3D-printed soft scaffolds by introducing hydrogen bonds. **Q. Liu**, C. Peng, T. Jain, F. Peng, A. Joy

1:50 PMSE 624. Novel, plant-based polymers: An efficient target directed non-toxic delivery system for chemotherapeutic drugs. **R. Srinivasan**, J. Speshock, D. Edwards

2:10 PMSE 625. Highly stretchable and tough hydrogel consisting of physical and chemical crosslinks. **R. Wijayapala**, S. Hashemnejad, B. Morgan, S. Kundu

2:30 Intermission.

2:50 PMSE 626. Novel glycopolymer-based biomaterials for tissue engineering. **R. Liu**, H. Screen, R. Becer

3:10 PMSE 627. Synthesis of poly(ester-peptide) materials and their potential in biomedical applications. **R.P. Brannigan**, A. Heise



TECHNICAL PROGRAM

3:30 PMSE 628. Lithium electrodeposition in crosslinked polymer electrolytes. **S. Stalin**, H.E. Johnson, G.W. Coates, L.A. Archer

3:50 PMSE 629. Generating an optimum icephobic silicone coating by simple manipulation of processing conditions. **S.S. Nair**, K.J. Wynne

Dispersity in Block Copolymers: Synthesis, Characterization, Modeling & the Effects on Self-Assembly

Dispersity in Block Polymer Amphiphiles

Sponsored by POLY, Cosponsored by PMSE

Producing Equilibrium Amorphous Packings

Making & Transforming Stable Glasses

Sponsored by PHYS, Cosponsored by COLL and PMSE[‡]

Innovative Chemistry & Materials for Electrochemical Energy Storage

Advanced Materials & Synthesis

Sponsored by ENFL, Cosponsored by CATL, INOR and PMSE

New Frontiers in Aerospace Polymers: Advances & Challenges in Experiments & Simulations

Stimuli-Responsive Composites

Sponsored by POLY, Cosponsored by PMSE

WEDNESDAY EVENING

Section A

Rosen Centre Hotel
Grand A

PMSE-POLY Plenary Lecture & Awards Reception

M. Becker, S. E. Morgan, *Organizers, Presiding*



TECHNICAL PROGRAM

5:30 Reception.

6:00 **PMSE 630.** Power of polymer synthesis: Translation of basic materials research into social benefits. **C.J. Hawker**

6:40 Awards Presentation.

7:00 Reception.

THURSDAY MORNING

Section A

Rosen Centre Hotel
Salon 17

General Papers-New Concepts in Polymeric Materials

E. Harth, *Organizer*
N. Kanbargi, P. McCormack, *Presiding*

8:30 **PMSE 631.** Biopolymer-based superhydrophobic surface assisted by electrostatic deposition. **N. S, V. Katiyar**

8:50 **PMSE 632.** High-performance nanocomposites of lignin-based thermoplastics. **N. Kanbargi**

9:10 **PMSE 633.** New class of soft dendritic polymer fibroid materials with extraordinary adhesive and structuring capabilities. **O.D. Velez**, S. Roh, A. Williams, S.D. Stoyanov

9:30 **PMSE 634.** Synthesis of ceramic and purely metallic aerogels from compressed *xerogel*/ powder compacts. **P. Rewatkar**, R. Soni, C. Sotiriou-Leventis, N. Leventis

9:50 Intermission.

10:10 **PMSE 635.** Poly(phenylene oxide) based ion conducting polymers for electrochemical applications. **P. McCormack**, G. Koenig, G. Geise

10:30 **PMSE 636.** Ultrasensitive diffraction gratings based on smart hydrogel for high-selective and rapid detection of trace heavy metal ions. **P. Hanyu**, W. Wang, L. Liu, X. Pu, Z. Liu, X. Ju, R. Xie, L. Chu

10:50 **PMSE 637.** Impact of architectural asymmetry on block polymer phase behavior. **A. Chang**, F.S. Bates

Section B

Rosen Centre Hotel
Salon 16

General Papers-New Concepts in Polymeric Materials



TECHNICAL PROGRAM

E. Harth, *Organizer*
T. Jain, S. A. Kedzior, *Presiding*

8:30 PMSE 638. Biodegradable polymeric microspheres: Preparation and evaluation. **S. Harsha**

8:50 PMSE 639. Interfacially-formed conductive nanocomposite films and their use as physical sensors. **S.A. Kedzior**, W. Kapadia, E.L. Gawron, R. Mayall, P. Egberts, M. Trifkovic, K. Karan, S. Bryant

9:10 PMSE 640. Alginate bio-film preparation with aloe vera and cat's claw, and their chemical, physical, and biological characterization. **S. Kim**, M. Elgegren, J. Nakamatsu

9:30 PMSE 641. Functionalization of self-healing polyelectrolyte multilayer films via thiol-ene click chemistry and its implication to refunctionalizable surface. **S. Cho**, N. Zacharia

9:50 Intermission.

10:10 PMSE 642. Structure-property relationships of multifunctional polyesters for extrusion-based 3D printing. **T. Jain**, S. Govindarajan, W. Clay, A. Joy

10:30 PMSE 643. Engineering of specialized 3D printer for rapid prototyping of thermoplastic materials. **T. Mensch**, B. Boyle, G. Miyake

10:50 PMSE 644. Evaluation of large-area projection sintering time and temperature on polyamide-12. **T. Kaur**

Section C

Rosen Centre Hotel
Salon 15

General Papers-New Concepts in Polymeric Materials

E. Harth, *Organizer*
T. W. Franklin, V. Romani, *Presiding*

8:30 PMSE 645. Flow-induced crystallisation of polymers. **T.W. Franklin**, A.J. Ryan, O. Mykhaylyk

8:50 PMSE 646. PEG-based nanocomposite hydrogels with controlled thermoresponsive gelation and hydrolytic degradation. **T. Maeda**, M. Kitagawa, S. Koizumi, A. Hotta

9:10 PMSE 647. Soft-templated synthesis of lightweight, elastic, and conductive aerogels. **W. Liang**, J. Fang

9:30 PMSE 648. Electrochemical patterning of tissue-mimetic conductive hydrogels. **V. Feig**, H. Tran, M. Lee, R. Huang, K. Liu, L. Baker, D. Mackanic, Z. Bao

9:50 Intermission.

10:10 PMSE 649. Active polymer films from agro-sources used to extend the shelf-life of Italian salami. **V. Romani**, B.D. Olsen, V.G. Martins



TECHNICAL PROGRAM

10:30 PMSE 650. Side-chain type multi-block anion exchange membranes functionalized with quaternary ammonium groups bearing long flexible alkyl moieties. **W. Khan**, A. Herrera, T. Tran, C.J. Cornelius

10:50 PMSE 651. Poly(L-lactide)-N-heterocyclic functionalised drug conjugates as drug carrier-systems: Synthesis, mechanistic, and kinetics study. **V. Katiyar**, M. Mili, A. Gupta

Section D

Rosen Centre Hotel
Salon 18

General Papers-New Concepts in Polymeric Materials

E. Harth, *Organizer*
Y. Lapitsky, Z. A. Page, *Presiding*

8:30 PMSE 652. Formation, rheology and long-term sustained release properties of polyelectrolyte/multivalent ion coacervates. P. Lawrence, U.K. de Silva, J. Brown, K.J. Zamora, S.S. Alam, Y. Huang, **Y. Lapitsky**

8:50 PMSE 653. Highly tough, mechanoresponsive, and self-recovery hydrogels used as strain-induced color sensors. **Y. Zhang**, B. REN, F. Yang, L. Tang, S. Xie, J. Zheng

9:10 PMSE 654. Fabricating stacked DE actuators of thermoplastic elastomer. **Y. Xiao**, Y. Luo

9:30 PMSE 655. 2D nanosheet: Self-assembly of poly[n]rotaxanes. **Y. Shi**, F. Stoddart

9:50 Intermission.

10:10 PMSE 656. Orthogonal chemistry for additive manufacturing of complex soft matter. **Z.A. Page**

10:30 PMSE 657. Improving the processability of thermally conductive polycarbonate/graphene/short carbon fiber composites. **Z. Yu**, J.H. Wang, Y. Bai, Y. Li, W. Wang

10:50 PMSE 658. Multilayers of graphene oxide to produce self-extinguishing, non-ignitable and flame-resistant flexible polyurethane foams. **A. Fina**, F. Carosio, L. Maddalena, J. Gomez, G. Saracco

Section E

Rosen Centre Hotel
Salon 8

General Papers-New Concepts in Polymeric Materials

E. Harth, *Organizer*
J. Budhathoki-Uprety, A. Jawaid, *Presiding*

8:30 PMSE 659. Basally modified layered transition metal dichalcogenides for optically active responsive composites. **A. Jawaid**, R.A. Vaia



TECHNICAL PROGRAM

8:50 PMSE 660. Polymer stereocomplexation as a platform for nanoparticle assembly. **A. Abdilla**, P. de Roos, J. Ming Ren, J. Lawrence, N. Dolinski, S.E. Seo, E. van der Woude, J. Read De Alaniz, C.J. Hawker

9:10 PMSE 661. Bioinspired thermal conductive polymeric composites. **C. Du**, B. Li

9:30 PMSE 662. Way to faster switching in photochromics using polyoligohedralsilsesquioxane nanoparticles. **J.G. Matisons**

9:50 Intermission.

10:10 PMSE 663. Polymer-functionalized fluorescent nanomaterials: Controlled assembly, properties and applications in biology. **J. Budhathoki-Uprety**, D.A. Heller

10:30 PMSE 664. Optical sensing of autoimmune disease related biomarkers containing solvent accessible lysines using hydrogel-coated gold nanoshells. **M.E. Wechsler**, H.J. Dang, S.D. Dahlhauser, J.F. Reuther, E.V. Anslyn, N. Peppas

10:50 PMSE 665. Tailoring of morphology and optical properties of metal-polymer interfaces during sputter deposition. **M. Schwartzkopf**, O. Polonskyi, T. Strunskus, V. Koerstgens, F. Faupel, P. Mueller-Buschbaum, S. Roth

Section F

Rosen Centre Hotel
Salon 14

General Papers-New Concepts in Polymeric Materials

E. Harth, *Organizer*
Y. Eygeris, M. Ghafari, *Presiding*

8:30 PMSE 666. Development of dynamically cross-linked hydrogels for 3D printing of cell-laden bioinks. **M.B. Baker**

8:50 PMSE 667. Nanocomposite polymer electrolytes based on poly(ethylene oxide) and Li single-ion conducting mesoporous organosilica nanoparticles. **U. Choi**, H. Jung, Y. Kim

9:10 PMSE 668. Responsive nanoporous materials from polymer-brush silica nanoparticles. **Y. Eygeris**, E. White, M. Görke, N. Ulery, I. Zharov

9:30 PMSE 669. Fabrication and characterization of high performance carbon molecular sieve membranes from a crosslinkable polyimide for propylene/propane separations. **C. Karunaweera**, J.P. Ferraris, K.J. Balkus, I.H. Musselman

9:50 Intermission.

10:10 PMSE 670. Topology transformation between cyclic and triarm star shaped macromolecules exploiting [c3]daisy chains as building blocks. **K. Cai**

10:30 PMSE 671. Clean block copolymer microparticles from supercritical CO₂: Universal templates for the facile and scalable fabrication of hierarchical mesostructured metal oxides. **T.M. Bennett**, G. He, R.R. Larder, M.G. Fischer, G.A. Rance, M.W. Fay, A.K. Pearce, C. Parmenter, U. Steiner, S.M. Howdle



TECHNICAL PROGRAM

10:50 PMSE 672. Hyper-cross-linking styrenic polymers with dichloroalkanes for improved adsorption of pollutants. **M. Ghafari**, J.D. Atkinson

Section G

Rosen Centre Hotel
Salon 11

General Papers-New Concepts in Polymeric Materials

E. Harth, *Organizer*
X. Kuang, D. Yang, *Presiding*

8:30 PMSE 673. One-step fabrication of chitosan microcapsules with nanowalls from single emulsion templates. **X. Mu**, X. Ju, L. Zhang, X. Huang, Y. Faraj, Z. Liu, W. Wang, R. Xie, Y. Deng, L. Chu

8:50 PMSE 674. Bio-inspired DOPA derivatives: Adhesion underwater and antifouling properties. **Z. Shafiq**

9:10 PMSE 675. Investigation of poly(ester urethane) degradations. **D. Yang**, J.A. Torres, A.S. Edgar

9:30 PMSE 676. Eco-designed polymers & composites from industrial waste valorization. **A. MIJA**

9:50 Intermission.

10:10 PMSE 677. Recycling of epoxy thermoset and composites via good solvent assisted and small molecules participated exchange reactions. **X. Kuang**, H.J. Qi

10:30 PMSE 678. Bio-based recyclable, reshapable and repairable (3R) fibre-reinforced epoxy composites for automotive and construction sector. **C. Di Mauro**, A. Mija, A. Graillot, A. Genua, S. Malburet, S. Montes

10:50 PMSE 679. Industrial feather waste valorisation for sustainable keratin-based materials. **R.M. Dinu**, A. Mija

Section H

Rosen Centre Hotel
Salon 13

General Papers-New Concepts in Polymeric Materials

E. Harth, *Organizer*
A. Punia, F. Yang, *Presiding*

8:30 PMSE 680. Surface-engineered biopolyimides nanohybrids with robust ITO nanolayer. **S. Dwivedi**, T. Kaneko

8:50 PMSE 681. Synthesis of novel ethylenediamine grafted graphene oxide for high performance epoxy polymer nanocomposite in structural applications. **A. Pathak**



TECHNICAL PROGRAM

9:10 PMSE 682. Mechanically tough and recoverable hydrogels via dual physical crosslinkings. **F. Yang**, Y. Zhang, B. Ren, T. Wang, Z. Feng, J. Zheng

9:30 PMSE 683. Imidazolium-functionalized Tröger's base-based ionene polymers with extraordinary membrane promises for enhanced CO₂ separation. **I. Kammakam**, J.E. Bara, K.E. OHarra

9:50 Intermission.

10:10 PMSE 684. Electrospun polymeric nanofiber mats based on poly(vinyl alcohol) and poly(vinyl acetate) for drug delivery. **A. Punia**, M. Gelb, S. Sellers, P. Kadakia, J. Ormes, N. Khawaja, J. Wylie, M. Lamm

10:30 PMSE 685. Nanomorphology-dependent mechanical properties: A case study based on aliphatic nanoporous polyurethanes with morphology controlled by the rate of polymerization with anhydrous metal salts from the first row of transition metals. **C. Mandal**, A. Doulah, S. Donthula, C. Sotiriou-Leventis, N. Leventis

Dispersity in Block Copolymers: Synthesis, Characterization, Modeling & the Effects on Self-Assembly

Discrete vs. Broad Block Polymer Dispersity

Sponsored by POLY, Cosponsored by PMSE

Producing Equilibrium Amorphous Packings

Hard Spheres & Jammed Systems

Sponsored by PHYS, Cosponsored by COLL and PMSE‡

Innovative Chemistry & Materials for Electrochemical Energy Storage

General

Sponsored by ENFL, Cosponsored by CATL, INOR and PMSE

Transport in Polymer Membranes

Molecular Transport & Fouling

Sponsored by POLY, Cosponsored by PMSE‡



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

New Frontiers in Aerospace Polymers: Advances & Challenges in Experiments & Simulations

Multiscale Modeling of Aerospace Composite

Sponsored by POLY, Cosponsored by PMSE

THURSDAY AFTERNOON

Dispersity in Block Copolymers: Synthesis, Characterization, Modeling & the Effects on Self-Assembly

Architectural Dispersity in Block Polymers

Sponsored by POLY, Cosponsored by PMSE

Producing Equilibrium Amorphous Packings

Glass Transition in Bulk & in Thin Films

Sponsored by PHYS, Cosponsored by COLL and PMSE

PROF

Division of Professional Relations

R. Libby, *Program Chair*

SUNDAY MORNING

Wolfrom Award

Sponsored by CARB, Cosponsored by CELL, MEDI, ORGN and PROF

Issues Challenging Entrepreneurs & Start-ups

Sponsored by SCHB, Cosponsored by PROF



TECHNICAL PROGRAM

Horton Award

Sponsored by CARB, Cosponsored by CELL, MEDI, ORGN and PROF

New Horizons: Early-Career Researchers in Renewable Materials: Symposium in honor of the Kingfa & PhD Student Prize Winners

Sponsored by CELL, Cosponsored by ANYL and PROF

Contributions of a Simple Chemist: How Professor Ronald Atlee Hites Changed Environmental Chemistry

Sponsored by ENVR, Cosponsored by PROF†

SUNDAY AFTERNOON

Section A

Hilton Orlando
Orange G

Leadership & Inclusive Excellence in STEM: Impact of Teacher-Scholars on Diversity

Cosponsored by PRES
P. K. Dorhout, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 **PROF 1.** Leadership and inclusive excellence in STEM: Impact of teacher-scholars on diversity. **P.K. Dorhout, M. Dennin**

1:55 **PROF 2.** One top-down evidenced-based approach to inclusive excellence in chemistry departments. **R. Hernandez**

2:15 **PROF 3.** Plugging the length of the leaky pipeline: The importance of mentoring and community. **K. Bjorkman**

2:35 **PROF 4.** You belong here: Creating safe spaces for failure. **J.M. Heemstra**

2:55 Panel Discussion.

3:25 Concluding Remarks.

Hudson Award



TECHNICAL PROGRAM

Sponsored by CARB, Cosponsored by CELL, MEDI, ORGN and PROF

Chemical Angel Network

Chemists Investing in Chemical Companies-Invited, Oral

Sponsored by BMGT, Cosponsored by PROF and SCHB†

Starting a Successful Research Program at a PUI

Sponsored by YCC, Cosponsored by PROF

Isabell Award

Sponsored by CARB, Cosponsored by CELL, MEDI, ORGN and PROF

Strengthening Your Patent Rights in Light of Recent Federal Circuit Court Decisions

Sponsored by CHAL, Cosponsored by PROF

Strengthening Your Patent Rights in Light of Recent Federal Circuit Court Decisions

Sponsored by CHAL, Cosponsored by PROF

Gin New Investigator Award

Sponsored by CARB, Cosponsored by CELL, MEDI, ORGN and PROF

New Horizons: Early-Career Researchers in Renewable Materials: Symposium in honor of the Kingfa & PhD Student Prize Winners

Sponsored by CELL, Cosponsored by ANYL and PROF

SUNDAY EVENING



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

CINF Scholarships for Scientific Excellence: Student Poster Competition

Sponsored by CINF, Cosponsored by PROF

MONDAY MORNING

Section A

Hilton Orlando
Orange A

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Cosponsored by AGFD, ANYL, BIOL, BIOT, CARB, CELL, CHED, CMA, COLL, COMP, ENVR, GEOC, I&EC, MEDI, MPPG, NUCL, ORGN, PHYS, PMSE, POLY, PRES, WCC and YCC

M. Morris, T. P. Yoon, *Organizers*

I. M. Blythe, *Presiding*

9:00 Introductory Remarks.

9:05 PROF 5. Blocky bromination of syndiotactic polystyrene via post-polymerization functionalization in the heterogeneous gel state. **K.F. Noble**, R.B. Moore

9:25 PROF 6. Design of ultra-robust supramolecular assemblies for engineering applications. **T. Christoff-Tempesta**, J. Tian, D. Kim, A. Lew, W. Lindemann, J. Ortony

9:45 PROF 7. Elucidating homeomorphic isomerism in macrobicycles of the pnictogen-series. **A. Ehnborn**, J.E. Kuszynski, L. Perez, M.B. Hall, J.A. Gladysz

10:05 Intermission.

10:15 PROF 8. Macroscale model for hands-on activities demonstrating transmission electron microscopy. **N.V. Hudson-Smith**, M. Cahill, N. Klein, M. Krause, C.L. Haynes

10:35 PROF 9. pH-dependent interaction of phosphate and lithium cobalt oxide nanoparticles: Combined spectroscopic and calorimetric study. **E. Laudadio**, P. Ilani-Kashkouli, D. Jones, J.W. Bennett, S.E. Mason, N. Kabengi, R.J. Hamers

10:55 Introductory Remarks.

11:00 PROF 10. Bridging biological inspiration and materials synthesis: Metal-organic framework artificial photosynthetic arrays. A. Chakraborty, W. Maza, **A.J. Morris**

Senior Chemists' Career Stories

Chemistry for New Frontiers



TECHNICAL PROGRAM

Sponsored by SCHB, Cosponsored by PROF, SCC[‡] and YCC

A Decade Later: The Death of Sheri Sangji as a Catalyst for a Change in Safety Culture

Sponsored by CHAS, Cosponsored by CCS and PROF

The Tenure-Track & Beyond: Academic Career Perspectives from Young Chemists

Sponsored by YCC, Cosponsored by CHED and PROF

New Horizons: Early-Career Researchers in Renewable Materials: Symposium in honor of the Kingfa & PhD Student Prize Winners

Sponsored by CELL, Cosponsored by ANYL and PROF

2019 Geochemistry Division Medal Symposium in Honor of Everett Shock

Sponsored by GEOC, Cosponsored by PROF[‡]

Excellence in Graduate Polymer Research

Biobased, Degradable & Chain-Exchange Polymers

Sponsored by POLY, Cosponsored by PRES, PROF[‡], SOCED[‡] and YCC[‡]

MONDAY AFTERNOON

Section A

Hilton Orlando
Orange A

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Cosponsored by AGFD, ANYL, BIOL, BIOT, CARB, CELL, CHED, CMA, COLL, COMP, ENVR, GEOC, I&EC, MEDI, MPPG, NUCL, ORGN, PHYS, PMSE, POLY, PRES, WCC and YCC
M. Morris, T. P. Yoon, *Organizers*
E. Laudadio, *Presiding*



TECHNICAL PROGRAM

1:00 Introductory Remarks.

1:05 **PROF 11.** Supporting diversity in the classroom with open-access chemical assessments. **J.R. Silverman**

1:25 **PROF 12.** Stereoselective synthesis of haemanthamine and related *Amaryllidaceae* alkaloids. **P.D. Parker**, G.A. Edwards, J.G. Pierce

1:45 **PROF 13.** Moving towards greener methods of intermolecular carbonyl-olefin metathesis. **I.M. Blythe**, C. Schindler

2:05 **PROF 14.** Applying automation to chiral resolutions: High-throughput preferential crystallization enabled by new technology. **R. Chung**, J. Hein

2:25 Intermission.

2:40 **PROF 15.** Biosynthesis of the side ring system of nosiheptide. **B. Wang**, J. LaMattina, E. Badding, S.J. Booker

3:00 **PROF 16.** Reactions of reactive electrophiles with mitoNEET. D. Arnett, A. Quillin, **M. Konkle**

3:20 **PROF 17.** Panel discussion: The LGBTQ+ community in chemistry – new frontiers for graduate students and postdoctoral scholars. **M. Morris**, T.P. Yoon

Frank H. Field & Joe L. Franklin Award for Outstanding Achievement in Mass Spectrometry

Sponsored by ANYL, Cosponsored by PROF‡

Kathryn C. Hach Award for Entrepreneurial Success

Sponsored by SCHB, Cosponsored by ANYL, BMGT and PROF

Beyond the Bench: Non-Traditional Careers in Chemistry

Sponsored by CHAL, Cosponsored by BMGT, PROF and YCC

Chemistry in Space: Future Directions

Sponsored by YCC, Cosponsored by AGFD, ANYL, BIOT, BMGT, CHAS, ENVR, FLUO, GEOC, HIST, I&EC, MEDI, POLY and PROF



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

New Horizons: Early-Career Researchers in Renewable Materials: Symposium in honor of the Kingfa & PhD Student Prize Winners

Sponsored by CELL, Cosponsored by ANYL and PROF

ACS Award for Research at an Undergraduate Institution: Symposium in Honor of Carol A. Parish

Sponsored by COMP, Cosponsored by PROF

2019 Geochemistry Division Medal Symposium

Sponsored by GEOC, Cosponsored by PROF

Excellence in Graduate Polymer Research

New Structures & Applications

Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC

MONDAY EVENING

Section A

Orange County Convention Center
West Hall C

Sci-Mix

8:00 - 10:00

18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32. See subsequent listings.

TUESDAY MORNING

ACS Award in Chromatography



TECHNICAL PROGRAM

Sponsored by ANYL, Cosponsored by PROF‡

ACS-CEI Award for Incorporation of Sustainability into Chemistry Education

Sponsored by CHED, Cosponsored by CEI and PROF

Bridging the (Safety) Gap between Academia & Industry

Sponsored by PRES, Cosponsored by CA, CCS, CHAS‡, CHED, PROF and YCC

ACS Award for Computers in Chemical & Pharmaceutical Research in Honor of Arnie Hagler

Sponsored by COMP, Cosponsored by PROF

ACS Award for Encouraging Women into Careers in the Chemical Sciences: Symposium in honor of Ruth Baltus

Sponsored by WCC, Cosponsored by PROF

Patent Insights for Pharmaceutical Companies

Sponsored by CHAL, Cosponsored by PROF

ACS Award for Achievement in Research for the Teaching & Learning of Chemistry

Sponsored by CHED, Cosponsored by PROF

ACS Award for Research at an Undergraduate Institution: Symposium in Honor of Carol A. Parish

Sponsored by COMP, Cosponsored by PROF

Excellence in Graduate Polymer Research



TECHNICAL PROGRAM

Approaches to Polymer Synthesis

Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC

TUESDAY AFTERNOON

Section A

Hilton Orlando
Lake Concord A

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Cosponsored by ENVR, GEOC, I&EC, MEDI, MPPG, NUCL, ORGN, PHYS, PMSE, POLY, WCC and YCC
M. Morris, T. P. Yoon, *Organizers*

3:00 - 5:00

PROF 18. Interaction of tumor homing LyP-1 peptide designed as lipid-polymer hybrid nanoparticle with overexpressed cell surface protein p32 using osteosarcoma tumor model. **R. Marasini**, T.D. Nguyen, S. Rayamajhi, S. Aryal

PROF 19. Correlation of shear response and temporal stability of supramolecular hydrogels as a function of gelation method. **E. Quigley**, B.L. Nilsson

PROF 20. Progress toward the total synthesis of falcatin A. **S.D. Mendoza**, S.E. Reisman

PROF 21. Insights into the complex electronic structure of CeB₆. **J. Mason**, H. Harb, J. Topolski, C. Huizenga, J. Ewigleben, H.P. Hratchian, C. Jarrod

PROF 22. Residue specific characterization of proline-rich motif recognition via infrared spectroscopy. **G. Bukowski**, M.C. Thielges

PROF 23. Oversaturation of the Carolacton scaffold leads to improved inhibition of *Streptococcus mutans* growth during biofilm growth. **A. Scharnow**, A. Solinski, J. Rosenfeld, A. Fraboni, W. Wuest

PROF 24. Development of chemical tools to probe quorum sensing in *Escherichia coli*. **S.A. Early**, M.J. Styles, H.E. Blackwell

PROF 25. Assessing the chemical water quality of Haitian waters: A non-targeted assessment of organic contaminants in the developing world. **J. Ulrich**, N. Madani, T. Sabo-Attwood, L. Ferguson

PROF 26. How spacial distance affects spin coupling of σ -type aromatic polyradicals. **D. Ding**, H.I. Kenttamaa

PROF 27. Interaction of a fluorescent teixobactin analogue with bacteria. **M. Morris**, M. Malek, M. Hashemian, J.S. Nowick

PROF 28. Tannic acid: A novel intumescent agent in epoxy systems. **M. Korey**, J.P. Youngblood, J.A. Howarter

PROF 29. Modeling the formation and fate of halogenated estrogens. **C. Hutchinson**, D.R. Griffith



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

PROF 30. Computational investigation of single nucleotide polymorphisms in human DNA polymerase κ . **E.M. Leddin**, A. Walker, N.M. Antczak, H. Stern, C. Palad, T.A. Coulther, R. Swett, P.J. Beuning, G.A. Cisneros

PROF 31. Family of isostructural actinide complexes with utilization of a redox active ligand for studying periodic trends across the series. **S.S. Galley**, S.C. Bart, T.E. Albrecht-Schmitt

PROF 32. Soluble zwitterionic poly(sulfobetaine) destabilizes proteins. **K.A. Miller**, L. Kisley, C. Davis, D. Guin, E.A. Murphy, M. Gruebele, D.E. Leckband

Improving Academic Safety Culture: Undergraduate & Graduate Student Leadership in Laboratory Safety

Sponsored by CHAS, Cosponsored by CCS and PROF

ACS Award in Analytical Chemistry

Sponsored by ANYL, Cosponsored by PROF

Eli Lilly Travel Awards 30th Anniversary symposium

Sponsored by WCC, Cosponsored by PROF

ACS Award for Computers in Chemical & Pharmaceutical Research in Honor of Arnie Hagler

Sponsored by COMP, Cosponsored by PROF

ACS Awards Lectures

Sponsored by COLL, Cosponsored by PROF

ACS Award for Achievement in Research for the Teaching & Learning of Chemistry

Sponsored by CHED, Cosponsored by PROF

ACS Award for Research at an Undergraduate Institution: Symposium in Honor of Carol A. Parish



TECHNICAL PROGRAM

Sponsored by COMP, Cosponsored by PROF

Excellence in Graduate Polymer Research

Conjugated & Electroactive Polymers

Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC

TUESDAY EVENING

Wiley Computers in Chemistry Outstanding Postdoc Award

Sponsored by COMP, Cosponsored by PROF

WEDNESDAY MORNING

Global Entrepreneurship: Business at the Frontiers of Chemistry

Sponsored by SCHB, Cosponsored by PROF

RUBB

Rubber Division

M.R. Morrow, *Program Chair*

MONDAY EVENING

Revamping Practical Chemistry Teaching for the New Frontier

Sponsored by CHED, Cosponsored by PMSE, POLY and RUBB

SCHB

Division of Small Chemical Businesses



TECHNICAL PROGRAM

J. Sabol, *Program Chair*

SUNDAY MORNING

Section A

Hilton Orlando
Orange A

Issues Challenging Entrepreneurs & Start-ups

Cosponsored by PROF
Financially supported by Saul Ewing Arnstein & Lehr LLP
J. E. Sabol, *Organizer*
P. C. Lauro, *Presiding*

9:30 Introductory Remarks.

9:45 SCHB 1. Board of directors and scientific advisory board: know the needs for your start-up. **J. Skinner**

10:30 SCHB 2. Cyber security: how to protect your information and resources and avoid common mistakes. **R. Scherer**

SUNDAY AFTERNOON

Section A

Hilton Orlando
Orange A

Frontiers in Cyber Security

Cosponsored by CINF
J. E. Sabol, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 SCHB 3. Cyber security horizon: where threats to your information technology are coming from today and tomorrow. **R. Scherer**

1:35 SCHB 4. Secure integration of computing systems into laboratory environments. **G.R. Bishop**, D. O'Gwynn

2:05 SCHB 5. Best practices cyber security. **R. Scherer**

2:35 Intermission.

2:50 SCHB 6. Panel discussion. **R. Scherer, G.R. Bishop, D. O'Gwynn, J.E. Sabol**



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

Chemical Angel Network

Chemists Investing in Chemical Companies-Invited, Oral

Sponsored by BMGT, Cosponsored by PROF and SCHB†

Careers in Chemical Information

Sponsored by CINF, Cosponsored by SCHB

SUNDAY EVENING

Section A

Orange County Convention Center
West Hall C

Chemical Business Poster Session

G. W. Ruger, *Organizer*

6:00 - 8:00

SCHB 7. SCHB is the hub for entrepreneurs in ACS. **P.C. Lauro, G.W. Ruger, A. Kantak, D.J. Deutsch,** M. Chorghade, J.L. Bryant, C.A. Burton, J.E. Sabol, J.L. Maclachlan, J. Crotty, N.A. Vaidya, A. Rahman

SCHB 8. Chemical Angel Network chemical professionals investing in chemistry-based deals. **S.S. White,** M. Vreeke, J.C. Giordan

SCHB 9. Science activities promoted by small businesses can have a big impact. **J.R. Berk, G.W. Ruger**

SCHB 10. Innovation and commercialization in green chemistry. **L. Zarama**

MONDAY MORNING

Section A

Hilton Orlando
Orlando V

Senior Chemists' Career Stories



TECHNICAL PROGRAM

Chemistry for New Frontiers

Cosponsored by PROF, SCC[†] and YCC
E. Meyer, *Organizer*
J. E. Sabol, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 SCHB 11. Sixty-nine years and counting: A very long career. **E. Meyer**

8:25 SCHB 12. It's been a good life: A linear career in academia. **M.Z. Hoffman**

8:45 SCHB 13. African American women chemists in the modern era. **J.E. Brown**

9:05 SCHB 14. Career opportunities with a U.S. National Laboratory. **E.B. Fox**

9:25 SCHB 15. Caring for your brand and your career. **W.F. Carroll**

9:45 SCHB 16. Have a plan, but not in stone. **L.H. Latimer**

Section A

Hilton Orlando
Orlando V

C&EN's Start-Ups to Watch: Entrepreneurs Discuss Chemistry for New Frontiers

Financially supported by C&EN
J. E. Sabol, *Organizer*
M. Bomgardner, *Organizer, Presiding*

10:30 Introductory Remarks.

10:35 SCHB 17. C&EN's start-ups to watch: Entrepreneurs discuss chemistry for new frontiers. **R.J. Hamers, N. Mainolfi, C.T. Liu, O.K. Farha, A.N. Koehler, M. Bomgardner**

MONDAY AFTERNOON

Section A

Hilton Orlando
Orlando V

Kathryn C. Hach Award for Entrepreneurial Success

Cosponsored by ANYL, BMGT and PROF
Financially supported by PID Analyzers, Inc.
J. L. Maclachlan, *Organizer, Presiding*



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

1:00 Introductory Remarks.

1:05 **SCHB 18. Award Address** (Kathryn C. Hach Award for Entrepreneurial Success sponsored by the Kathryn C. Hach Award Fund). Photoionization detector for gas chromatography: From inception and PPB analysis of VOC's to PPT analysis of heavy metals. **J.N. Driscoll, J.L. Maclachlan**

1:45 **SCHB 19.** Growing up the daughter of the father of photoionization: Perspectives on life with a serial entrepreneur. **J.L. Maclachlan**

2:15 **SCHB 20.** Oceanographic applications for photoionization detection. **G.A. Cutter**

2:45 **SCHB 21.** Arthur Obermayer and the billion-dollar SBIR program. **J.N. Driscoll, J.L. Maclachlan**

3:25 Panel Discussion.

4:05 Concluding Remarks.

ACS – A Place to Do Business

Sponsored by BMGT, Cosponsored by SCHB[†]

MONDAY EVENING

Section A

Orange County Convention Center
West Hall C

Sci-Mix

G. W. Ruger, *Organizer*

8:00 - 10:00

8-10. See previous listings.

25, 30, 34. See subsequent listings.

TUESDAY MORNING

Section A

Hilton Orlando
Orlando V



TECHNICAL PROGRAM

Frontiers in Green Chemistry for Small Businesses

Cosponsored by CEI
J. Y. Tanir, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 SCHB 22. Green chemistry: The technology greenhouse. **J.C. Warner**

8:50 SCHB 23. Green chemistry as a business model: it is sustainable. **R.D. Rogers**

9:35 Intermission.

9:55 SCHB 24. From concept through growing a company: A clean-tech story. **R. Gilliam**

10:25 SCHB 25. Mango materials journey towards commercialization of a biodegradable polymer, PHA. **A. Schauer-Gimenez**

10:55 SCHB 26. Experiences of a faculty entrepreneur in the “greener” bioplastic products space. **R. Narayan**

11:25 Panel Discussion.

TUESDAY AFTERNOON

Section A

Hilton Orlando
Orlando V

Frontiers in Green Chemistry for Small Businesses

Cosponsored by CEI
J. Y. Tanir, *Organizer*
G. W. Ruger, *Presiding*

1:00 Introductory Remarks.

1:05 SCHB 27. Lab to market: A difficult journey. **D.J. Constable**, I. Martinez

1:35 SCHB 28. Power of customer discovery and other tips for green chemistry entrepreneurs. **J.Y. Tanir**

2:05 SCHB 29. Regulatory landscape for novel substances. **R. Engler**

2:35 Intermission.

2:55 SCHB 30. Remover products development: Remooble is following the right trends. **B. Engendahl**, T. Fennelly

3:25 SCHB 31. Commercialization opportunities in green chemistry. **L. Zarama**



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

3:55 **SCHB 32.** Mirror, mirror on the wall, we have the best porphyrin of them all. **M. Chorghade**

4:25 **SCHB 33.** Harnessing the economic, nutritive, and commercial potential of food waste employing principles of green-chemistry extraction and functional product development. **F. Madiyar**

WEDNESDAY MORNING

Section A

Hilton Orlando
Lake Mizell A/B

Global Entrepreneurship: Business at the Frontiers of Chemistry

Cosponsored by PROF
M. Chorghade, *Organizer, Presiding*

8:00 Introductory Remarks.

8:10 **SCHB 34.** Small-business initiative on green manufacturing: MCAT-53 for API/API intermediate synthesis in water and global collaborations. **A. Mehta**

8:35 **SCHB 35.** Game changing: The future challenges in process chemistry and technology. **c.j. steele**

9:00 **SCHB 36.** Therapies for global diseases: discovery in chemical biology with worldwide implications. **V. Montanari, K. Kumar**

9:25 **SCHB 37.** Origins, launch, evolution, and growth of Snapdragon Chemistry, Inc. **T.F. Jamison, M.M. Bio**

9:50 Intermission.

10:05 **SCHB 38.** Creating the quantified skin category: An entrepreneur's journey. **R. Mehendale**

10:30 **SCHB 39.** ROAR: The UK's 'Dial-a-Molecule' Grand Challenge Institute. **M. Hii**

10:55 **SCHB 40.** How the funding process works for scientific-based start-up companies. **J. Skinner**

11:20 **SCHB 41.** Fascinating adventures in observational therapeutics: A personal perspective. **M. Chorghade**

11:45 Concluding Remarks.

CCS



TECHNICAL PROGRAM

Committee on Chemical Safety

R. Stuart, *Program Chair*

SUNDAY AFTERNOON

Educating the Educators

Sponsored by CHAS, Cosponsored by CCS

MONDAY MORNING

A Decade Later: The Death of Sheri Sangji as a Catalyst for a Change in Safety Culture

Sponsored by CHAS, Cosponsored by CCS and PROF

MONDAY AFTERNOON

The Chemistry of Disasters

Sponsored by PRES, Cosponsored by CCS and CHAS[†]

TUESDAY MORNING

Bridging the (Safety) Gap between Academia & Industry

Sponsored by PRES, Cosponsored by CA, CCS, CHAS[‡], CHED, PROF and YCC

TUESDAY AFTERNOON

Improving Academic Safety Culture: Undergraduate & Graduate Student Leadership in Laboratory Safety

Sponsored by CHAS, Cosponsored by CCS and PROF



TECHNICAL PROGRAM

Ask Doctor Safety about New Materials, Processes & Products

Sponsored by CHAS, Cosponsored by CCS

CCA

Committee on Community Activities

M. McGinnis, *Program Chair*

WEDNESDAY AFTERNOON

Fundamentals of Chemistry Outreach Education: From Program Design to Assessment

Sponsored by CHED, Cosponsored by CCA, LSAC, SOCED and YCC

CA

Committee on Corporation Associates

D. G. Schmidt, *Program Chair*

TUESDAY MORNING

Bridging the (Safety) Gap between Academia & Industry

Sponsored by PRES, Cosponsored by CA, CCS, CHAS‡, CHED, PROF and YCC

CEI

Committee on Environmental Improvement

C. Middlecamp, *Program Chair*



TECHNICAL PROGRAM

SUNDAY AFTERNOON

Green and Sustainable Chemistry Theory & Practice: Chemistry for New Frontiers

Sponsored by CHED, Cosponsored by CEI

MONDAY MORNING

**Chemistry & Our Common Future: 2019 George C. Pimentel Award Symposium in Honor of Cathy Middlecamp
Symposium in Honor of Cathy Middlecamp**

Sponsored by CHED, Cosponsored by CEI⁺

MONDAY AFTERNOON

UN Sustainable Development Goals: Unique Opportunities for the Chemical Enterprise

Sponsored by CHED, Cosponsored by CEI

Undergraduate Research Posters

Green Chemistry & Sustainability

Sponsored by CHED, Cosponsored by CEI and SOCED

TUESDAY MORNING

ACS-CEI Award for Incorporation of Sustainability into Chemistry Education

Sponsored by CHED, Cosponsored by CEI and PROF

Frontiers in Green Chemistry for Small Businesses



TECHNICAL PROGRAM

Sponsored by SCHB, Cosponsored by CEI

TUESDAY AFTERNOON

Frontiers in Green Chemistry for Small Businesses

Sponsored by SCHB, Cosponsored by CEI

Perspectives on Climate Change Literacy & Education: Local to International

Sponsored by CHED, Cosponsored by CEI

IAC

International Activities Committee

J. Breffke, *Program Chair*

SUNDAY MORNING

International Perspectives on Chemistry Education & Olympiads

Sponsored by CHED, Cosponsored by IAC

LSAC

Committee on Local Section Activities

J. Ritchie, *Program Chair*

WEDNESDAY AFTERNOON



TECHNICAL PROGRAM

Fundamentals of Chemistry Outreach Education: From Program Design to Assessment

Sponsored by CHED, Cosponsored by CCA, LSAC, SOCED and YCC

CMA

Committee on Minority Affairs

J. Sarquis, *Program Chair*

SUNDAY AFTERNOON

Here We Are: Leading & Emerging Black Chemists in Analytical Chemistry

Sponsored by ANYL, Cosponsored by CMA[‡], CTA[‡] and MPPG[‡]

MONDAY MORNING

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Sponsored by PROF, Cosponsored by AGFD, ANYL, BIOL, BIOT, CARB, CELL, CHED, CMA, COLL, COMP, ENVR, GEOC, I&EC, MEDI, MPPG, NUCL, ORGN, PHYS, PMSE, POLY, PRES, WCC and YCC

Therapeutic Developments in Health Disparities

Sponsored by MEDI, Cosponsored by CMA[‡]

MONDAY AFTERNOON

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Sponsored by PROF, Cosponsored by AGFD, ANYL, BIOL, BIOT, CARB, CELL, CHED, CMA, COLL, COMP, ENVR, GEOC, I&EC, MEDI, MPPG, NUCL, ORGN, PHYS, PMSE, POLY, PRES, WCC and YCC



TECHNICAL PROGRAM

COMSCI

Committee on Science

M. Fisher, *Program Chair*

TUESDAY MORNING

Section A

Orange County Convention Center
Room W314B

Exploring the Frontiers of Chemistry through NASA Research

Getting There: Advanced Materials for Space Travel

Cosponsored by ANYL, BIOL, BIOT, CELL, COLL, ENFL, I&EC, INOR, NUCL, PHYS, PMSE and POLY
M. G. Kociolek, R. P. Viggiano, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 COMSCI 1. Role of advanced materials and manufacturing in future NASA exploration missions. **M.A. Meador**

8:35 COMSCI 2. Molecular design and development of polybenzoxazines that protects astronauts from galactic cosmic rays: Low-temperature polymerization and improved shelf-life benzoxazine resin. D. Iguchi, S. Ohashi, G. Abarro, X. Yin, S. Winroth, C. Scott, M. Gleydura, L. Jin, N. Kanagasagar, C. Lo, C. Arza, P. Froimowicz, **H. Ishida**

9:05 COMSCI 3. Progress on high-performance carbon nanotubes materials. **M. Pasquali**

9:35 Intermission.

9:45 COMSCI 4. Ion propulsion for solar system exploration. **M. Patterson**

10:15 COMSCI 5. Carbon-based metal-free electrocatalysis for efficient energy conversion and storage. **L. Dai**

10:45 COMSCI 6. Neutron scattering studies of polyimide aerogels saturated with ionic liquids. S.J. Rinehart, B. Nguyen, R.P. Viggiano, M. Meador, **M.D. Dadmun**

11:15 Discussion.

TUESDAY AFTERNOON

Section A



TECHNICAL PROGRAM

Orange County Convention Center
Room W314B

Exploring the Frontiers of Chemistry through NASA Research

Living There: Science for the Future of Manned Space Exploration

Cosponsored by ANYL, BIOL[‡], BIOT, CELL, COLL, ENFL[‡], I&EC[‡], INOR[‡], NUCL[‡], PHYS[‡], PMSE[‡] and POLY[‡]
M. G. Kociolek, R. P. Viggiano, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 **COMSCI 7.** Role of synthetic biology in NASA's missions. **L. Rothschild**

2:05 **COMSCI 8.** Making biopharmaceuticals on Mars. K. Karuppanan, M. McNulty, D. Antonio, J. Delzio, N.E. Lane, A.M. Dandekar, S. Nandi, **K. McDonald**

2:35 **COMSCI 9.** Biochemical process modeling and optimization for a space biomanufacturing factory. **A.A. Menezes**

3:05 **COMSCI 10.** Synthetic biology: A key technology to enable long-term space exploration. **M.A. Blenner**, M. Spagnuolo, M. Brabender, E. Mabry, M. Bailey

3:35 Intermission.

3:45 **COMSCI 11.** Synthetic biology for microbial production of protein-based materials. **F. Zhang**

4:15 **COMSCI 12.** Metal–organic frameworks to the rescue. **O.K. Farha**

4:45 **COMSCI 13.** Designing metal-organic frameworks for trace CO₂ capture. **C.R. Wade**, C.E. Bien

5:15 Discussion.

WEDNESDAY MORNING

Emerging Frontiers in BIOT

Beyond Earth: BIOT's Role in Space

Sponsored by BIOT, Cosponsored by COMSCI

SCC



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

Senior Chemists Committee

T. Beattie, *Program Chair*

MONDAY MORNING

Senior Chemists' Career Stories

Chemistry for New Frontiers

Sponsored by SCHB, Cosponsored by PROF, SCC⁺ and YCC

SOCED

Society Committee on Education

S. Tremain, *Program Chair*

SUNDAY MORNING

Section A

Orange County Convention Center
Room W314B

Forensic Science: Innovative Applications of Chemistry

S. M. Tremain, *Organizer, Presiding*

9:00 Introductory Remarks.

9:05 SOCED 1. Forensic chemistry: Providing actionable intelligence in criminal investigations. **C. Bridge**, M. Maric

9:35 SOCED 2. Chemical forensics in an international context. **M.E. Sigman**

10:05 Panel Discussion & Q&A.

10:15 Concluding Remarks.



TECHNICAL PROGRAM

MONDAY MORNING

Excellence in Graduate Polymer Research

Biobased, Degradable & Chain-Exchange Polymers

Sponsored by POLY, Cosponsored by PRES, PROF[‡], SOCED[‡] and YCC[‡]

Green Chemistry Student Chapters: Stories of Success

Sponsored by CHED, Cosponsored by SOCED

MONDAY AFTERNOON

Section A

Orange County Convention Center
West Hall F1

Eminent Scientist Lecture with Dr. Teri Odom

S. M. Tremain, *Organizer, Presiding*

2:30 Introductory Remarks.

2:35 SOCED 3. Follow the nano-brick road. **T.W. Odom**

3:35 Q&A.

3:50 Concluding Remarks.

Excellence in Graduate Polymer Research

New Structures & Applications

Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC



TECHNICAL PROGRAM

Undergraduate Research Posters

Agricultural & Food Chemistry

Sponsored by CHED, Cosponsored by AGFD and SOCED

Undergraduate Research Posters

Analytical Chemistry

Sponsored by CHED, Cosponsored by ANYL and SOCED

Undergraduate Research Posters

Biochemistry

Sponsored by CHED, Cosponsored by BIOL and SOCED

Undergraduate Research Posters

Biotechnology

Sponsored by CHED, Cosponsored by BIOT and SOCED

Undergraduate Research Posters

Chemical Education

Sponsored by CHED, Cosponsored by SOCED

Undergraduate Research Posters

Colloid & Surface Chemistry

Sponsored by CHED, Cosponsored by SOCED



TECHNICAL PROGRAM

Undergraduate Research Posters

Computational Chemistry

Sponsored by CHED, Cosponsored by COMP and SOCED

Undergraduate Research Posters

Environmental Chemistry

Sponsored by CHED, Cosponsored by ENVR and SOCED

Undergraduate Research Posters

Geochemistry

Sponsored by CHED, Cosponsored by GEOC and SOCED

Undergraduate Research Posters

Green Chemistry & Sustainability

Sponsored by CHED, Cosponsored by CEI and SOCED

Undergraduate Research Posters

Inorganic Chemistry

Sponsored by CHED, Cosponsored by INOR and SOCED

Undergraduate Research Posters

Medicinal Chemistry

Sponsored by CHED, Cosponsored by MEDI and SOCED



TECHNICAL PROGRAM

CHEMISTRY FOR NEW FRONTIERS

Undergraduate Research Posters

Nanochemistry

Sponsored by CHED, Cosponsored by SOCED

Undergraduate Research Posters

Organic Chemistry

Sponsored by CHED, Cosponsored by SOCED

Undergraduate Research Posters

Physical Chemistry

Sponsored by CHED, Cosponsored by SOCED

Undergraduate Research Posters

Polymer Chemistry

Sponsored by CHED, Cosponsored by PMSE, POLY and SOCED

MONDAY EVENING

Successful Student Chapters

Sponsored by CHED, Cosponsored by SOCED

TUESDAY MORNING

Excellence in Graduate Polymer Research

Approaches to Polymer Synthesis

Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC



TECHNICAL PROGRAM

TUESDAY AFTERNOON

Excellence in Graduate Polymer Research

Conjugated & Electroactive Polymers

Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC

WEDNESDAY AFTERNOON

Fundamentals of Chemistry Outreach Education: From Program Design to Assessment

Sponsored by CHED, Cosponsored by CCA, LSAC, SOCED and YCC

CTA

Committee on Technician Affairs

C. Libby, *Program Chair*

SUNDAY MORNING

Strategies Promoting Success of Two-Year College Students

Sponsored by CHED, Cosponsored by CTA

SUNDAY AFTERNOON

Strategies Promoting Success of Two-Year College Students

Sponsored by CHED, Cosponsored by CTA

Here We Are: Leading & Emerging Black Chemists in Analytical Chemistry

Sponsored by ANYL, Cosponsored by CMA[‡], CTA[‡] and MPPG[‡]



TECHNICAL PROGRAM

SUNDAY EVENING

Analytical Division Poster Session

Sponsored by ANYL, Cosponsored by CTA[†]

TUESDAY EVENING

I&EC General Posters

Sponsored by I&EC, Cosponsored by CTA

WEDNESDAY AFTERNOON

Advances in Spectroscopy

Novel Applications of Fluorescence, Absorption & SEM-EDS Spectroscopy

Sponsored by ANYL, Cosponsored by CTA

THURSDAY MORNING

Advances in Spectroscopy

Novel Applications of Raman Spectroscopy

Sponsored by ANYL, Cosponsored by CTA

Advances in Spectroscopy

Advances in EPR, NMR & Infrared Spectroscopy

Sponsored by ANYL, Cosponsored by CTA

I&EC General Papers



TECHNICAL PROGRAM

Sponsored by I&EC, Cosponsored by CTA

WCC

Women Chemists Committee

R. Cole, *Program Chair*

MONDAY MORNING

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Sponsored by PROF, Cosponsored by AGFD, ANYL, BIOL, BIOT, CARB, CELL, CHED, CMA, COLL, COMP, ENVR, GEOC, I&EC, MEDI, MPPG, NUCL, ORGN, PHYS, PMSE, POLY, PRES, WCC and YCC

MONDAY AFTERNOON

Section A

Orange County Convention Center
Room W330B

WCC Rising Star Award Symposium

M. A. Kane, *Organizer, Presiding*

1:30 Introductory Remarks.

1:40 **WCC 1.** On the importance of studying faculty's instructional practices and mindsets. **M.N. Stains**

2:00 **WCC 2.** Multiphase atmospheric chemistry: Continuum across phase states and career. **A. Carlton**

2:20 **WCC 3.** Impacting the future energy landscape through catalyst design and education. **E. Nikolla**

2:40 **WCC 4.** Science: A universal language. **N.V. Garizi**

3:00 **WCC 5.** Chemistry shaping life, life shaping chemistry. **A. Converso**

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium



TECHNICAL PROGRAM

Sponsored by PROF, Cosponsored by AGFD, ANYL, BIOL, BIOT, CARB, CELL, CHED, CMA, COLL, COMP, ENVR, GEOC, I&EC, MEDI, MPPG, NUCL, ORGN, PHYS, PMSE, POLY, PRES, WCC and YCC

TUESDAY MORNING

Section A

Orange County Convention Center
Room W330B

ACS Award for Encouraging Women into Careers in the Chemical Sciences: Symposium in honor of Ruth Baltus

Cosponsored by PROF
R. Taylor, *Organizer*
E. J. Podlaha-Murphy, *Organizer, Presiding*

9:00 Introductory Remarks by E. Podlaha-Murphy.

9:10 WCC 6. Women in engineering: Personal observations of progress or lack thereof over 50 years. **J.L. Anderson**

9:30 WCC 7. Award Address (ACS Award for Encouraging Women into Careers in the Chemical Sciences sponsored by The Camille and Henry Dreyfus Foundation, Inc.). Are we 'there' yet? **R.E. Baltus**

9:55 WCC 8. What pioneering women engineers tell us: Choices and challenges in context. **L. Ettinger**, N. Conroy, W. Barr

10:15 Intermission.

10:30 WCC 9. Journey to leadership in the federal government. **J. Livengood**

10:50 WCC 10. Millennial perspective: Growing up with female role models. **M. Ball**

11:10 WCC 11. Tipping the gender scale in STEM: The power of mentoring. **L. Napolione**

11:30 Concluding Remarks by **R. Baltus**.

TUESDAY AFTERNOON

Section A

Orange County Convention Center
Room W330B

Eli Lilly Travel Awards 30th Anniversary symposium

Cosponsored by PROF
M. Jeffries-El, *Organizer, Presiding*

1:30 Introductory Remarks.



TECHNICAL PROGRAM

- 1:45 WCC 12.** Silanediols in enantioselective catalysis and complex molecule synthesis. **A.E. Mattson**
- 2:05 WCC 13.** Recombineering: in vivo genetic engineering with bacteriophage recombination functions. **L.C. Thomason**
- 2:25 WCC 14.** Scientific communications at the academic, small business, and international company levels. **J. Olson**
- 2:45 WCC 15.** Combining science, teaching, and design. **A. Joplin**
- 3:05** Intermission.
- 3:20 WCC 16.** There and back again: My journey through academia. **D.E. Williams**
- 3:40 WCC 17.** Making use of the Women Chemists Committee to navigate professorship, parenting, and personal satisfaction as a female chemistry professor. **M. Levine**
- 4:00 WCC 18.** Trans 101: Background on the transgender population and how to create a safe, inclusive and productive environment within both, academia and industry. **J.D. Burnett**
- 4:20** Concluding Remarks.

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Sponsored by PROF, Cosponsored by ENVR, GEOC, I&EC, MEDI, MPPG, NUCL, ORGN, PHYS, PMSE, POLY, WCC and YCC

YCC

Younger Chemists Committee

D. Williams, M. Brann and J. Kelly, *Program Chairs*

SUNDAY MORNING

Extraterrestrial Organic Analysis: Past, Present & Future

Past & Present

Sponsored by ANYL, Cosponsored by YCC[‡]

SUNDAY AFTERNOON



TECHNICAL PROGRAM

Section A

Orange County Convention Center
Room W414D

Starting a Successful Research Program at a PUI

Cosponsored by PROF
M. L. Druelinger, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 YCC 1. What is undergraduate research and why do it at a predominantly undergraduate institution. **A.M. Schoffstall**

1:55 YCC 2. Collaborative research with undergraduates: Research project and research group design. **K.K. Karukstis**

2:15 YCC 3. Taking an entrepreneurial approach to finding small pockets of funding to jump-start your research. **B.L. Gourley**

2:35 YCC 4. Art and necessity of gaining internal support from institutional administrators. **M.L. Druelinger**

2:55 Intermission.

3:05 YCC 5. Undergraduate new investigator grants at the ACS petroleum research fund. **T. Clancy**

3:25 YCC 6. Tips and tricks for maintaining balance between teaching, research, service, and life at primarily undergraduate institutions (PUIs). **B.L. Gourley**

3:45 YCC 7. Funding opportunities at the National Science Foundation of interest to faculty at primarily undergraduate institutions (PUIs). **T. Sammakia**

4:05 YCC 8. Writing competitive research grants. **K.A. Wheeler**

4:25 Concluding Remarks.

MONDAY MORNING

Section A

Orange County Convention Center
Room W414D

The Tenure-Track & Beyond: Academic Career Perspectives from Young Chemists

Cosponsored by CHED and PROF
J. Houck, D. E. Williams, *Organizers, Presiding*



TECHNICAL PROGRAM

8:45 Introductory Remarks.

8:50 YCC 9. Opportunities in the university: Discipline-Based Education Research (DBER). **J. Harshman**

9:10 YCC 10. Career in teaching: Professional insights from a teaching professor. **J. Houck**

9:30 YCC 11. Interdisciplinary science in the academic job market. **L. Zarzar**

9:50 YCC 12. Getting over the tenure activation barrier. **E.E. Rodriguez**

10:10 YCC 13. From bench to boardroom: Making the transition from chemist to academic administrator. **K. Finch**

10:30 Intermission.

10:40 YCC 14. From postdoc to assistant professor: Navigating the academic job market. **D.E. Williams**

11:00 YCC 15. Why did nobody tell me this? Reflections on the journey from Assistant to Associate Professor. **S.K. Zingales**

11:20 YCC 16. The whirlwind journey of the first decade of an academic career at PUIs. **S.A. Toledo**

11:40 Networking.

Senior Chemists' Career Stories

Chemistry for New Frontiers

Sponsored by SCHB, Cosponsored by PROF, SCC[†] and YCC

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Sponsored by PROF, Cosponsored by AGFD, ANYL, BIOL, BIOT, CARB, CELL, CHED, CMA, COLL, COMP, ENVR, GEOC, I&EC, MEDI, MPPG, NUCL, ORGN, PHYS, PMSE, POLY, PRES, WCC and YCC

Extraterrestrial Organic Analysis: Past, Present & Future

Planned & Proposed

Sponsored by ANYL, Cosponsored by YCC[†]



TECHNICAL PROGRAM

Excellence in Graduate Polymer Research

Biobased, Degradable & Chain-Exchange Polymers

Sponsored by POLY, Cosponsored by PRES, PROF[‡], SOCED[‡] and YCC[‡]

MONDAY AFTERNOON

Section A

Orange County Convention Center
Room W414D

Chemistry in Space: Future Directions

Cosponsored by AGFD, ANYL, BIOT, BMGT, CHAS, ENVR, FLUO, GEOC, HIST, I&EC, MEDI, POLY and PROF
R. F. Hirsch, *Organizer*
F. Darvas, A. E. Pavlath, *Organizers, Presiding*

12:30 Introductory Remarks.

12:35 YCC 17. Decentralized pharmaceutical manufacturing. **F. Gupton**

1:00 YCC 18. On-demand reagents. **D.T. Mc Quade**

1:25 YCC 19. Perspectives on continuous-flow capture and conversion of CO₂ in martian space. **D. Kim**

1:50 YCC 20. Polymers and nanomaterials for space manufacturing: Flow chemistry demonstration. **R.C. Advincula**

2:15 YCC 21. Towards compact configurable flow devices for synthesis and crystallisation. **V.S. Sangorin**

2:40 Intermission.

2:55 YCC 22. Harvesting solar energy for pharmaceutical production in outer space using flow chemistry. **T. Noel**

3:20 YCC 23. Hands-on solar spectroscopy for introductory chemistry classes. **J.M. Newman**

3:45 YCC 24. Flow chemistry applications in microgravity: Innovative approaches to chemical synthesis and microreactor systems. **J. Stoudemire**

4:10 YCC 25. Exploring the chemistry of spaceflight with the National Air and Space Museum. **V.L. Miller**

4:35 Concluding Remarks.

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium



TECHNICAL PROGRAM

Sponsored by PROF, Cosponsored by AGFD, ANYL, BIOL, BIOT, CARB, CELL, CHED, CMA, COLL, COMP, ENVR, GEOC, I&EC, MEDI, MPPG, NUCL, ORGN, PHYS, PMSE, POLY, PRES, WCC and YCC

Beyond the Bench: Non-Traditional Careers in Chemistry

Sponsored by CHAL, Cosponsored by BMGT, PROF and YCC

Excellence in Graduate Polymer Research

New Structures & Applications

Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC

TUESDAY MORNING

Bridging the (Safety) Gap between Academia & Industry

Sponsored by PRES, Cosponsored by CA, CCS, CHAS[‡], CHED, PROF and YCC

Excellence in Graduate Polymer Research

Approaches to Polymer Synthesis

Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC

TUESDAY AFTERNOON

Assessing Chemistry Outreach

Sponsored by CINF, Cosponsored by PRES and YCC

Young Investigators in Nuclear & Radiochemistry

Sponsored by NUCL, Cosponsored by YCC



TECHNICAL PROGRAM

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Sponsored by PROF, Cosponsored by ENVR, GEOC, I&EC, MEDI, MPPG, NUCL, ORGN, PHYS, PMSE, POLY, WCC and YCC

Excellence in Graduate Polymer Research

Conjugated & Electroactive Polymers

Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC

WEDNESDAY MORNING

Section A

Orange County Convention Center
Room W414D

Young Chemist: Earth & Space

Cosponsored by PHYS
S. E. Brown, R. C. Fortenberry, N. Hammer, *Organizers*
J. T. Kelly, *Organizer, Presiding*

9:30 Introductory Remarks.

9:35 YCC 26. Probing the effects of environment on novel CCC-NHC-Pt(II) pincer complexes. **S. Autry**, M. Zhang, E. Dornshuld, T. Hollis, C.E. Webster, N. Hammer

10:00 YCC 27. Gas-liquid interface studies by molecular beam scattering on water surfaces. **C. Lee**, I.A. Ramphal, D.M. Neumark

10:25 YCC 28. Bridging theory and experiments of ion hydration with the MB-nrg potential energy functions. **M. Riera Rimbau**, S.E. Brown, D. Zhuang, J.T. Kelly, F. Paesani

10:50 YCC 29. Near-infrared spectroscopy and anharmonic theory of protonated water clusters: Higher elevations in the hydrogen bonding landscape. **D.C. McDonald II**, J. Wagner, A.B. McCoy, M.A. Duncan

11:15 YCC 30. Vibrational spectroscopy and structure of complex atmospheric clusters. **J.J. Kreinbihl**, Y. Yang, C.J. Johnson

11:40 YCC 31. Prediction of a non-valence temporary anion shape resonance for a model (H₂O)₄ system. **A. Kairalapova**, K.D. Jordan, D.N. Maienshein, M.C. Fair, M.F. Falcetta

12:05 YCC 32. Calculation of the peak progression in the vibrational spectrum of HCO₂⁻(H₂O) in the OH stretch region: application of a one-dimensional adiabatic model. **B. Henderson**, K.D. Jordan



TECHNICAL PROGRAM

12:30 Concluding Remarks.

WEDNESDAY AFTERNOON

Section A

Orange County Convention Center
Room W414D

Young Chemist: Earth & Space

Cosponsored by PHYS
R. C. Fortenberry, N. Hammer, J. T. Kelly, *Organizers*
S. E. Brown, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 YCC 33. Interaction of metals and metal oxides with CO₂ in anionic complexes studied by infrared photodissociation spectroscopy. **L.G. Dodson**, M.C. Thompson, J. Weber

1:30 YCC 34. Molecular-level origin of the carboxylate head group response to divalent metal ion complexation at the air-water interface. **J.K. Denton**, P.J. Kelleher, C.J. Mundy, H.C. Allen, K.D. Jordan, M.A. Johnson

1:55 YCC 35. Shedding light on the elusive cyanofomate anion. **T.L. Ellington**, J.T. Kelly, S. Schmahl, T.M. Sexton, K.R. Asmis, G.S. Tschumper

2:20 YCC 36. Revealing the nature of chemical bonding with anion photoelectron spectroscopy. **G. Liu**, S. Ciborowski, C. Martinez-Martinez, X. Zhang, K.H. Bowen

2:45 YCC 37. Quantum chemistry & spectroscopy: Match made in the heavens. **R.C. Fortenberry**

3:10 YCC 38. Semi-empirical anharmonic vibrational calculations of astrochemical species. **J.P. Layfield**, R.C. Fortenberry, T.J. Lee

3:35 YCC 39. Spectral fingerprint of ammonium halide complexes by cryogenic ion trap vibrational spectroscopy. **J.T. Kelly**

4:00 Concluding Remarks.

Fundamentals of Chemistry Outreach Education: From Program Design to Assessment

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