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CIEC

Division of Carbohydrate Chemistry
Advop Company, Limited, China
Alectos Therapeutics

Division of Cellulose and Renewable Materials
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CelluForce Performance Biofilaments Spectra Research Corporation
College of Natural Resources, NC State
CP Kelco
Daniel E. Saloni
Department of Forest Biomaterials, NC State
Dupont Biomaterials
Eastman Chemical Company
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Hasan Jameel
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Division of Chemical Education
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Division of Organic Chemistry
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Division of Polymer Chemistry
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Division of Polymeric Materials Science and Engineering
NSF
TOSOH Bioscience, LLC
Biomaterials Science (RSC journal)
Carbon Nexus
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Polymer Competence Center Leoben
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PPG Industries
The Institute of Molecular Engineering at the University of Chicago

Division of Small Chemical Businesses
C&EN
PID Analyzers, Inc.
Saul Ewing Arnstein & Lehr LLP
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
2:30 PRES 2. Hurricane María: Forging the future of science in Puerto Rico. I. Montes

3:00 Intermission.


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


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


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
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


9:55 Intermission.

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


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


9:45 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
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


Section B

Orange County Convention Center
Room W314A

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


3:00 Awards Presentation.


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
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


9:30 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
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


9:55 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
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.


3:50 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.
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, GECO, I&EC, 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.


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


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


9:50 Intermission.


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
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


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
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 absed 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


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.


4:10 Concluding Remarks.

SUNDAY EVENING

Section A
General Posters

X. Fan, Organizer

5:30 - 7:30


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 aestivalis (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 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 cinnamyl 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 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 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 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 64. Determination of rate constants and activation energies associated with cannabidiol (CBD) formation and decomposition. B. Bailey, B.M. Canfield
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 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 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 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
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. Szwedo, 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. Jarunglumlert, P. Pavasant, A.E. Flood


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 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
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 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


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

10:00 Intermission.
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


11:30 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


9:50 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
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.


3:40 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

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.


3:35 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, GECO, I&EC, MEDI, MPPG, NUCL, OGNN, PHYS, PMSE, POLY, PRES, WCC and YCC

Chemistry in Space: Future Directions

Sponsored by YCC, Cosponsored by AGFD, ANYL, BIOT, BMGT, CHAS, ENVR, FLUO, GECO, 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
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.


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


9:35 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

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


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 enduration 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
1:15 Introductory Remarks.


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.


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. Kortesniemi, B. Yang, J. Zheng


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

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. Irey

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**


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
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


9:45 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
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 trifoliate orange (Poncirus trifoliata) leaf polyphenols. J.A. Manthey, D.G. Hall


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.


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
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


2:45 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


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.
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.


10:30 AGFD 197. Nanotechnology application to remediation of soils and plant nutrition through amphiphile enantiomorph 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


8:45 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.

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**
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


9:55 Intermission.


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


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


9:55 Intermission.


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
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

Sponsored by CELL, Cosponsored by ANYL and BIOL

Bio-Based Materials for Energy Conversion & Storage Applications

Electrodes for Battery Applications

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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
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 (TAMS-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.


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


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


1:30 ANYL 30. Effects of antimicrobials on bacteria membrane permeability probed by second harmonic light scattering. H. Dai
2:00 ANYL 31. SERS monitoring of quorum sensing in bacteria colonies. L. Liz Marzan


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


1:55 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
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**


4:40 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**


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**

4:40 ANYL 56. Bioinspired Copolymers-Cu$^{2+}$ 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
Sponsored by CELL, Cosponsored by ANYL and BIOL

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


ANYL 69. Distribution of the stereoisomers of VX in guinea pig tissues following intravenous exposure. J.M. McGuire, L. Wright, R. Kristovich, M. Busch
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 mineralogy 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 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 82. Co-immunocapture and electrochemical quantitation of total and phosphorylated amyloid-β40 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
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 $\theta_{HnHn+1}$. 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 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 101. Determination and comparison of antioxidant levels in Moringa oleifera leaves and fermented seeds. A.G. Gonzalez, H.M. Morales, A. Mar


ANYL 104. Multi-chamber plasma oxidation apparatus for radiocarbon dating of ancient rock art paintings. A. Arykbayeva, K.L. Steelman


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 115. Development of colorimetric sensor array for discrimination of heavy metal ions. Y. Huang, P. Cheng, C. Tan, Y. Tan


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


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


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
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 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 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. Cerveny, 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

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$_2$Cl$_2$-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 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 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 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 Ti$_3$C$_2$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 $^3$$\text{J}_{HH}$ and torsional angles ($\theta_{n\text{H}n+1}$) 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
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 178. Gold microtubes to electrolessly synthesize manganese dioxide particles. E. Johnson, J. Experton, C.R. Martin


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


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 plasmas - mass spectrometry analysis of dokha, Middle-Eastern tobacco product, to measure nictoine. E. Hondrogiannis, R. Albozek, A. Belunis
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 196. Withdrawn


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 203. Chiral analysis of amino acid distributions in Europa and Enceladus analogues using analyte pre-concentration. **K.M. Seaton, A. Stockton**


ANYL 205. Au nanotube 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 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**


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 illinoinsensis (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 illinoinsensis (pecan), Acer negundo (box alder), Quercus palusris (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 illinoinsensis (pecan), Acer negundo (box alder), Quercus palustric (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 illinoinsensis (pecan), Acer negundo (box alder), Quercus palustris (pin oak), and Populous alba (white poplar). C. McCullum


ANYL 218. Expression, purification, and separation of Notch1 EGF25. K.D. Jenkins, M. Macnaughtan


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 conductiometric 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


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
Sponsored by CELL, Cosponsored by ANYL and CARB

General Posters
Sponsored by CELL, Cosponsored by ANYL and CARB

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.


8:35 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
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


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.


10:40 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
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


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

9:45 Intermission.


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

9:10 Intermission.


10:25 Intermission.


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
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


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 MSN measurements of individual ions with charge detection mass spectrometry. E.R. Williams, C. Harper, A. Elliot

Section B

Hyatt Regency Orlando
Orlando Ballroom N
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


2:30 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.


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


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
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 NOx at different relative humidities. A.C. Morales, T. Jayarathne, J. Slade, A. Laskin, P.B. Shepson


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


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.


1:40 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
2:10 Intermission.


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.


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

Sponsored by SCHB, Cosponsored by ANYL, BMGT 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

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

Sponsored by CELL, Cosponsored by ANYL and PROF
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.
ANYL 289. Distinctive fluorescence of water-soluble flavonol induced by the surface bonding on ZrO$_2$ nanoparticle 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 $^{13}$C-NMR chemical shift and tetrahedral angles. C. Mitan, R.M. Moriarty, P. Filip, E. Bartha, C. Draghici, M.T. Capriu


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. Grinisas

10:10 Intermission.


Section B

Hyatt Regency Orlando
Orlando Ballroom N
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.


10:50 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

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

10:00 Intermission.


10:40 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


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

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

**Sustainable Materials in High Performance Applications**

Sponsored by CELL, Cosponsored by ANYL and COLL

**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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**Planetary & Meteoritic Chemistry**

Sponsored by GEOC, Cosponsored by ANYL and PHYS

**Understanding Cellulose Crystallinity & Non-Crystalline Aggregated States of Cellulose**

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**Failed Brilliance in Nanocellulose Science & Technology**
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
Sponsored by CHED, Cosponsored by ANYL

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
Advances in Ligand-Binding Assays Involving Integral Membrane Proteins

C. Chen, A. Vaish, Organizers, Presiding

1:00 Introductory Remarks.


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.


3:20 ANYL 330. Withdrawn


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
3:00 Intermission.


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


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


1:55 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. Minbiole


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

Lignocellulosic Materials & Multiphase Systems

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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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Planetary & Meteoritic Chemistry

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Failed Brilliance in Nanocellulose Science & Technology

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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.


8:30 ANYL 348. Mechanism of remarkable surface enhanced raman scattering based on graphene-TiO$_2$ 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
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. Sali pro 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


11:20 Panel Discussion.

Section C

Hyatt Regency Orlando
Orlando Ballroom L

Advances in Electrochemistry

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


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


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 tetramethysilane: 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


8:50 ANYL 370. Excited-state CH2Cl2-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


9:40 Intermission.


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


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
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.


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


2:25 Intermission.


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**
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


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.


3:45 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. Forohar

4:45 ANYL 390. Withdrawn

Nanocellulose: From Fundamentals to Function
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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
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 \(^3J_{\text{HH}}\), \(^1\text{H}\) and \(^{13}\text{C}\)-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.


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


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

Nanostructuration of Gels & Aerogels & their Use as Sensors
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Valorization of Renewable Resources & Residuals into New Materials & Multiphase Systems
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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
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. Pfleger, Program Chairs
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


9:50 Intermission.


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

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


9:50 Intermission.


Section B

Rosen Centre Hotel
Grand B

Spotlights on Research Areas

Welcome to 2018 BIOT

J. Neville, B. Pfleger, 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
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


9:30 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


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


8:50 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
9:50 Intermission.


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**


8:50 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


9:50 Intermission.


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


**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**


3:00 BIOT 45. Optimization of a platform hydrophobic interaction chromatography step for robust aggregate removal in flow-through mode. M. Dolan, O. Bhave, 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


Section C

Rosen Centre Hotel
Salon 4

Biomolecular Technologies

Protein Conjugates & Fusions

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


2:40 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

4:20 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


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.


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


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

SUNDAY EVENING

Section B
General Biochemical Technology

BIOT Tank

N. Jacob, A. Kantardjieff, Organizers, Presiding

5:00 Introductory Remarks.

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


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. GSKÕs manufacturing technology roadmap for biopharmaceuticals: learnings and a look ahead. D. Bhanushali

9:10 BIOT 70. Continuous processing of biotech therapeutics Ð 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.
10:10 BIOT 72. Keynote: Smart agricultural systems: Designing plant-microbe communities. C.A. Voigt


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


Section C

Rosen Centre Hotel
Salon 4

Upstream Processes
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. Pfleger


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


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


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


9:50 Intermission.


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. Asoka, 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


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


9:50 Intermission.
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
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


2:40 BIOT 110. Investigating selectivity trends of a bispecific antibody from key impurities on multimodal cation exchange systems. S.S. Parasnavis, 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. Norman, K. Esfandiarfard, 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
2:20 BIOT 117. Modeling and manipulation of microbial communities through the integration of machine learning and evolutionary algorithms. **R. Srivastava**, S. Lincoln, J. Benjamine, J. Graf


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.


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


4:40 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**


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


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**


2:40 BIOT 134. Synthetically facile stable and reversible cell-surface functionalization for cell based therapeutic applications. **J. Majumder, G. Chopra**


3:20 Intermission.


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**

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

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Undergraduate Research Posters

Biotechnology

Sponsored by CHED, Cosponsored by BIOT and SOCED

MONDAY EVENING

Section A

Orange County Convention Center
West Hall C

Sci-Mix

J. Neville, B. Pfleger, Organizers

8:00 - 10:00


TUESDAY MORNING

Section A

Rosen Centre Hotel
Grand A
Spotlights on Research Areas

End-to-End Biomanufacturing

J. Bender, J. C. Love, V. Roy, Organizers
B. Pfieger, 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. Stjerndorff, 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


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


9:50 Intermission.
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


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


9:50 Intermission.


10:50 BIOT 158. Systems approaches for engineering microbial biocatalysts. J. Reed

Section D
Rosen Centre Hotel
Salon 5

Biomolecular Technologies

Therapeutic Protein Discovery

B. Hackel, B. F. Marques, Organizers
J. Jardine, G. J. Rocklin, Presiding


8:50 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


9:50 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


Section E
Rosen Centre Hotel
Salon 6

Biomedical Technologies

New Strategies for the Delivery & Targeting of Therapeutics

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


9:50 Intermission.

10:10 BIOT 172. ‘Antimicrobial peptide’-functionalized catheter for efficacious antimicrobial protection. S.S. Leong


11:10 BIOT 175. Targeted breast cancer imaging and therapy enabled by tumor-targeting peptides. C. Mao

Exploring the Frontiers of Chemistry through NASA Research

Getting There: Advanced Materials for Space Travel

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Polymer Bioconjugates for a Changing World

Sponsored by POLY, Cosponsored by BIOT

TUESDAY AFTERNOON

Section A

Rosen Centre Hotel
Grand A

Spotlights on Research Areas
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

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.


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


2:40 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


4:40 BIOT 193. Expansion of NOTCH$^{\text{high}}$ and CD133$^{\text{high}}$ GSC-enriched niche model using a small scale bioreactor. J. Park, Y. Kim

Section D

Rosen Centre Hotel
Salon 5
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 Sahberg, P. Sjöholm, M. Soulsioti, S. Musunuri, E. Wallby, A. Akerblom, A. Lagerlof, M. Lundgren


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.


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


Section E

Rosen Centre Hotel
Salon 6

Biomolecular Technologies

Engineering & Design

Cosponsored by BIOL³
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


3:00 BIOT 205. Engineering the local environment for enhanced enzyme biocatalysis. I.R. Wheeldon

3:20 Intermission.


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

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Polymer Bioconjugates for a Changing World

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TUESDAY EVENING

Section A

Orange County Convention Center
West Hall E2

Biomedical Technologies

Poster Session

BIOT 211. Structural basis for protein energy landscapes in a de novo designed proteome. G.J. Rocklin, S. Houliston, C. Arrowsmith, M. Guttman, D. Baker


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 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 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
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 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 234. ZIGIRs for the fluorescence imaging of Zn²⁺ in secretory granules. E.H. Ghazvini Zadeh, W. Li


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 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 243. Evaluation of bare and functionalized reduced graphene oxide as a platform for organelle targeting. M. Farell, E. Gomez, M. Kumar

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 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 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
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 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 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 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 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

BIOT 274. Artificial duel-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 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 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
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 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


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 305. Streaming 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 308. Prediction of mass transfer coefficients in linear pH and salt gradient elution. J. Hedrich, C. Frech


BIOT 310. Single use centrifuge, uniFuge, in bioprocessing of mammalian cell. D. Richardson


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 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 D a case study D 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 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 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 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 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 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 343. Improving mAb purification process using a high capacity anion exchange resin coupled with buffer modulation. Q. Zhang, R. Mal, B. Thiyagarajan, N. Deokar


BIOT 345. Effects of substrate morphology on protein binding and elution for responsive hydrophobic interaction chromatography applications. S. Chen, S. Wickramasinghe, X. Qian


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 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 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
BIOT 355. Visualization technique of protein bind and elute processes on a IEX membrane adsorber. A. Ley, D. Stein, J. Hubbuch, V. Thom


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 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, L. Chen, X. He

BIOT 365. Raw material evaluation of a novel chromatography resin. J. Quang


BIOT 367. Accelerated resin lifetime methodology to de-risk resin cycling in commercial processes. Y. Feng


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. Hirotomi

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

BIOT 374. Development of a small-scale freeze thaw methodology using Blast Freezer 4002. A. Alva, A.C. Dumetz, S. Parimal


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 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 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 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 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 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 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 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. Thieves, 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 408 | High-capacity multimodal anion-exchange membranes for purification of biologics. | J. Osuofa, A. Forsyth, J. Zhou, S.M. Husson |
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 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 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

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


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 428. Mapping the ultramorphological changes of SPION-induced cell death in Glioblastoma Multiforme. **M.A. Tovar**


BIOT 430. Withdrawn


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. Rieht

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 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


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 455. 3d printed bioreactors: Enabling rapid process optimization. G.E. Barringer, A. D'Ambruoso, T. Walvoort


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
| BIOT 463 | Debottlenecking manufacturing capacity using high seed density production processes. R. Ottman, Y. Gowtham, S. Mostafa |
| 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 477 | Novel stable isotope approaches to identify flux bottlenecks in photosynthetic microbes. J. Young, Y. Cheah, Y. Xu, C. Johnson |

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 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 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
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. Pfleger


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. Pfleger

BIOT 500. Genetic engineering of *Pseudomonas putida* for the heterologous production of polyketides and nonribosomal peptides. T.B. Cook, B. Pfleger


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. Pfleger

BIOT 504. Microbioreactors for high-cell density CHO perfusion scale-down and personalized T-cell manufacturing. K. Lee, H. Lee


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


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

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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
### 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


### 9:30 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

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


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. Madhavaraao, 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


Section D

Rosen Centre Hotel
Salon 5

Biomolecular Technologies

Engineering Cellular Interactions


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


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

9:30 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


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


2:40 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
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


2:40 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


3:20 Intermission.


4:00 BIOT 564. In-silico aided strategy for efficient and rapid design of integrated purification processes. N. Vecchiarello, S.M. Cramer


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
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.


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

3:20 Intermission.


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 ecoloical driver of microbiome structure and function: microdroplet co-cultivation technology and its applications. X.N. Lin


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


Polymer Bioconjugates for a Changing World

Sponsored by POLY, Cosponsored by BIOT

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


9:30 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


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 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


9:50 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


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-Rodriguez, D.F. Jarosz
8:30 BIOT 608. Functional characterization of 3-hydroxyacyl ACP:CoA transferase for production of medium-chain-length oleochemicals. Q. Yan, B. Pfleger

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. Hebbi, G. Thakur, A.S. Rathore

9:50 Intermission.


11:10 Panel Discussion.

Section E
Rose 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


9:10 BIOT 622. Visualization and modulation of EF-G power stroke in ribosomal translocation. H. Yin, S. Xu, Y. Wang


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. Raeeszadeh Sarmazdeh, B. Sankaran, D. Radisky, E. Radisky


Polymer Bioconjugates for a Changing World

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THURSDAY AFTERNOON
Section A
Rosen Centre Hotel
Grand A

Emerging Frontiers in BIOT

E\text{2}E 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


2:40 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
2:00 BIO 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 BIO 636. Enablers for QbD implementation: Mechanistic modeling of liquid chromatography. A. Tiwari, V. Kumar, L. Kanwar, A.S. Rathore

2:40 BIO 637. Using knowledge for downstream process design. R. Khalaf, A.T. Hanke, L.W. Pampel

3:00 BIO 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.


4:00 BIO 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 BIO 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. Thorn

4:40 BIO 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 BIO 643. Rapid optogenetic inverter circuits for yeast metabolic engineering. E.M. Zhao, J.L. Avalos


2:40 BIO 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 BIO 646. Parallel integration and chromosomal expansion of metabolic pathways. G. Goyal, N. Hillson, T. Lee, H. Garcia Martin

3:20 Intermission.
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


4:20 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


2:40 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


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


11:20 BIOL 6. Chemical approaches for analyzing RNA structure inside cells. R. Spitale

Section B

Orange County Convention Center
Room W240C
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


9:15 BIOL 12. Redefining the protein kinase conformational space with machine learning. R. Rahman, P.M. Ung, A. Schlessinger


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. Miksovska

10:00 BIOL 15. Realization of unnatural codon translation in mammalian cells. A.X. Zhou, F.E. Romesberg


11:30 BIOL 21. Do supramolecular catalysts mimic enzymes? V. Vaissier
Interdisciplinary Chemistry for New Frontiers in Biology and Medicine

NanoBio

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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
1:55 BIOL 24. Conformational motions and electrostatics facilitate proton-coupled electron transfer in BLUF photoreceptor proteins. S. Hammes-Schiffer


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


3:50 BIOL 28. Hole hopping through tryptophan and tyrosine chains in proteins. H.B. Gray


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


2:45 Intermission.

3:00 BIOL 34. Understanding oxygen tolerant [Fe-Fe] hydrogenase. A. Silakov, P.S. Corrigan


4:15 BIOL 37. Atomically precise hybrid nanoparticles with multivalent capabilities. A.M. Spokoyny
Interdisciplinary Chemistry for New Frontiers in Biology and Medicine

Microbia

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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

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-Dheelaan, P. Russo, S. Padden, A. Amaya, Y. You


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 cyclopropenones. **A.J. Ferreira**, S. Nguyen, D. Row, J.A. Prescher


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 55. Examination of neurod4 in retinogenesis. **A. Saunders**, T. Bailey


BIOL 57. Intracellular assembly for enhancing drug efficacy and combating resistance. **C. Yanyan**, S. Wang
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 ?-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 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 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-∆NTD. K.R. Perroz, M. Arnold, I. Garcia

BIOL 73. N-Amino peptide inhibitors of Aβ1-42 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
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 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 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 sclerotialus. Y. Fu, Y. Wang, I. Shin, A.D. Horwitz, A. Liu, K.L. Colabroy
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 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 vermicomposting for domestic wastewater treatment. **X. Ma**, Y. Wang


BIOL 103. Synthesizing building blocks for bioactive lipids: Biocatalytic approach using 5-aminolevulinic acid synthase. **A. Kim**


BIOL 106. Attenuation of G-wire self-assembly using G-quadruplex ligands. **E. Kinfu**, T.C. Marsh


BIOL 108. Development of an assay for antimicrobial susceptibility testing of *Coxiella burnetii*. **M. Khan**, C.N. Miller, M.L. Hale


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

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 thermophillic and mesophillic 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 Ca²⁺ binding: A computational study. Y. Eken, A.K. Wilson

BIOL 125. Neuronal calcium sensor DREAM interactions with insulinitropic agent repaglinide. M.D. Santiago, M.D. Santiago, J. Miksovska

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 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

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 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 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 Aβ42 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 144. Effect of the cell penetrating peptide Pep-1 on vesicles containing lipid rafts. B.M. Almarwani, A. Sunda-Meya, N. Phambu


BIOL 146. Pulmonary fibroblasts influence epithelial cells response to air pollution. N. Aponte, E. Vitucci, N. Mallek, S.D. McCullough


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

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. McDonell, 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 156. ANS binding of Halobacterium salinarum cysteinyl-tRNA synthetase. S. Li, C.M. Evilia


BIOL 158. Withdrawn

BIOL 159. Withdrawn


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

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**
8:45 BIOL 176. Controlling protein folding via de novo design of small molecules. S.R. McAlpine


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


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‡

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
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


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
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
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
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
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


10:15 BIOL 202. Phosphorylation control of homologous recombination. M.S. Smolka


Section B

Orange County Convention Center
Room W240C

Mid-Career Investigators in Biological Chemistry
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
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


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 dinitroindolinyl 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 glycyl 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-phenylglycinyl 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-ethynlypyridine 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
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
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. Enediyne functionalization by a cofactor-promiscuous methyltransferase. A. Adhikari


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


10:15 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


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


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


10:50 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
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
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
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.


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
SUNDAY MORNING

Section A

Orange County Convention Center
Room W221B

Wolfrom Award

Cosponsored by CELL, MEDI, ORGN and PROF
Financed 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.


10:00 Discussion.

Section A

Orange County Convention Center
Room W221B

Horton Award

Cosponsored by CELL, MEDI, ORGN and PROF
Financed 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.
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
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.


4:40 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
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 Cs₂CO₃-mediated anomeric O-alkylation: Mechanistic investigations and syntheses of complex carbohydrate molecules. X. Li, S. Meng, B. Bhetuwal, H.P. Nguyen, J. Zhu


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 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 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 27. Optimizing polysaccharides and cyclodextrin blends for electrospinning: Sustainable biomaterials for active packaging. D. Poudel, S.F. Okeefe, C. Fernandez Fraguas


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 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 40. Synthesis and Testing of dipicoloylated thiosialosides. C. Dean, B. Jones, M. Shadrick, C. De Meo

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 44. Comparison of fructose-1,6-bisphosphate (fbp) aldolase inhibitors by structure and Ki 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.


9:35 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
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.


9:55 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
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


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
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 isomorphic, 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.


5:00 Discussion.

5:05 CARB 69. DNA-based precision glycocalyx engineering. S. Purcell, N. Marroquin, T. MacCulloch, N. Stephanopoulos, K. Godula

5:20 Discussion.

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium
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


9:30 CARB 72. Fast and high-throughput detection of glycan-binding proteins. P.G. Wang

9:55 Intermission.

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
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.


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
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


4:50 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 GPls. 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
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


2:25 CARB 106. Lectin microarrays for intact cell analysis. S. TAO


3:15 Intermission.


Bioactive Delivery: Frontiers in Biomaterials
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


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

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.


8:50 CATL 11. Mechanochemical routes for the synthesis of Schiff base ligands and coordination compounds relevant to catalysis. T. Jurca


9:30 Intermission.


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


11:30 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

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


10:00 Intermission.


10:45 CATL 23. Imaging and chemical probing of the catalytic NOₓ and O₂ reduction over Pt and Rh with sub-nanoscale lateral resolution. N. Kruse


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


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

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


9:40 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


Section F

Orange County Convention Center
Room W310A

Computational Electrocatalysts
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-Melchôr

8:20 CATL 43. Computational rational design of high-performance water oxidation electrocatalysts. M. Garcia-Melchôr, 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


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
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. Mendelev, 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 fivetwinned 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 Ive Hermans
1:00 CATL 61. Getting the most from molecular oxygen: Low overpotential $\text{O}_2$ 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**


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. Mechnochemical synthesis of supported nanoparticles on poreous 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. Prodingher**, R.F. Lobo

2:00 CATL 71. Understanding mechanocatalytic reaction pathways: Surface chemistry at the solid-solid interface. **W.T. Tysoe**

2:40 Intermission.
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


2:00 CATL 78. Activation of H-H and C-H bonds on oxide supported single Pd atoms. Z. Dohnalek


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 NOx 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


4:55 CATL 84. Catalysis for energy and the environment: A research career (so far). C.H. Peden
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


3:15 CATL 89. Addressing uncertainty in machine learning model predictions for inorganic complex discovery. J. Janet, A. Nandy, C. Duan, H.J. Kulik


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

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
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


4:20 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


2:50 Intermission.
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 CO$_2$ 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 RuO$_2$. 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 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
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


9:00 CATL 125. Supported bimetallic noble metal catalysts prepared by use of bifunctional organic chelates. S. Soled, S. Miseo, C.E. Kliwer, M.P. Lanci, J. Guzman

9:30 CATL 126. Elucidating structure-performance relationships in zeolite catalysis. J.D. Rimer

10:00 Intermission .


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.


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


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
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


9:45 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

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.


8:55 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 heterogeneous metal catalysis. M.S. Wong, Y. Yin, S. Guo, K.N. Heck, C.A. Clark, C.L. Coonrod

9:45 Intermission.


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. Sundararaman, 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. Martirez, C. Krauter, J.A. Gauthier, E.A. Carter, A.C. Luntz, K. Chan, J.K. Norskov
Unofficial Technical Program draft as of 2/19/2019

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. Ruzsinzsky

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


10:10 Intermission.

10:20 CATL 174. Plasma-enhanced catalysis for ammonia production. J. Hong, S. Prawer, A.B. Murphy
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 CATL² 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
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
Sponsored by ENFL, Cosponsored by CATL and I&EC

MONDAY AFTERNOON

Section A
Orange County Convention Center
Room W306A
Ipatieff Prize: Symposium in Honor of Ive 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


2:00 CATL 180. Oxidative methane activation over Cu-containing zeolites. R.F. Lobo


3:00 Intermission.

3:10 CATL 182. Role of heterogeneous catalysis in biomass conversion. B. Sels


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.

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


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


3:45 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
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.


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


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


1:55 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
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 Electro catalysis

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


4:10 Concluding Remarks.

Section G

Orange County Convention Center
Room W310B

Recent Advances in Plasma-Enhanced Catalysis

1:30 CATL 222. Coupling of heterogeneous catalysts with non-thermal plasma for CO\textsubscript{2} methanation: probing the reaction mechanisms using \textit{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 CO\textsubscript{2} into value-added fuels and chemicals. X. Tu

2:20 CATL 224. Plasma catalysis for methane dissociation: Investigation of optimal reaction conditions for C\textsubscript{2}H\textsubscript{x} formation. Y. Engelmann, P. Mehta, E.C. Neyts, W.F. Schneider, A. Bogaerts

2:40 CATL 225. Energy-efficient CO\textsubscript{2} conversion with renewable electricity storage by plasma catalysis. J. Liu

3:10 Intermission.


4:05 CATL 228. Cold plasma catalysis for SO\textsubscript{2} reduction with CH\textsubscript{4} over metal sulfide catalysts. M. AlQahtani, S. Knecht, X. Wang, S. Bilén, C. Song


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

Supercapacitors

Sponsored by ENFL, Cosponsored by CATL, INOR and PMSE

Carbon Dioxide Conversion & Utilization

CO\textsubscript{2} as an Oxidant
Celebrating 50 Years of ExxonMobil's Corporate Strategic Research Laboratories: A View Forward from a Retrospective

Sponsored by ENFL, Cosponsored by CATL and I&EC

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
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 SO\textsubscript{2} 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.


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 WO\textsubscript{3} 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
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. Kenvin, 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


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


8:55 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


10:45 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
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


9:35 Intermission.

9:50 CATL 259. Time resolved in operando optical spectroscopy of (photo)electrochemical water oxidation. J.R. Durrant


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
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)arylmethals. 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.


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
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 specied during deoxydehydration. B.E. Sharkey, F. Jentoft

9:45 Intermission.


10:25 CATL 280. TiO_2 morphology effect in Au-TiO_2 catalysis. W. Huang


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
Carbon Dioxide Conversion & Utilization

Electrocatalysis

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Carbon Dioxide Conversion & Utilization

Electrocatalysis

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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 TiO\textsubscript{2} supported catalysts in the vapor phase. L. Herrera, A. Gomez, T. Pham, L. Barrett, D. Jones, N. Briggs, B. Wang, S. Crossley


2:20 Intermission.

2:40 CATL 287. Molecular mechanism of ethanol steam reforming on bifunctional nickel-cerium oxide catalysts. L. Baker, Y. Mueangern

3:00 CATL 288. Intermetallic nanoparticles with atomic precision for selective catalytic transformations. W. Huang, Y. Pei
3:20 CATL 289. First principles microkinetic analysis on water-gas shift reaction over Rh/ZrO$_2$. 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


4:40 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. H$_2$O$_2$ formation in alcohol-assisted catalytic oxidation of water. J. Ye, J. Dombrowski, R. Han, A. Prokofjevs, M. Kung, H. Kung


2:35 Intermission.

2:55 CATL 297. In search of an efficient approach to condensed phase catalyst design. L.T. Roling


Section C

Orange County Convention Center
Room W309A
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


2:50 CATL 304. New routes to engineer the physicochemical properties of zeolite catalysts. J.D. Rimer


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
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 CO$_2$ 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.


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
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


1:30 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


Section G

Orange County Convention Center
Room W310B

Catalytic Chemistry over Metal Oxides

Titania Catalysis

S. D. Senanayake, Organizer
1:00 Introductory Remarks.

1:05 CATL 333. Structure, polarization and sum frequency generation spectrum of the anatase TiO$_2$-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


2:45 Intermission.


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


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
General Catalysis

A. Savara, Organizer

7:00 - 9:00


CATL 342. Photoreduction of carbon dioxide by biomimetic polyimide-supported cuprous oxide/graphitic carbon nitride photocatalytic films. I. Tseng, Y. Chen, P. Chang


CATL 344. Photocatalytic production of $\text{H}_2\text{O}_2$ through selective two-electron reduction of $\text{O}_2$. W. Choi, G. Moon, P. Zhang, S. Kim

CATL 345. Tunable doping of chromium Cr$^{3+}$ in TiO$_2$ nanocrystals via ion diffusion. R. Hossain, J.D. Hoefelmeyer


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 350. Synthesis and catalytic performance of a dual-sites Fe-Zn catalyst based on ordered mesoporous Al$_2$O$_3$ for isobutane dehydrogenation. M. 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 MnWO$_4$ for selective oxidation of toluene to benzaldehyde. D. Mal, D. Pradhan


CATL 356. Specific metal–support interactions of layered nanoparticle catalysts in catalytic methanol oxidation. S. Yoon, K. An


CATL 359. Effective structural descriptor to quantify the reactivity of lattice oxygen in CeO2 subnanoclusters. C. Zhou, H.F. Wang, P. Hu


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
CATL 373. CO\(_2\) reduction on defect rich 2D-TaS\(_2\) 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 376. Withdrawn


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 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 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 gC\(_3\)N\(_4\) 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


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 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 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 408. Catalytic conversion of carbon dioxide via hydrogenation to light olefins over Fe2O3 supported Cu-CO catalysts. D. Triger, C. Zhang
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 414. Intermittent plasma-assisted selective catalytic reduction of NOx 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.


9:55 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. Waegle

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


9:50 Intermission.

10:00 CATL 425. Oxidative coupling of light alkanes using isobutane as oxygen carrier: Alkane structure reactivity relationship. K. Wang, J.E. Mitchell


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


11:40 CATL 430. Light alkanes activation using ALD modified catalysts. Z. Gan, Y. Lei

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
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

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


10:55 CATL 445. Exciton dynamics and photoreduction of water in 1D and 2D semiconductor/metal nanoheterostructures. T. Lian


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


8:40 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


9:20 Intermission.

9:50 CATL 452. Insights into the electrochemical conversion of biomass derivatives to fuels and chemicals. A. Román, Z. Barton, A. Holewinski
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


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\textsubscript{2-x}(111). C. Zhao, C. Watt, P. Kent, S.H. Overbury, D.R. Mullins, F.C. Calaza, Y. Xu, A. Savara


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
11:20 CATL 466. Grain-boundary-supported active sites in heterogeneous electrocatalysis. X. Feng


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\textsuperscript{1} and Ru\textsuperscript{1}) on catalyst surface for reforming CH\textsubscript{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 IrO\textsubscript{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


Innovative Chemistry & Materials for Electrochemical Energy Storage
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
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


4:40 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


4:20 CATL 495. Implications of electron scavenging character of sulfated titania for photochemistry. A. Mahdavi-Shakib, A. Rahman-Chokanlu, T.J. Schwartz, R.N. Austin, B.G. Frederick


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


1:55 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**


3:55 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*
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


3:30 Intermission.


4:10 CATL 514. Dynamic catalytic interfaces: statistical ensembles of multiple metastable states dictate the properties. A. Alexandrova


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


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.
2:50 CATL 520. Metal encapsulation in zeolites: An approach for stable catalysts. J. Guzman


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


2:25 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


3:55 CATL 531. Identifying the active structures of metal nanoparticles supported on CeO₂ for CO oxidation. J. Liu, M. Yang, E. Hensen, B.R. Goldsmith

4:35 CATL 533. Controlling the concentration of oxygen vacancies in CeO$_2$-ZrO$_2$ 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 NaBH$_4$ 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.


10:20 CATL 539. Synthesis and catalytic properties of Graphene based mesoporous silica (SBA-15) doped titania nanocomposites(Graphene/SBA15/TiO$_2$). 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
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


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
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/\(\text{CeO}_2\) catalysts. Y. Li, M. Kottwitz, R.G. Nuzzo, A. Frenkel

9:00 CATL 555. Catalytic oxidation of 2-propanol on SnO\(_2\)(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 \textit{in situ} environmental and liquid STEM. M. Chi

9:50 Intermission.

10:00 CATL 557. \textit{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


10:50 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 TaS\(_2\)/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 \(\text{CO}_2\) 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

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 form biomass derived small oxygenates conversion. K.K. Ramasamy, A. Devaraj


10:30 CATL 568. Hydrodeoxygenation of biomass-derived intermediates to paraffins for blending into jet or diesel fuels. D.K. Johnson


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


8:40 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.


10:00 CATL 575. Solvation effects on deoxygenation reactions over bimetallic phosphide catalysts. V. Jain, N. Rai


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


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


10:10 CATL 584. Design principles for dihydrophenazine-mediated photoredox applications. **J. Cole**


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**
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


2:00 CATL 591. Mn-promoted cobalt catalysts for light olefin production. E.Ø. Pedersen, I. Svenum, E.A. Blekkan


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
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


2:30 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


3:30 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


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
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.


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. Prodinger, 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
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


4:40 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


1:40 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


2:40 Intermission.
2:50 CATL 632. Computational study of the selective hydrogenation of alkynes to alkenes on 2D materials. E. Mates-Torres, M. Garcia-Melchor


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 C$_6$-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


2:40 Intermission.

3:00 CATL 643. NO + 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
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


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. Martín García, 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

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
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


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

11:40 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. Gonâalves, E. Lizundia, M.M. Silva, C. Costa, S. Lanceros-Mendez

8:30 CELL 19. Cellulose-inspired solid electrolytes membranes. K. Fu


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

10:50 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


9:45 Intermission.

10:00 CELL 30. New eco-friendly high-performance cellulosic fibers for the textile and packaging industries. M. Alam, L. Christopher


10:50 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
Interplay of Cellulose & Other Biopolymers in Biological & Designed Materials Systems

Interactions of Plant Polymers in Model Systems

Cosponsorred 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


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


11:15 CELL 41. Interactions between the building blocks of plant cell walls. M.S. Skaf

11:40 Concluding remarks.

Wolf from Award

Sponsored by CARB, Cosponsored by CELL, MEDI, ORGN and PROF

Horton Award
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

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.


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. Nystrom, 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


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


4:30 CELL 57. Bio-inspired Photonics: from nature to applications. S. Vignolini

5:15 Concluding remarks.
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


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
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.


1:45 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


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
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-Guerente, 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


3:00 Intermission.


4:05 CELL 80. Investigation of the structure and dynamics of plant cell wall polysaccharides at acidic pH by solid-state NMR. M. Hong


4:55 Concluding remarks.

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

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 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 sono-enzymatically generated bioadhesive. J. Hoyo, T. Tzanov


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
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 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 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 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 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 117. Using zinc salts from spent alkaline batteries to produce activated carbon from rice husk. J. Leiton


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

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 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 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 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
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 bifurcral. 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 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 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 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 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

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 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 168. Obtaining pure spectra of hemicellulose and cellulose from poplar cell wall Raman imaging data. X. Zhang, F. Xu


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 175. Xyloglucan and cellulose nanocrystals biomimetic aerogels produced by freeze-casting. Z. Jaafar, B. Quelennec, 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 Fique 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
CELL 179. Withdrawn


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 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 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 Desertiillum sp.. S. Meléndez-Antonio, I. Hernández-Martinez, 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 193. Withdrawn


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
CELL 197. Withdrawn


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 201. Two-dimensional antifouling fluidic channels on cellulose nanopaper. K.A. Solin, H. Orelma, M. Borghei, M. Vuoriluoto, R. Koivunen, 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 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 210. Xylan-lignin hydrogels. G. Toriz, A. Escalante, P. Gatenholm


CELL 212. Towards interfacial applications of soybean hull pectins. V. French, C.E. Frazier


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
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


9:45 Intermission.

10:00 CELL 220. Diol reactivity in polysaccharides. E. Bedini


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


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


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 sidetreams. M.S. Peresin, S. Sanchez Diaz, A. Restrepo Osorio, C. Alvarez Lopez, M.C. Arango, T.J. Elder


11:15 CELL 232. Fungal chitosan-glucan in water remediation applications. A. Mautner, J. Janesch, A. Bismarck

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, T. Larsson, Organizers
A. D. French, S. H. Kim, Organizers, Presiding

8:00 Introductory Remarks.


8:30 CELL 234. Crystallinity: Why is cellulose different from other polymers and what are we measuring? W.T. Winter


9:20 CELL 236. Determining cellulose I crystallinity by CP/MAS $^{13}$C-NMR. T. Larsson

9:45 Intermission.

10:00 CELL 237. The pseudo-crystallinity of native cellulosics. 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
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


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
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


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


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
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
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. Renneckar, M. Karaaslan, M. Cho, L. Liu, L. Ji


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


3:50 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
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


3:00 CELL 267. Cellulose nanofibrils as building blocks for advanced structures and applications. F. Jiang


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.


1:45 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

3:00 CELL 273. Dissolution of unbleached wood pulp from low temperature (≤ 90 °C) acid hydrotropic fractionation in an ionic liquid. J. Zhu, H. Wang, C. Liu


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
Hemp Processing: From Weed to Values

Cosponsored by AGRO and ANYL
Financially supported by EPNOE
S. H. Renneckar, Organizer
N. Sathitsuksanoh, Organizer, Presiding

1:15 Introductory remarks.


1:45 CELL 283. Medical cannabis products and Cannabinoids: Medicinal value through chemistry. L.P. Kotra

2:10 CELL 284. Withdrawn


3:50 CELL 288. One-pot acid-catalyzed 5-hydroxymethylfurfural production from industrial hemp: from controversies to commodity chemicals. N. Sathitsuksanoh, S. Tulaphol, N. Grisdanurak, L. Liu, S. Renneckar, 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
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
L. Bergstrom, Presiding

8:00 Introductory remarks.


8:30 CELL 290. Microstructure and properties of polysaccharide based cryogels. D. Petri


9:45 Intermission.

10:00 CELL 293. Hierarchical films from cellulose. T. Nypelo, M. Liebi, R. Kádár, R. Bordes


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
8:55 CELL 299. Magnetic and electric field alignment of cellulose nanocrystal suspensions. A. Fouques, B. Frka-Petesic, S. Vignolini, L. Heux


9:45 Introductory remarks.

10:00 CELL 301. Functional materials from cellulose: colours, magnetism and charge storage. S.J. Eichhorn


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.
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


10:50 CELL 311. Correlating structure-properties of TEMPO-treated cellulose nanofibers. G. Salazar-Alvarez, S. Kumar, V. Guccini


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


9:45 Intermission.

10:00 CELL 317. Where does surface stabilisation end and bulk modification begin? T. Koso, E. Kontturi, A. King

10:25 CELL 318. Filed surface coating for PET with bamboo-ACC nanocellulose to allow to find a suitable container for the resin-adsorbable nanocellulose. T. Kondo, G. Ishikawa


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. Pfrengle


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


10:50 CELL 327. Engineered polysaccharides: Control of morphology & colloidal structure and applications in wood adhesives. C. Lenges, M. Harvey, N. Behabtu


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
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
S. S. Kelley, Organizer, Presiding

1:15 Introductory remarks.


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
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.


1:45 CELL 337. Metal chloride deep eutectic solvents for biomass fractionation: Experimental and computational approach. L. Das, A. Ladera, A. George, B. Simmons, J. Gladden


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


3:50 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  
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


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
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.


1:45 CELL 355. Extraction and modification of hemicellulose to produce high value super absorbent gels. **R.A. Venditti**, W. Geng, J. Pawlak, H. Chang


3:00 CELL 358. Enzymatic polymerization: Engineered polySaccharides and unique properties in coating systems. C. Lenges, N. Behabtu, M. Harvey, **K. Kim**


3:50 Concluding remarks.
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


9:45 Intermission.

10:00 CELL 364. One-component nanocomposites based on polymer-decorated cellulose nanocrystals. S. Wohlhauser, J.O. Zoppe, C. Weder


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


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. Benselfelt, 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


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


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


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


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
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


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
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.
1:20 CELL 408. Withdrawn


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.


3:40 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


4:55 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


Unofficial Technical Program draft as of 2/19/2019

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


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.


Unofficial Technical Program draft as of 2/19/2019
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. Filipponen, T. Nypelo, J. O. Zoppe, Organizers
M. Ek, S. Spirk, Organizers, Presiding

1:15 Introductory Remarks.


3:00 Intermission.


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


4:55 Concluding remarks.
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. Gestranius, 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. Borghei, A. Tripathi, L. Garcia Greca, O. Rojas


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. Magdasi, O. Shoseyov


10:50 CELL 446. Orientation and alignment of cellulose nanofibrils in shear and extensional flows. K. Vijayakumar, D. Söderberg, F. Lundell


11:40 Concluding remarks.
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. Hausmman, 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


9:45 Intermission.

10:00 CELL 452. Conductive 3D printed structures based on nanocellulose for electro-responsiveness and controlled drug release. R. Ajdary, N. Zanjaniadeh 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


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
8:00 Introductory Remarks.


8:30 CELL 457. Ultra-light and flexible nanochitin aerogel prepared from ice templating. L. Liu, L. Bai, Y. Fan, O. Rojas


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
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


9:45 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


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.


8:30 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


9:20 CELL 475. FLIPPR²: Future lignin and pulp processing research in Austria. T. Timmel
9:45 Intermission.

10:00 CELL 476. Marine pollution: Exposing some of the myths and facts. M. Kogler, S. Rahbaran, K. Schuster, S. Kulka


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-Al³⁺ composite for effective removal of fluoride from water. S. Sharma, P.R. Sharma, K.I. Johnson, B.S. Hsiao


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

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


3:00 Intermission.


3:40 CELL 493. Evaluating the processing of keratin-based copolymer systems into 4D responsive materials. M. Plowman Holmes, S. Scott, W.J. Grigsby


4:30 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.


1:45 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.


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
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. Filipponen, 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.


3:40 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. Filipponen, 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
2:10 CELL 514. Is it possible for lignin molecules to become oriented during processing? M. Cho, F.K. Ko, S. Renneckar


3:00 Intermission.


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. Kostiainen, 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 Registatation.

8:30 Introductory Remarks.
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


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

10:45 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


9:35 Intermission.


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.
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.


10:00 CHED 23. Using short videos to regularly review common misconceptions: A change inspired by the cCWCS Active Learning in Organic Chemistry. **R. DeCicco**


11:00 CHED 26. Hybrid learning in large and small organic chemistry lectures. **C.G. McDaniel**

11:20 Intermission.


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.

8:55 CHED 31. Comparison of course modalities for a fundamental chemistry course using novel multimedia instruction. **N. Lapeyrouse, C. Yestrebsky**


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**
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.


10:30 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.
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. Cabreros, G. Muller


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


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


10:45 Intermission.
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 TiO$_2$-graphene oxide inverse opal substrates. L.E. Perez, E.J. Atkinson

11:15 CHED 65. Withdrawn


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
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
3:10 CHED 81.  $^1$H NMR investigation of acid-catalyzed enolization of acetophenones. N.M. Wachter, H. Tarbox


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


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
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

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


2:55 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. Ruhlantd-Senge

3:45 CHED 104. Chemical principles in public policy, and vice versa. J.D. Soper

4:05 Intermission.


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.


2:40 Intermission.


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.


1:45 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


2:05 CHED 116. Force generation and encapsulation of fluorophores in swellable organically modified silica. R. Reffner, P.A. Bonvallet, R. Silvestri


2:25 Intermission.


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

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. Balija


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 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. Fahlman
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 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 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
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 156. Investigative comparison between drinking water quality and socioeconomic status in Los Angeles County. **H. Hakopian, M. Hasan, V.I. Jaramillo**


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 164. Teaching mathematical methodology in general chemistry. **P.K. Yuen, C. Lau, A. Yuen**


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**
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 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 175. Using an assessment design and critique activity to investigate secondary chemistry teachers’ assessment beliefs and practices. A.G. Schafer, E.J. Yezierski

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 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
CHED 186. Students’ responses to making mistakes in the undergraduate chemistry teaching laboratory. S. Fullington


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


9:35 Intermission.

9:45 CHED 197. Introducing undergraduate students to environmental chemistry and sustainability: From turrets to sheep to Baraboo. N.J. Pienta

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


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


11:10 Intermission.

11:25 Panel Discussion.
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


10:45 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


9:35 Intermission.


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


11:05 CHED 221. How does active learning classroom affect STEM faculties in tertiary STEM Classes? S. Gao, J. Harshman


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


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
9:55 Intermission.


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. Yarberry

9:10 CHED 233. Transforming lives through green chemistry. S.M. Pérez Lajara, D.I. Oyola Soto, L.I. Santiago


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

10:10 Intermission.


10:30 CHED 239. Getting crafty: Artistic applications of green chemistry. M. Youmans, M. Pavlac, N. Fitzpatrick, D. Defazio, H. Arcure, A. Black


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


11:30 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

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**


10:40 Intermission.


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.


8:45 CHED 256. Qualitative and quantitative elemental analyses of total gunshot residue with TXRF. **N.C. Homburger**, M. Oliva, J. Berger, L. Huang


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**


9:25 Intermission.

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


10:05 CHED 263. Applications of naturally-sourced waste ingredients in cosmetics. K. Westergaard, K. Gilcrease, T. Filipova


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


11:35 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
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


3:45 Concluding Remarks.

Section B

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
1:55 CHED 278. OMIS: The Open Millifluidic Inquiry System for small scale chemical synthesis and analysis. R.J. Lesuer


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.


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.


1:55 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. Sevian


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
1:30 Introductory Remarks.


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.


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.


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
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**
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


1:55 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


2:25 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


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


4:05 CHED 330. Development of lectin-based biosensors for the detection of flaviviruses. N. Mercer, K.T. Hamorsky
4:15 CHED 331. Utilization of maltotetraose during a nine generation serial repitching experiment. **A.D. Smith**, W. Deutschman


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 335. Response of *Megacopta cribraria* to insect exposed soybeans plants in a Y-track olfactometer. **R. Ortiz**


CHED 337. Effect of ozone on barley malt quality. **S.L. Miller**, D.J. Oostendorp, A. MacLeod, K. Miller


CHED 339. Novel compounds extracted from endophytes isolated from *Populus nigra*. **J.M. Taylor**, M.D. Halling


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
CHED 344. Investigation into the potentially devastating diastatic activity of the hop. L. Benedict, N. Mesloh, M. Ackerman, Z. Bodah


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. Wieczorkowski, 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. Jordan, 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
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 makeup 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 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 373. Electrodeposition of Cu$_2$O from O$_2$ saturated deposition solution as an attempt for enhancement of Cu$_2$O 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 *Ilicium c.f. ekmanii* Smith from the Dominican Republic using HD, SPME, and GC-MS. K. Soun, M. Bida, A. Guerrero, T.E. Pagano
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 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 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 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
CHED 394. Analysis of sucrose, glucose, and fructose present in maple sap and syrup. M. Meyers, C. Chant


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 luminescers by explosives. D.R. Ogburn, K.D. Sienert

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 408. Cytochrome c adsorbed to peptide SAM modified evaporated gold electrodes. T. Yawitz, K. Patterson, B. Onkst, R.A. Clark


CHED 411. Development of a quality control lab for a microbrewery. G. LeBlanc, M. Symcox, K.D. Symcox

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. Surovic

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 428. Nutraceutical properties of several commercial herbal tea samples. V. Carranza, E.E. Mojica


CHED 431. Blood alcohol testing using SPME and head-space gas chromatography. T. Rinehart, R. Montgomery

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 435. Preparation and characterization of magnetic nanoparticles functionalized with molecularly imprinted polymers (Fe₃O₄@TEOS@MIP) for the extraction of ibuprofen from water samples. N. Middeeleer, Y. Mei-Ratilff

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 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 isotachophoresis. F. Matthews, M. Hossan, S. Gamagedara


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 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. Dunnavant, 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 460. Method development and determination of metal complex pKₐ’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 466. Mercury concentration in water fowl in Wisconsin. S. Frisque, M.D. Schuder


CHED 468. Spectroscopic characterization of aged historic inks for their rapid detection and remediation. T. Huntington, D. Rothfels, R.P. Jensen, N.A. Swartz

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 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 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 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

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 493. Forensic ink analysis with miniaturized UV-Vis spectrometry. M. Morrill, L. Huang, M. Chambers

CHED 494. Further studies of chalcone-like derivates 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 496. Development of an analysis method of forensically significant reduced-size STRs by MALDI-TOF-MS. A. Osenbach, 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

Undergraduate Research Posters

Biochemistry
Cosponsored by BIOL and SOCED
N. Di Fabio, J. Roberts, Organizers

12:00 - 2:00


CHED 503. Construction of mntn 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 *Arthospira platensis*. T.D. Williams, C.K. Saner, C. Hartwig

CHED 507. Exotic butter formulation to enhance bacterial resistance and UV protection. R. Persaud


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 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 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 Rhamnosidase 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 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
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 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. MihaiIescu

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 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 anticancer 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 555. Effects of novel napthoquinone derivatives on topoisomerase activity. A. Rowe, O.J. Alao, J.C. Dicesare, R.J. Sheaff

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 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 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 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. Ceesay, 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 571. MMP-9 cleavage of self-assembling amyloid peptides. J. Bell, J.E. Smith-Carpenter


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
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 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 595. Investigation of carnosic acid mitigation of amyloid beta (Aβ) 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-deoxynyboquinone and beta-lapachone in a BRCA1-mutant breast cancer cell line expressing elevated NQO1 levels. K. Brokaw, L. Palquist, 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 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 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. Aldakhllallah, M. Salemi, 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 614. Template-based engineering of stacked c-type hemes. C. Sommerville, J. Kleingardner


CHED 617. Analysis of antibacterial properties of *Phlox divaricata*. A. Orourke, 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 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 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 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 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 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 nocadione natural products. **K. Patterson**, A. Lane
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 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 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. Burridge, I. Sahu, C. Dabney-Smith, R. Edelmann, 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

CHED 672. Development of multimodal drugs targeting the inhibition of the methylerthritol phosphate (MEP) pathway. P. Gross, C. Grosdemange-Billiard, D. Lièvremont, 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 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 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 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

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-κB to κBDNA. 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 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 701. Investigation of antiferromagnetic properties of Co₃O₄ nanoparticles produced via bacterial medium. R. Loughran, S. Nellutla, J. Mendell

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 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 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 715. Diversifying STEM through community college social integration. A. Peck, E. Salazar, A. Wilt, A. Sanderlin, M. Hoyle
CHED 716. Investigating the alignment between secondary inquiry chemistry activities and assessments. **V. Borland**, A.G. Schafer, E.J. Yezierski

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. Campise**, 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 724. Withdrawn


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. Yezierski, 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 731. Increasing the accessibility of the rainbow flame test by utilizing household chemicals. **A. Rossi**, A.J. Carroll


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. Ancharski, D.P. Predecki, J. Kegerreis


CHED 740. Utilization of GC-MS for arson accelerant determination. C. Slezak, C.V. Gauthier


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 744. Using 3D printing technology to recreate historically accurate teaching models from the 1800s. C.E. Caldwell, J.D. Mendez


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 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-sakes 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. Laulhe

CHED 770. Development of an online organic chemistry course and the most faced challenges. M. Cordero, J. Figueroa

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 777. Feasible synthesis of high surface area, porous and magnetic graphitic carbon spheres. J.G. Jeskey, M. Jaroniec, A.C. Dassanayake


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
CHED 783. NMR investigation of micelle formation by phenylalanine-containing biosurfactants. **E. Pieroni**, F.H. Billiot, E. Billiot, Y. Fang, K.F. Morris


CHED 785. Exploring the addressability of DNA decorated multifunctional gold nanoparticles with DNA origami template. **R. Nixon**, W. Liu, S. Yang, R. Wang


CHED 791. Amino acid behavior studied at relevant conditions with EC-STM. **I. Baljak**, J.A. Phillips, K. Boyd, 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 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 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 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
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 829. Computational modeling of the absorption spectrum of gold nanorods in explicit solvent. A. Tran, E.B. Guidez


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 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 840. Theoretical studies on the length dependence of molecular rectification. I.F. Guzmán González, J.L. Palma


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 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

12:00 - 2:00


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 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. Dearrington**, K. Roberts


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 866. Pertechnetate reduction by reactive rhodochrosite, a common Mn(II) mineral. **A. Cadet**, **N. Tran**, V. Anagnostopoulos
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 878. Determination of PAH levels in Lake Champlain sediment. A.C. Flueckiger, C. Chant


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 884. Effects of soil redox conditions on riparian zone ecosystem services and disservices. W. Chace, A.J. Gold, K. Addy

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 895. Factors affecting eutrophication: The health of the Chicago River. J. Ramos, T. Lam, F. Calderon, R. Sepulveda, M. Musa, D. Espiritu


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. Heinl

CHED 903. Sulfur dioxide is to dye for. A. Eckert, P. Hymas, J. Rosentreter

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 909. Determining the metal pollutants from the Elizabeth Mine: An EPA superfund site in Vermont. S. Vaal, S.M. Lamos


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 914. Wastewater-based epidemiology. K.J. Bisceglia, G. Kroening, M. Lakuleswaran, O. White


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 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 922. Withdrawn
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 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 930. Investigation of microplastic contamination of Pacific sea salts. T. Potts, K.A. Woznack, G. Gould


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


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 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. Biflouride 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


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. Cestrone, 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 962. Fuel property assessment of Shorea robusta seed and oil from physico-chemical properties and thermal analysis. M. Hasan, M. Islam, M. Ismail


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
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 trismethimazolylborate 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. Milsmann

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 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 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
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 $\text{H}_3\text{N}–\text{GeX}_3\text{CH}_3$ 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 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 991. Synthesis and characterization of a novel Zn(II) porphyrin incorporating TAMRA for use as a PDT agent. S. Harris, J.E. Bradshaw


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

CHED 1000. Nuclear magnetic resonance analysis of atrazine chlorohydrolase small molecule mimics. C. Carbajal, S.S. Rocks


CHED 1002. Reaction of a copper(II) centered Schiff-base complex with strong acid: A kinetic investigation. C.J. Hansen, J.J. Stace


CHED 1004. Different coordination stoichiometries using a novel pincer ligand with Eu(III) and La(III) ions. N. Battaglia, M. Guino-o


CHED 1006. Synthesis of titanium oxofluorides under hydrothermal conditions. E.P. Miller, D.H. Johnston


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 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 1016. Moving anion sensing towards the finish line. M.O. Odago, Z.F. Peterson

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 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. Alkhazalah, A. Akinniyi, **A.A. Christopher**, C.R. Fraire, A. Gaspar-Mendoza, J. Logan, C. Perez, J. Pham, G. Scott, E. Theard, M. Omary


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 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 Cd$^{2+}$, Pb$^{2+}$, and Zn$^{2+}$ 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 SF$_6$ and its analogs SF$_5$Cl and SF$_5$CF$_3$. W.S. Taylor, **C.L. Foscue**, C. Emmerling, A.L. Harris


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 1033. Synthesis and characterization of a new Anderson-Evans polyoxotungstate with Cu(II) in its central cavity. **M. Pina**, S. Nellutla

CHED 1035. Modeling cytochrome \(c_{552}/\text{Cu}_{A}\) interfacial electron transfer at gold electrodes modified with functionalized SAMs. **C. Cullip**, S. Hunter, N. Muren, K. Yokoyama, M.G. Hill


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-MoS\(_2\) electrodes for CO\(_2\) 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 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 1052. Synthesis and characterization of manganese carbon monoxide releasing molecules bearing ferrocenyl thiosemicarbazone ligands. **M. Lawrence**, F.A. Beckford
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. Thananatthanachon

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 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 1064. Development of nanoprecipitated water-insoluble gallium complexes for treatment of infections caused by cystic fibrosis. K.M. Greskovich, S. Huang


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 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
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<tr>
<td>CHED 1072. Complexation of lanthanides with the rhodizonate anion.</td>
<td>C.A. Nodarse, J.A. Silverman, K. Kavallieratos</td>
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<td>CHED 1073. o-Phenylenediamine derived sulfonamides for lanthanide and</td>
<td>A.A. Rains, E.V. Govor, K. Kavallieratos</td>
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<td>actinide extraction from alkaline aqueous media.</td>
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<td>CHED 1074. Silylation of pyridine and pyridine derivatives with</td>
<td>J. Prybil, R.M. Chin</td>
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<td>diruthenium complexes.</td>
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<td>CHED 1075. Solution vs. mechanochemical syntheses of lanthanide</td>
<td>B.J. Cooper, R.E. Cooper, A.A. Brown, L. Sylvain, E.M. Fatila</td>
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<td>coordination complexes.</td>
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<td>CHED 1076. Synthesis and characterization of titanium tantalum metal</td>
<td>M.L. Emmons, J.L. Hunting</td>
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<td>oxides.</td>
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<td>CHED 1077. Investigation in to the fundamentals of metal-organic</td>
<td>R.M. Marusko, J.F. Eubank</td>
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<td>frameworks and their potential biomedical applications.</td>
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<td>CHED 1078. Synthesis and stability of bis(imino)pyridine iron methyl</td>
<td>G. Pombar, P.J. Chirik</td>
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<td>complexes.</td>
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**Undergraduate Research Posters**

**Medicinal Chemistry**

Cosponsored by MEDI and SOCED  
N. Di Fabio, J. Roberts, Organizers

12:00 - 2:00

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<td>CHED 1079. Apoptosis induction and the effect of novel naphthoquinone</td>
<td>R. DeWeerd, M. Manpadi</td>
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<td>analogues on the JAK-STAT pathway.</td>
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<td>DCM-MJ-I-21 isoprenylated coumarin.</td>
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<td>substituted-2,4-triazolium salts with lipophilic and hydrophilic</td>
<td>K.L. Shelton</td>
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<td>substituents.</td>
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<td>CHED 1084. Optimization, characterization and encapsulation</td>
<td>G. Torres, N. Günday Türeli, A. Türeli</td>
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<td>efficiency analysis of Eudragit L100 nanoparticles loaded with</td>
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<td>fenofibrate by nanoprecipitation method.</td>
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<td>CHED 1085. Synthesis and characterization of pyruvic aldehyde-1-</td>
<td>S.B. Crum, E.C. Lisic</td>
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<td>oxime thiosemicarbazones and their complex formation with Cu(II).</td>
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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 1094. Drug repositioning and diversification strategy for discovery of compounds with anti-cancer activity. M. Chapa, D. Gibson, D. Bateman


CHED 1096. Characterization of erlotinib polymorphs by solid-state NMR. A. Viggiano, R. Iuliuucci, R. Quinones

CHED 1097. Green synthesis of cholic acid derivatives as novel antimicrobials. D. Bolding, D.C. Bromfield-Lee


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 isoindolinyl 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

CHED 1106. Analysis of the folding and misfolding of Shadoop by nuclear magnetic resonance (NMR). E.Q. Williams, C. Chant


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 enaminones inhibiting voltage-gated sodium channels. J. Kirkland, I. Amaye, P. Jackson-Ayotunde, Y. Fang


CHED 1111. Biophysical characterization of a G quadruplex structure within MBNL 1 mRNA. A. Moses, M. Mihailescu


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-benzyol-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 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
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 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 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 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 1135. Microencapsulation of anthocyanins in alginate hydrogels for potential applications in anti-β amyloidosis therapies. A.D. Santiago-Mercado, C.M. Osorio-Cantillo


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 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
CHED 1141. Fractionation of Hierba Santa extracts via flash column chromatography and their effects on HeLa cells. **A. Aceves, S. Deprele, L. Nogaj**


CHED 1144. Development of novel inhibitors to modulate trained immunity. **A. Cipriano, F. Janssen, A. Lacour**


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 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. Knechtle**

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**
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 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 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 1170. Coating and biofunctionalization of gold nanospheres and nanorods using polytannic acid and polypyrrogallol. 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 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 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 1189. Repeated immersion of silver ion exchange glasses in a single molten bath. C.M. Nichols, R.M. Magruder, D.W. Ferrara


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


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 1201. S_n1 alkylation of heterocycles in aqueous reaction mixtures. F.H. Lundy, C. Ballard
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 1205. Fluorination and reduction of 1-indanone as a method to study carbon-fluorine hydrogen bonding. **S. Gooding**, R.E. Rosenberg


CHED 1208. Synthesis of 1-pentyl-3-(1-napthoyl)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 cyclopropenones in strain-releasing methodologies. **B.M. Klootwyk**, J.E. Muir, G.R. Boyce


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 1217. Efforts towards cycloadditions with pyridoxal via an ortho-pyridinone methide intermediate. **M.X. Bozor**, G.R. Boyce


CHED 1219. Utilization of green chemistry for the synthesis of resveratrol analogues to target cancer cells. **C.L. Knudstrup**, H. Benmerabet, D. Paull


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 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 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 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 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 1239. Convergent synthesis of photoactive naphthalamide 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
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 $^{15}$N labeled amino acids from simple starting materials. T. Pinto, W. Carroll


CHED 1244. Absorption spectra of juglone in its anionic and neutral form in aqueous solutions of basic pH. I. Crouch, T. Majors, O.A. Cojocaru

CHED 1245. Modelling for polymer chemistry: Using $^{19}$F 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. Cojocaru


CHED 1248. Diastereoselective synthesis of syn-$\beta$-hydroxy-$\alpha$-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 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. Cojocaru

CHED 1259. Synthesis of an extended matrix metalloproteinase inhibitor. J. Hungerford, D.A. Fish


CHED 1262. Synthesis of isoxazoles and isoxazolines as lavendamycin analogues. G.S. Taylor, R.E. Sammelson, H.D. Beall

CHED 1263. S_{n}1 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 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-b-D-muramic acid. J. Bomhof, J.E. Hanson


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 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 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 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 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 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 1297. Investigation of Rhamnus crocea leaf extract effect on Hermes copper butterfly. J. Dang, L. Malter, J.A. Trischman


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 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 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-diamine) 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 1312. Solubility of albuterol-NSAIDs ionic salts. J. Scantland, O.A. Cojocaru

CHED 1313. Synthesis of novel linked viologen and Py2TTz dimers to enhance radical stability in cucurbit[8]uril. B. Cousineau, J.J. Reczek

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.  

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. Cojocaru, 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. Cojocaru, T.W. Majors

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.  

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. Cojocaru

CHED 1335. Efforts toward the synthesis of Fischer carbenes for intramolecular decarboxylative allylation. P. Thai, M.C. Slade


CHED 1337. Substituent effect on aromatic imine basicity. N. Javaly, 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 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-fluorenlymethoxycarbonyl-N-benzyloxy carbonyl-L-homoglutamine. B. Belcher, K. Harris


CHED 1347. Synthesis of electron withdrawing oxoammonium salts. V. Rapela, L.J. Tilley


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 1352. Synthesis and evaluation of NSAID active pharmaceutical ingredient ionic liquids. J. Pelton, K. Callahan, R.N. Manchanayakage

CHED 1354. Nickel-catalyzed borylation of aryl sulfamates. A. Bulger, M. Merriman, A. Judy, A.L. Silberstein


CHED 1356. Application of (cyclopentadienone)iron catalysts to the lactonization of diols. Y. Tang, R. Meador, T.W. Funk


CHED 1358. Investigation of the scope of substituted benzaldehyde substrates for use in a non-traditional method of N-sulfonfyl imine formation. Z.C. Brandenburg, A.J. Hanson, 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 1370. Synthesis of a triazacyclic amine metalloenzyme mimic building block. A. Lajmi, C. Pizza, A. Condoroteanu-Orovean, M. Harris, P. Sandoval-Sanchez, A. Porter
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 1379. Synthesis of cinnamaldehyde phenylsemicarbazones and exploration of their photochromicity. E.J. Hose, E. Treadwell

CHED 1380. Quinazolin-4(3H)-ones and 5,6-dihydropyrimidin-4(3H)-ones from β-aminoamides and orthoesters. J.T. Gavin, R.A. Bunce


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. Kruel, A. Authement


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 1388. Synthesis of a 2,4-methylenedianiline (MDA) derivative. M.J. Graham, D.E. Janzen, J. Wollack

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 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 1399. Palladium-catalyzed direct α-C(sp³) heteroarylation of ketones under microwave irradiation. A. Rosen, M. Neiser, Q. Nguyen, L. Ma, T. Atesin


CHED 1401. Synthesis of new chiral N-heterocyclic carbene ligand for catalysis. J. Payne, P.J. Lombardi


CHED 1403. Continuous preparation of alkylidene malonates. E. Stryker, C. Kong, F. Gupton


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 isoconamiums 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 carba[porphyrinoids using a ‘3 + 1’ approach. S.J. Kempel, T.D. Lash
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 1416. Mechanistic insights into deboronofluorination of alkyl-Bpin substrates with selectfluor and silver catalyst. **T. Taylor**, T.M. Perrone, B.V. Popp


CHED 1420. Synthesis of symmetrical trisubstituted 1H-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 1H-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 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[4.3.0.0²,4.0³,8.0⁵,7]non-4-ene. **C. DeAngelo**, E. Brutschea, M.A. Forman


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 1436. Tunable removal of carbonyl compounds through rapid bisulfite extraction: Method optimization and selective carbonyl compound removal. M. Furigay, C. Brindle


CHED 1439. Synthesis of 1,2-dihydroisoquinolines. A. Palaia, A.K. Isaacs

CHED 1440. Stereocchemical 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 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 1449. Efficiency of reductive amination in a variety of solvents. J.J. Marcantonio, J. Bennett
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 1455. Synthesis of 2-(2-furymethylidene)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. Moumné


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 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 \(\text{bis}(2\text{-fluorophenyl})\text{furoxan}\). M. Stodolka, W.H. Ojala
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 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 1477. Copper mediated trifluoromethylation of benzylic Csp³−H bonds. W.P. Carson, M. Paeth, W. Liu


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
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 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 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 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 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 mordançage, a historic photographic process. C. Fudala, R.M. Jones


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 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 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
<table>
<thead>
<tr>
<th>Session</th>
<th>Title</th>
<th>Authors/Institutions</th>
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<tbody>
<tr>
<td>CHED 1517.</td>
<td>Will the spins align? Theoretical investigations into the magnetism of oxo-centered tri-metallic clusters decorated with nitoxide groups.</td>
<td>E. Hess, S. Nellutla, S.C. Haefner</td>
</tr>
<tr>
<td>CHED 1519.</td>
<td>Role of the spectator ion in the &quot;reverse chemical garden&quot; reaction.</td>
<td>C. Cowley, M.A. Horn</td>
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<td>CHED 1521.</td>
<td>Computational modeling of lithiated carbon phophonitride electrolyte materials.</td>
<td>M. Lanetti, M. Dorko</td>
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<tr>
<td>CHED 1522.</td>
<td>Comparison of ionic association indicators: Lithium triflate in polyamine and polyether systems.</td>
<td>H. Lee, M. Vogt, K. Elder, R.N. Mason</td>
</tr>
<tr>
<td>CHED 1523.</td>
<td>Revisiting the properties of fluoro-pyridine-SiF₄ complexes: Condensed-phase structural changes.</td>
<td>R. Mooney, P. Treacy, A. Ley, B. Zehner, J.A. Phillips</td>
</tr>
<tr>
<td>CHED 1526.</td>
<td>Plasticizing effect of water on highly viscous sucrose films.</td>
<td>T.S. Qin-Terrill, A. Edwards</td>
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<tr>
<td>CHED 1528.</td>
<td>Understanding the photophysical properties and self-assembly of meso-tetrakis(4-sulfonatophenyl)porphyrin in aqueous solution.</td>
<td>H. Schmidt, O. Makinde, J. Hollingsworth</td>
</tr>
<tr>
<td>CHED 1530.</td>
<td>Usage of localized surface plasmon resonance to study interfacial effects on environmental electron transfer mediators.</td>
<td>N. Nguyen, N. Slenning, P. Hall, A. Pavitt, P.G. Tratnyek</td>
</tr>
<tr>
<td>CHED 1531.</td>
<td>Effect of electron-donating and withdrawing groups in the photophysical, electrochemical, and spectr Electrochemical characterization and solvent effect on the tautomerism of free-base corrole.</td>
<td>K. Webb, V.E. Hernandez, C. Reed, E.A. Aleman</td>
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<td>CHED 1532.</td>
<td>Noble metal nanoparticles as targeted drug delivery vehicles.</td>
<td>A. Alfaro, B.D. Gilbert</td>
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<tr>
<td>CHED 1533.</td>
<td>Photophysical, electrochemical, and spectroelectrochemical characterization and solvent effect on the tautomerism of free-base corrole.</td>
<td>K. Webb, V.E. Hernandez, C. Reed, E.A. Aleman</td>
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<tr>
<td>CHED 1534.</td>
<td>Observation of photobleaching lifetimes of Cy3-alkyne and Cy5-alkyne fluorescence.</td>
<td>I.A. Orantes-Orellana, M.A. Garcia, D. Cooper</td>
</tr>
</tbody>
</table>
CHED 1535. Taming polypyrrole oligomer synthesis with mass spectrometry. **J.L. Stair**, D. Moore


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-butyn-1-yl and 1-butyn-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 1544. TATP: An exploration of practical applications for highly sensitive explosives. **A. Nance, L. Brock**, M.B. Jacobs


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 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


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 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 1561. Synthesis of heterotelechelic polymers via RAFT polymerization for tagging red blood cells as drug carriers. Y. Huang, J. Niu


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 1565. Synthesis of horseradish peroxidase (HRP)-polymer bioconjugates by grafting-from HRP-initiated RAFT polymerization. **C. Kozuszek, K. Burridge, 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 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 1570. Heavy metal water filtration by chitin with varying degrees of acetylation. **S. Baumgartner, J.D. Mendez**


CHED 1572. Stereolithographic 3D printing of photocurable resins for tissue engineering. **T. Colpitts, J.A. Morrill**


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:DMHQ (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**
CHED 1582. Encapsulation and controlled release of G-quadruplex DNA through PMAA/PVPON microcapsules. J. Gearhart, A. Alford, N. Gupta, E.P. Kharlampteva

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 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 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 1595. Chemical Repellents in polymers undergo environmental strains. B. Halliwell, D.A. Fish


CHED 1597. Imidazoliuim-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
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.


Section B

Orange County Convention Center
West Hall C
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 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 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 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 1616. American Chemical Society student chapter at the University of Texas at Tyler. J.M. King, T. Rashid, L. Johnson, L.E. Boyd


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 Tecnologico de Monterrey. N. Baeza, P. Uribe Jimenez, G. Torres, M. Medina, J. Gómez, M. Medina, A. Medrano, J. Arriaga, I. Palestino, A. Murrieta


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. Yarberry

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 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 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
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 1642. Inspiring today’s youth through science & geochemistry. J.P. Stetzler, M.E. Olsson


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 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 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

CHED 1656. Catalyzing a community in chemistry with UCSD American Chemical Society-Student Affiliates. J.A. Chiong, R. Ananth, R. Helsel, 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 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 1662. Chemistry is the science of matter, and it definitely matters @ St. Xavier University, Chicago. L. Lomeli, B. Alappat

CHED 1663. ACS student chapter at the University of Utah. H. Ponce, C. Coplan, R.P. Baskin, A. Thomas, M. Pham, A. Reifsnyder, 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. Bogan, A.R. O'Connor, B.C. Chan


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 1670. Olivet College Gruen Chemistry Society: Student affiliate activities. B. Sturgeon, J. Kiess, I. York, S. Verlinde, S.M. Lewis

CHED 1672. Developing an engaging ACS chapter at a private, liberal arts institution. C.A. Azaldeguí, J. Jaimez, A. Roth-Rodriguez, D. Saldana, B. Westbrook, M. Kopecki Fjetland


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 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. Jocic, M. Roach, K. Parrott, C. Snyder, J. Tibbs


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. Abeыта, F. Delacruz, G. Carrion-Gonzales, L. Perez

CHED 1683. Blazing a path across National Chemistry Week. L. Buchan, R. Andersen


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 1689. SMSU chemistry club: Striking a balance. E.J. Popma, S.M. Erickson, N.J. Beyer


CHED 1692. Temple University Chemical Society. L. Popilock, T. Tran, S.A. Fleming


CHED 1695. National Chemistry Week annual themes demonstrations at Plaza del Caribe. D. Soler, L. Santos


CHED 1698. ACS Alexandria University: Activities, events and community outreach. S.M. Elnztawy, A. Elshamy


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 1703. Pasadena City College (PCC) chemistry club: Every student can contribute. B. Clairday, R. Fukuda, A. Martinez, E. Albert-Minckler, V.I. Jaramillo


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 1708. Cypress Bay ACS Chem Club: In our element! M. Ballester, A. Tracey


CHED 1714. Passion that drives frontiers. Y. Hernandez-Perez, S. Valle-Cortes, R. Estremera-Andujar, B.J. Ramos-Santana


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 1720. Marvelous science outreach in South Texas. C. Ventura, Y. Sanchez, K. Moreno, L. Avila


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


CHED 1728. Growing and sustaining outreach practices for a Student Affiliates chapter. **S. Kempf**, E. Michael McLaughlin


CHED 1731. ACS-UPRB promoting the Chemical Education and impacting the community. **D. Avellanet Ramos**, A.M. Varela Martinez, L.I. Santiago

CHED 1732. Student involvement the heart of UA Little Rock ACS. **J. Desai**, C. Kornelsen, E. Anderson, T. Lee


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**


10:10 Intermission.
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<th>Time</th>
<th>Session</th>
<th>Title</th>
<th>Presenter(s)</th>
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<tbody>
<tr>
<td>10:20</td>
<td>CHED 1737</td>
<td>Teaching environmental sustainability using real-world problems in project-oriented chemistry laboratories.</td>
<td>J. Zhang</td>
</tr>
<tr>
<td>10:45</td>
<td>CHED 1738</td>
<td>Incorporation of environmental chemistry and sustainability into the graduate and undergraduate curriculum.</td>
<td>E. Roberts-Kirchhoff</td>
</tr>
<tr>
<td>11:10</td>
<td>CHED 1739</td>
<td>Innovative approaches to educate students environmental remediation strategies.</td>
<td>M.A. Benvenuto</td>
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<tr>
<td>11:35</td>
<td></td>
<td>Concluding Remarks.</td>
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**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

<table>
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<th>Time</th>
<th>Session</th>
<th>Title</th>
<th>Presenter(s)</th>
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<tr>
<td>8:30</td>
<td></td>
<td>Introductory Remarks.</td>
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<td>8:40</td>
<td>CHED 1740</td>
<td>Method to significantly improve bottom quartile performance in large general chemistry classes.</td>
<td>C.H. Atwood</td>
</tr>
<tr>
<td>9:00</td>
<td>CHED 1741</td>
<td>Benefitting unambiguously: Notable collaborations in education.</td>
<td>J. Moore, E.A. Moore</td>
</tr>
<tr>
<td>9:20</td>
<td>CHED 1742</td>
<td>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.</td>
<td>T.J. Greenbowe</td>
</tr>
<tr>
<td>9:40</td>
<td>CHED 1743</td>
<td>Inclusive and collaborative chemistry education research with chemistry teachers in schools.</td>
<td>H. Sevian, S.A. Murray, R.D. Lewis, G. Banks</td>
</tr>
<tr>
<td>10:00</td>
<td>CHED 1744</td>
<td>POGIL Project: A case study for diffusion of innovation.</td>
<td>R.S. Moog</td>
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<td>10:20</td>
<td></td>
<td>Intermission.</td>
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<td>10:30</td>
<td>CHED 1745</td>
<td>Using symbolic forms and graphical forms to characterize student mathematical reasoning in a chemistry context.</td>
<td>M.H. Towns, J.G. Rodriguez, K. Bain</td>
</tr>
<tr>
<td>10:50</td>
<td>CHED 1746</td>
<td>The relationship of mathematics fluency and success in general chemistry: How collaborations lead to better research.</td>
<td>V.M. Williamson</td>
</tr>
<tr>
<td>11:10</td>
<td>CHED 1747</td>
<td>Beyond content knowledge: Measuring transferrable skills connected to experience as a peer-leader in a PLTL program.</td>
<td>A. Chase, G. Kline, A. Rao, P. Varma-Nelson</td>
</tr>
<tr>
<td>11:30</td>
<td>CHED 1748</td>
<td>Answering questions about teaching and learning in chemistry.</td>
<td>R.S. Cole</td>
</tr>
</tbody>
</table>
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. Trajectory based thermodynamics and kinetics of molecular machines. R.D. Astumian


10:35 Intermission


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.
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. Yezierski

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
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.


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.
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**


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**
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


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

Porphyrrins & 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 carbaporphykinoid systems. T.D. Lash

2:15 Intermission.

2:30 CHED 1793. Investigating metalloporphyrins as water oxidation catalysts with undergraduate researchers. W.M. Ames
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.


3:45 CHED 1796. Ever-versatile porphyrin: Host-guest studies of porphyrin-based M₈Pore metalloccubes. **J.D. Thoburn**

4:05 Intermission.


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.


2:55 Intermission.


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

3:55 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, ORGN², 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.


2:15 CHED 1809. Analyzing the retention of knowledge among general chemistry students. **J.T. Kingsepp**, S.E. Lewis
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


3:35 Intermission.


4:05 CHED 1821. Undergraduate research in the chemistry department at Randolph-Macon College. S.H. Schreiner
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**


5:25 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**
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

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.


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


10:45 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
CHED 1851. Communicating chemistry to adult non-scientists with concepts from *Don't Be Such a Scientist*. S.K. St Angelo

CHED 1852. Tips to help art-students distinguish justified beliefs from opinions in college chemistry classes. B. Budy


CHED 1854. Chemical synthesis of color in art: Curricular innovation at The Thacher School. C. Vyhnal, E. Mahoney, Y. Lin

CHED 1855. Infusing cCWCS “Chemistry in Art” workshop activities into the college curriculum. M.R. Nahm Garrett

CHED 1856. Chemistry in art within an analytical chemistry course. K. Jansen Labby

CHED 1857. Perfume Chemistry: Combining artistry, science, and culture. J.L. Bayline

CHED 1858. Atomic Narratives: Exploring the Manhattan Project through writing, ethics, history, and chemistry. A.L. Smalley, N. Kuroiwa-Lewis

CHED 1859. Linking chemistry and political science: Topics related to weapons of mass destruction. L. Davis, K. Taylor

CHED 1860. Leveraging philosophy to cultivate a culture of ethical and responsible conduct in chemistry and beyond. S.M. Kuebler, J. Beever

CHED 1861. Humanities formation in chemistry: Evidence-based argument and Primo Levi’s *The Periodic Table*. J. Heising, S. Gorman
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


9:55 Intermission.


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
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


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
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


10:45 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


11:55 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


9:35 Intermission.

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


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.


8:55 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


9:55 Intermission.

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


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


9:55 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

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 Sega, 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


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


4:35 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

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.


1:55 CHED 1928. Faculty perceptions of science practices in undergraduate chemistry laboratory courses. C. Schnoebele, T.J. Bussey, S. Brydges
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.


3:50 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.


2:35 Intermission.

2:50 CHED 1937. Exploring teacher noticing, interpreting and acting in response to written student work. S.A. Murray, H. Sevian

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.
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.


2:35 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.


4:15 CHED 1946. Simulating the real-world research experience through course clustering. R.G. Aslanian, M. Bendaoud, R. Carroll


4:55 Concluding Remarks.

Section F

Orange County Convention Center
Room W311C
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


2:35 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.


1:55 CHED 1954. Flipping and restructuring an OB course: Improved student performances and positive longitudinal student survey responses. D.M. Schirch


2:35 Intermission.

2:45 CHED 1956. Withdrawn
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 cCWCS Green Chemistry and Environmental Chemistry workshops. D.W. Carpenetti


9:00 CHED 1960. Fun with forensic chemistry. A.A. Hazari

9:20 Intermission.


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
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


8:45 CHED 1975. Benefits of collaboration between colleges and high schools. L. Aronne

9:05 Intermission.
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


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


8:45 CHED 1982. Embedded math in chemistry: A case study of students' attitudes and mastery. A.M. Preininger

9:05 Intermission.


9:40 CHED 1984. Withdrawn


10:20 Concluding Remarks.

Section E

Orange County Convention Center
Room W311B
Observing & Measuring Classroom Instructional Practices

E. Saitta, Organizer, Presiding

8:00 Introductory Remarks.


9:05 CHED 1989. Withdrawn

9:25 Intermission.


10:35 Intermission.


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


11:45 Concluding Remarks.

CHAS
Division of Chemical Health & Safety

J. Pickel and D. Decker, Program Chairs
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


2:50 CHAS 4. Engaging students to gain understanding of chemical safety information. E. Sweet

3:15 Intermission.


4:15 CHAS 7. Using a “mock safety sort” to raise the many issues a high school science teacher may face. S.D. Wiediger


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
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
9:45 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
2:50 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
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
9:00 Opening Remarks.


9:30 CHAS 28. Formulation of customized cannabis concentrates. T. Trah


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
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.


11:20 CHAS 45. Novel formation of THC isomers in cannabis oil distillate. N. Mosely, Z. Iszard
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


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


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
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


Section A

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


4:30 CINF 20. Data-driven drug discovery for rare diseases: tales from the trenches. F. van den Broek

Section B

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
1:55 CINF 22. Careers in publishing chemical information: From the lab bench to the editorial office to the database. G. Jones


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


3:45 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
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 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

10:05 Intermission.


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


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


10:55 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
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 Eufracio, 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

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
1:30 Introductory Remarks.


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


3:55 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
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


10:05 Intermission.

10:20 CINF 68. MOEsaic: The application of matched molecular pair analysis to SAR exploration. G. Fortin


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.


8:35 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. Haghighatlari, J. Hachmann

10:05 Intermission.


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


1:35 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
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.


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


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.
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


10:40 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. Asil

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

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.


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


1:55 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


3:15 Intermission.

3:45 CINF 118. Methods for *in silico* screening of use and exposure data in authority databases. **S. Fischer**


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


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**
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


10:45 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


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


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


9:35 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


11:15 COLL 6. Impact of pH on the orientation of antibody adsorbed onto gold nanoparticles. J.D. Driskell, G. Ruiz, K. Tripathi


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


Unofficial Technical Program draft as of 2/19/2019
10:00 COLL 12. pH-Driven hierarchical assembly of DNA origami nanostructures. S. Yang, W. Liu, R. Wang


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 MoS\(_2\)/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


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
<table>
<thead>
<tr>
<th>Time</th>
<th>Session</th>
<th>Title</th>
<th>Authors</th>
</tr>
</thead>
<tbody>
<tr>
<td>8:30</td>
<td>COLL 24</td>
<td>Water-based environmentally benign flame retardant nanocoatings for textiles.</td>
<td>J.C. Grunlan, S. Lazar</td>
</tr>
<tr>
<td>9:30</td>
<td>COLL 26</td>
<td>Functional, biobased poly(phosphazene) flame-retardant coatings for textiles.</td>
<td>A. Pich, A. Deniz</td>
</tr>
<tr>
<td>10:00</td>
<td>COLL 27</td>
<td>Functionalized fabrics for chemical protection.</td>
<td>B.J. Johnson, B.J. Melde, M.H. Moore</td>
</tr>
<tr>
<td>11:00</td>
<td>COLL 29</td>
<td>Decontamination of toxic organophosphates using metal hydroxide/polymer textiles: Particle aggregation and its effects on material performance.</td>
<td>D.B. Dwyer, J. Gomez, A. Davoodabadi, T. Tovar, W. Bernier, J. DeCoste, W.E. Jones</td>
</tr>
<tr>
<td>11:30</td>
<td>COLL 30</td>
<td>Aminated polyacrylonitrile fiber coated with Fe$_2$O$_3$ as a high-capacity adsorbent for phosphorus removal.</td>
<td>J. Youngkyun, T. Do, Y. Ko, U. Choi</td>
</tr>
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Section E

Orange County Convention Center
West Hall B4 - Theater 5

Nanomaterials

Applications: Colloid & Surface Chemistry Influencing Function

<table>
<thead>
<tr>
<th>Time</th>
<th>Session</th>
<th>Title</th>
<th>Authors</th>
</tr>
</thead>
<tbody>
<tr>
<td>8:30</td>
<td>COLL 31</td>
<td>Hybrid dual-functional Ag@Au based nanofilms with high sensitivity for in-situ SERS monitoring of catalytic reaction.</td>
<td>S. He, F. Tian</td>
</tr>
<tr>
<td>8:50</td>
<td>COLL 32</td>
<td>Degradation studies on organophosphate methyl parathion mediated by silver-titania core-shell nanoparticles.</td>
<td>S. Talebzadeh Farooji, F. Forato, B. Bujoli, S. Trammell, S. Grolleau, H. Pal, c. queffelec, D. Knight</td>
</tr>
<tr>
<td>9:10</td>
<td>COLL 33</td>
<td>Self-assembled monolayer of 2D metal oxides: Applications in gas sensing.</td>
<td>J. Miao, L. Meng, C. Chen, J.Y. Lin</td>
</tr>
<tr>
<td>9:30</td>
<td>COLL 34</td>
<td>Hydrophilic/hydrophobic self-converting nanoreactors.</td>
<td>H. Jia, J. Gohy</td>
</tr>
<tr>
<td>9:50</td>
<td>COLL 35</td>
<td>Encoding molecular information to plasmonic gold nanostars for anti-counterfeiting.</td>
<td>Y. Huo, S. Curry, C. Jiang</td>
</tr>
</tbody>
</table>


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


9:30 COLL 44. Electrochemically generated superhydrophobic meshes for efficient separation of oil from water. N. Baig, T. A. Saleh


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
11:20 COLL 49. Theoretical study on the conversion mechanism of methane on surface single atom catalysts. Y. Liu


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


9:00 COLL 53. Mechanism of nanocrystal self-assembly at an interface, followed by oriented attachment. D. Vanmaekelbergh


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
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


9:40 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


11:20 COLL 66. Dynamic interplay between PA and DGPP regulates lipid negative charge and protein-lipid interactions. E. Kooijman


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
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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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
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. Noureddine**, L. Tang, R. Serda, J. Brinker


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**
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**


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 repellant additive for fiber forming thermoplastics. **L. Wei, P. Brown, I.A. Luzinov**


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**
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


3:40 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


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
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


3:20 Intermission.


4:10 COLL 115. Standing, lying, and sitting: Unique properties of diyne phospholipid striped phases in templating inorganic and organic nanomaterials. S.A. Claridge


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.


Unofficial Technical Program draft as of 2/19/2019
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


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
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**


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

**Cellulose Nanocrystals Enabling Sustainable Materials**

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**Molecular Processes at Mineral-Water Interfaces: Predictions via Linking Theory & Experiments**

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**Interdisciplinary Chemistry for New Frontiers in Biology and Medicine**

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**SUNDAY EVENING**

Section A

Orange County Convention Center
West Hall C

**Fundamental Research in Colloids, Surfaces & Nanomaterials**

R. Nagarajan, **Organizer**
6:00 - 8:00

COLL 139. Preparation and characterization of a new erlotinib polymorph. S.A. Nickel, R. Quinones


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 147. Preparation of sol-gel GeO₂ and GeO₂-SiO₂ nanoparticles for use in 3D printed optics. A.C. Vahle, J.F. Destino


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 152. Silver selenide nanoparticles as a gateway to diverse quantum dot compositions. A. Fall, P.G. Van Patten


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

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 160. Antibacterial coating on aluminum alloy: SERS detection. B. Baruah


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 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 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 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
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 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. Litle, 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 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 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 198. Colloidal synthesis of hexagonal FeIn₃S₄ and its layer-dependent band structures. H. Kim, H. LEE


COLL 203. Dopamine surface adhesion via spin casting. J. Byun, Y. Zhou, M. Le, W. Chen


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
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. Soufrant, A. Bigio, E. Bonyi, K. Aslan


COLL 215. Magnetism and luminescence property of Mn$^{2+}$-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 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 228. Emulsions stabilized by chemically heterogeneous nanoparticles. L.D. Capre, C. Acevedo
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 236. Shiga and cholera toxins induce roll-up of membranes. **M. Berg Klenow**, J. Camillus Jeppesen, A.C. Simonsen


COLL 239. Improving the functionality of carbon dots via doping and functionalization. **M. Prado**


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 248. Metal nanocrystal-based sensing platform for the quantification of water in water-ethanol mixtures. D. Kim, M. Kim


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 Au_{25} 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 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 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 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. Sebők, I. Szilágyi


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 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 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 Fe^{3+} 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
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 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


Section C
Orange County Convention Center
West Hall C

Supramolecular Assemblies at Surfaces: Non-covalent, Covalent & Coordination Bonding

Posters
F. Rosei, S. L. Tait, Organizers

6:00 - 8:00


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. Polaron 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
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


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


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


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

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.


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

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


9:00 COLL 328. Chemical self-assembly strategies for designing molecular electronic circuits. D. Olson, W.T. Tysoe


10:30 Intermission.


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
Colloidal Nanoparticle Synthesis & Assembly

O. Chen, T. Li, Organizers
F. Bai, H. Fan, Organizers, Presiding


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 perovskite nanocrystals. L. Manna

10:00 Intermission.

10:10 COLL 337. Synthesis and assembly of chiral nanoparticles. N. Kotov


11:10 COLL 339. Colloidal cesium and formamidinium lead halide perovskite nanocrystals: Genesis, properties and applications. M. Kovalenko


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


9:15 COLL 343. Molecular interactions between cell membranes and surface immobilized peptides. Z. Chen

10:05 COLL 345. Mapping membrane receptor dynamics, self-association, and oligomerization: Applications of homo-FRET and super-resolution microscopy. C. Yip


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.


10:45 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
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
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


2:50 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


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
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


3:00 COLL 373. Combination of SERS and fluorescence for detection and/or characterization in biological systems. R.A. Alvarez-Puebla


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

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
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


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


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
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


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

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**


2:45 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 lipds. **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**


Section I

Orange County Convention Center
West Hall B4 - Theater 9

**Surface Chemistry of Colloidal Nanocrystals**
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


3:30 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
Section A

Orange County Convention Center
West Hall C

Sci-Mix

R. Nagarajan, Organizer

8:00 - 10:00


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, Organizer
J. A. Boscoboinik, F. C. Calaza, Organizer, Presiding

8:00 Intermission.


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
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 hematin 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


9:40 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


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


Section C

Quantitative Particle Cell Interaction

L. Liz Marzan, W. J. Parak, Organizers
N. Feliu, Organizer, Presiding

9:00 COLL 438. Live-cell encoding by single-nanoparticle FRET multiplexing. C. CHEN, N. Hildebrandt


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


11:00 COLL 444. Deciphering uptake and trafficking of nanostructured materials built from immune signals. M.L. Bookstaver, C. Jewell


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
11:30 COLL 451. Cancer diagnosis and response to treatment with plasmonic nanoprobes. 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


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
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


9:40 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


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.
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


8:55 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


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

Unofficial Technical Program draft as of 2/19/2019
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


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

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Interdisciplinary Chemistry for New Frontiers in Biology and Medicine
Structure, Imaging & Sensing
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


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. Nauillage, A.A. Bertolazzo, V. Molinero

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


4:40 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


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


Section E
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


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 NaPnE₂ nanocrystals (Pn = Sb, Bi; E = 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


2:40 COLL 524. Chemical fusion of the soft matter under the mechanical stirring. M. Lisunova
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


4:10 COLL 528. Improving BFFT of waterborne polyurethane coating by building encapsulated polycyanate emulsion with hydrophobic inter-facial agent. R. Wang, Z. Jiang, Z. Wang, M. Zhao, J. Zhang, J. Li


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


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


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

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


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
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**


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**


**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**

**Lignocellulosic Materials & Multiphase Systems**

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**Exploring the Frontiers of Chemistry through NASA Research**

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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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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


9:50 Intermission.


10:40 COLL 558. Surface chemistry of colloidal Cu₂₋ₓS 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
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


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


11:00 COLL 567. Dynamic surfactant behaviour and interface coverage during single droplet formation in microfluidics. I. Kiratzis, D. Vigolo, M. Simmons


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
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 MoS$_2$-based nanoplatform for multimodal synergistic inactivation of superbugs. P.C. Ray


10:40 COLL 575. Physicochemical characterisation of PAMAM dendrimer as multifunctional nanocarriers. B. Jachimska

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


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


Section E
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 nanoprobes. 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


10:30 COLL 589. Computational design of nanoparticles with tunable water-mediated interactions. B.C. Dallin, R. Van Lehn


Section F

Surface Chemistry

Biomaterials & Membranes

S. L. Tait, Organizer
N. Jiang, S. Youm, Presiding
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


9:50 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


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
10:00 Intermission.

10:10 COLL 607. Architecting nanomaterials for naval applications. **A. Smith**

10:40 COLL 608. Crystal structure of Au$_{36}$(SPhCH$_3$)$_{24}$ gold nanomolecules. **V. Ganesh Raj**, A. Antonysamy

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**


10:05 COLL 616. Determination of biomembrane elastic properties via analysis of thermal fluctuations of lipid orientation in molecular simulations. **F.L. Brown**


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


Producing Equilibrium Amorphous Packings

Vapor Deposited Glasses

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Producing Equilibrium Amorphous Packings

Vapor Deposited Glasses

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Environmental Interfaces under Nano-scale Confinement
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Bio-Based Gels & Porous Materials
3D printing & Rheology of Cellulose & Nanocellulose
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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.

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


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
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


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

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

2:50 COLL 653. Switchable surfactants for the preparation of monodisperse, sinter-resistant, supported nanoparticle catalysts. K.N. Bryant, S.R. Saunders


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-CsPbX$_3$ heterostructure nanoparticles. F. Rodriguez Ortiz, B. Roman, N. Mireles Villegas, J. Wen, M. Sheldon

4:10 COLL 657. Light-assisted cation exchange in CsPbX$_3$ nanocrystals. T. Qiao, D.H. Son


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


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


4:10 COLL 664. Nanostructured graphite-based materials for hydrogen energy storage. Y. Zhang
4:30 COLL 665. Atomistic simulations of carbon nanotube deposition on functionalized silicon substrates. Z. Shen, R. Van Lehn, J. Dwyer, P. Gopalan


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


2:20 COLL 669. Optimized surface functionalization with self-assembled monolayers for enhanced alpha detection from uranium hexafluoride (UF₆). 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 NO₂-functionalized N-heterocyclic carbene monolayers on Au (111) surface. E. Gross


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


4:30 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
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


2:40 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


3:40 Intermission.


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


Section H
Orange County Convention Center
West Hall B4 - Theater 8
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


2:45 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. McClennon, S. Lecommandoux

3:35 COLL 693. Connecting cell plasma membrane lipid oxidation to cell dysfunction in oxygen toxicity. K. Ren, N. Malmstadt


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.
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


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
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. Schuleit, A. Millqvist-Fureby, M.W. Rutland


10:50 COLL 709. Mapping surface wetting with trifunctional organosilanes bound at the vapor/solid interface. J.C. Garno, 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


Section B

Orange County Convention Center
West Hall B4 - Theater 2

Basic Research in Colloids, Surfactants & Interfaces

Surfactant Science
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


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


8:50 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

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


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


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

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**


9:10 COLL 741. Metal amidinate precursors for general solution-phase synthesis of intermetallic nanocrystals. **A. McGrath, F. Ronning, S. Ivanov**


9:50 COLL 743. Structural transformations of functional nanoparticles. **Z. Quan**


Section F

Orange County Convention Center
West Hall B4 - Theater 6

**Surface Chemistry**

**Nanomaterials**

S. L. Tait, *Organizer*
M. Ganguly, I. Schweigert, *Presiding*

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


9:30 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


10:40 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


9:50 COLL 758. Reversible aggregation of covalently cross-linked gold nanocrystals by linker oxidation. Z. Luan, A. Abelson, M. Law

10:10 Intermission.


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


9:50 COLL 768. Activation of the EphA2 receptor tyrosine kinase by a conditional transmembrane peptide. **F.N. Barrera**


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


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


8:50 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


9:50 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
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
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.


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. Ozcelik, 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


10:15 Intermission.

11:00 COMP 13. Control of electronic properties of two-dimensional materials: Bilayer graphene, porous crystalline 2D materials, and heterostructures. J.L. Mendoza-Cortes


11:50 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


10:05 Intermission.

10:20 COMP 19. Predicting new molecular properties with multimodal learning. O. Isayev


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
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


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


10:45 COMP 29. Affinity and selectivity determinants of bitropic ligands targeting D2 and D3 dopamine receptors. H.S. Hayatshahi, R. Luedtke, J. Liu


Section E

Orange County Convention Center
West Hall B4 - Theater 24

Molecular Mechanics

J. Shen, Organizer
C. Devereux, Presiding


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
9:15 COMP 33. Coarse-grained simulation of cation interactions with lipid bilayers. **R.D. Hills**


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.


11:15 COMP 38. No more histograms: Variational and Bayesian approaches to estimating potentials of mean force. **M.R. Shirts**, A. Ferguson


12:00 COMP 40. Calculating free-energy differences by conveyor belt thermodynamic integration. **D. Hahn**, P. Hunenberger


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**
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 Electro catalysis**

Sponsored by CATL, Cosponsored by COMP and ENFL

**Sustainable Software for Computational Molecular Science**
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. Furche

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


4:50 COMP 54. Dissociative electron attachment in microhydrated molecules. J. Fedor

Section B
Orange County Convention Center
West Hall B4 - Theater 22
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


2:45 COMP 58. Modeling 2D materials with electron correlations and randomly distributed defects. D. Gunlycke

3:10 Intermission.


3:50 COMP 60. Exploring PtXnY(2-n) (X, Y= S, Se and Te; 0≤n≤2) monolayers: Is Janus PtXY the most favorable one? F. Ersan, C. Ataca


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
<table>
<thead>
<tr>
<th>Time</th>
<th>Session</th>
<th>Title</th>
<th>Presenter(s)</th>
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<tbody>
<tr>
<td>2:25</td>
<td>COMP 66</td>
<td>Distance-based Boolean applicability domain for category QSAR.</td>
<td>F. Berenger, Y. Yamanishi</td>
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<td>2:45</td>
<td>COMP 67</td>
<td>Mindfulness and care of the foundation of AI.</td>
<td>T.R. Stouch</td>
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<td>3:05</td>
<td>COMP 68</td>
<td>Comparison of random forest and deep learning approaches for ADMET endpoint prediction.</td>
<td>E.N. Feinberg, V.S. Pande, A.C. Cheng</td>
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<td>3:35</td>
<td>Intermission</td>
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<td>3:50</td>
<td>COMP 69</td>
<td>Machine learning methods to evaluate correlations and causalities in allosteric signaling in proteins.</td>
<td>S. Varma</td>
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<td>4:20</td>
<td>COMP 70</td>
<td>Machine learning to predict molecular interactions.</td>
<td>J. Cheoh</td>
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<td>4:40</td>
<td>COMP 71</td>
<td>PotentialNet for molecular property prediction.</td>
<td>E.N. Feinberg, V.S. Pande</td>
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<td>5:00</td>
<td>COMP 72</td>
<td>Learning molecular models from microscopic simulation and experimental data.</td>
<td>C. Clementi</td>
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**Section D**

Orange County Convention Center  
West Hall B4 - Theater 23

**Undergraduate Research Roundtable & Career Panel**

M. C. Nagan, Organizer, Presiding

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<td>1:35</td>
<td>COMP 73</td>
<td>Modeling Fe(II)-based chromophores for solar energy conversion with quantum mechanical calculations.</td>
<td>E. Jakubikova</td>
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<td>2:25</td>
<td>COMP 74</td>
<td>Delineating function from protein conformational ensembles.</td>
<td>D. Hamelberg</td>
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**Section E**

Orange County Convention Center  
West Hall B4 - Theater 24

**Molecular Mechanics: Computational Studies of Transmembrane Proteins**
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
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
Computational Electro catalysis
Sponsored by CATL, Co-sponsored by COMP and ENFL

Advances in Methods for Comparing Molecular & Supramolecular Simulations to Experiments
Sponsored by CATL, Co-sponsored by CINF, COMP and PHYS

Sustainable Software for Computational Molecular Science
Workflows
Sponsored by PHYS, Co-sponsored 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, Organizer
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
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


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


11:55 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

9:25 COMP 107. Travelling through levels of resolution with machine-learning methods. T. Lemke, S. Hunkler, O. Kukharenko, C. Peter


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


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 aryienes. J. Scanlon, P. Willoughby, J. Lilly, G. Mraz
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.


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.


10:50 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
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**


**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 GEC

**Data Science for Catalysis Research**

Sponsored by CATL, Cosponsored by CINF, COMP and ENFL

**Modeling Dynamics in Dense Manifolds of Electronic States**
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, Organizer
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


2:30 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.


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


2:40 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
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


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


3:10 Intermission.

3:25 COMP 158. Molecular simulations in the study of reactive intermediates towards discovery of novel materials. V. Glezakou, R. Rousseau
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.


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
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


4:45 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
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 transability in molecular simulations. J.R. Schmidt

9:30 Discussion.


10:40 Discussion.
11:00 Intermission.


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 ETA 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


11:05 Intermission.


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
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.


10:50 COMP 192. Minimally parametrized exchange–correlation functional for static, dynamic, and strong correlation, including dispersion corrections. E. Proynov, J. Kong, R. Peverati


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


10:10 Intermission.

10:55 COMP 199. Modeling catalytic reactions with multireference electronic structure theories. S. Stoneburner, C.A. Gaggioli, L. Gagliardi


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


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
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.


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
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.


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
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


2:20 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
3:50 COMP 228. Relativistic quantum chemistry with reduced-density-matrices: The effect of angular momentum constraints. **R. Li**


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


2:30 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


3:40 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**
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


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


4:45 COMP 248. Insights into the mechanism of the PIK3CA E545K activating mutation using MD simulations. H. Leontiadou, I. Galdadas, C. Athanasiou, Z. Cournia
Division of Physical Chemistry Award Symposium
Sponsored by PHYS, Cosponsored by COMP

Deep Learning
Sponsored by CINF, 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 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


Section A
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 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 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 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
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 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 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
COMP 288. Symmetric and non-symmetric short iterative Lanczos integrators for time-dependent coupled-cluster theory. B. Cooper, A.E. DePrince


COMP 290. Computational investigation of binding energetics for selective lanthanide extraction. M.Y. Darrings, A. Perry, O. Sode


COMP 293. Conformational coupling to asymmetric ATP hydrolysis in the transport cycle of p-glycoprotein. S. Dehghanighanaviyeh, K. Kapoor, E. Tajkhorshid


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 300. Connecting the TraPPE force fields to the MoSDeF framework. B.L. Eggimann, K. Beardslee, C.E. Bunner, J.I. Siepmann


COMP 302. Describing transition metal chemistry with the random phase approximation. H. Eshuis, J. Chedid, N. Ferrara


COMP 305. Survey of quantum chemical methods for computing interaction energies in organometallic systems. R. Evans, L.W. Peterson, M.L. Cafiero
COMP 306. Molecular dynamics and metadynamics based studies of Brg1/DNA interaction. **s. evoli**, J. Wereszczynski


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. Mwongela

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 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 318. Effect of mutations on the binding of ligands in phenylalanine hydroxylase. **R.M. Giampapa**, L.W. Peterson, M.L. Cafiero


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**
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 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 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 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

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 349. Molecular dynamics study for the ion-channel opening of NMDAR. J. 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 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 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 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 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 375. Tamiflu: Analysis of drug binding and resistance. L. Oliver, J. Lu, Y. Zhang


COMP 377. Theoretical study of nonadiabatic relaxation dynamics in [Au$_{25}$(SeCH$_3$)$_{18}$] and [Au$_{13}$(P$_2$H$_4$C$_2$H$_4$)$_5$Cl$_2$]$^{3+}$. 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
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. Puzdakiewicz, 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 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 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 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 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 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 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


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 + CH₄. **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 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 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 tricarbazolo 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 CpRu(PPh$_3$)$_2$Cl and Mel. 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 451. Ab initio molecular dynamics simulations of imidazolium-based ionic liquids. K. Yue, O. Acevedo


COMP 453. Pyparam: A Python-based tool for force field parameterization and optimization. Q. Zeng
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. Rehmood, H.J. Kulik


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
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 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
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'-Cu₃V₂O₅. A. Parija, J.L. Andrews, J.V. Handy, S. Banerjee

8:55 COMP 474. New LaMnO₃ surface energy results obtained from density-functional theory. Y. Mantz


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


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
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


9:30 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. Raebber, D.A. Mazziotti

Section D

Orange County Convention Center
West Hall B4 - Theater 23

Drug Design

Al & Machine Learning

M. R. Landon, Y. Tseng, Organizers
E. M. Leddin, Presiding

8:30 COMP 489. Towards accurate and precise binding affinity predictions: the $\lambda$-SAMS and 2D-vFEP($\lambda$) methods. T. Lee, D.M. York


9:30 Intermission.

9:45 COMP 492. Designing for bias: Computational methods to drive rational design of G-protein biased agonists. R. Torella
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


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


10:00 COMP 500. Novel small molecule modulators of the hotspot PIK3CA mutants identified by computational and experimental approaches. Z. Cournia, P. Gikeka, 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
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
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.


3:30 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

3:30 COMP 511. Molecular mechanism for the role of histone tails in nucleosome repositioning. K. Chakraborty, M. Kang, S. Loverde

4:00 COMP 512. Critical inspection of the Varkud satellite ribozyme active site. A. Ganguly, D.M. York

4:30 COMP 513. Material Science

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


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

Unofficial Technical Program draft as of 2/19/2019
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


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


3:35 Intermission.


4:15 COMP 529. Investigating the anharmonic vibrational structure of van der Waals systems. O. Sode, M. Keceli


5:05 COMP 531. Spin splittings from first-order symmetry-adapted perturbation theory without the single exchange approximation. J. Waldrop, K. Patkowski

Section D
**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
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 Aβ 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 dyphteria 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
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

8:55 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.


10:50 COMP 562. Multiscale modeling of aqueous phase methane diffusion in zeolite frameworks. P.M. Kekenes-Huskey, T. Pace, H. Rahmainejad


11:40 COMP 564. Multi-scale modeling of Li-ion battery anode materials using reactive force fields. M. Bhati, T. Senftle


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 streptomycys 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.
10:25 COMP 571. Elucidating the role of the enzyme environment and mechanism of H₂ catalysis in FeNi hydrogenase. M.E. McGreal, J. Goodpaster


11:05 COMP 573. Understanding the structure and energy relationship of double helical amylose fragments. U. Schnupf


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


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


10:30 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

Sponsored by PHYS, Cosponsored by COMP
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 κB kinase-β. M.R. Jones, A.K. Wilson, B. Brooks


2:10 COMP 593. Hydration and dispersion forces in hydroxypropylcellulose phase behavior. G.W. Dayhoff, D. Rogers


2:50 COMP 595. ff18SB: Amino-acid specific protein backbone parameters trained against quantum mechanics energies in solution. C. Tian, K.A. Belfon, L. Ragquette, A.N. Migues, Q. Wu, C.L. Simmerling

3:10 Intermission.


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


4:45 COMP 600. Study of the pH-dependent properties for the *Escherichia coli* glycaminamide 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.


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**


5:05 COMP 611. Some computational experiments revealing anisotropic strain energies in C_{60} fullerene. **P. Deshpande**
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


2:45 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


4:40 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
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


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


2:50 Intermission.
3:05 COMP 633. Water as described by the random phase approximation. H. Eshuis, J. Chedid


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

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Sustainable Software for Computational Molecular Science

Methods

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ENFL

Division of Energy and Fuels

H. Lin, Program Chair

SUNDAY MORNING

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

8:30 Introductory Remarks.

8:35 ENFL 1. My research partner, Chunshan Song. X. Guo

9:00 ENFL 2. Overview of gaseous carbon waste streams utilization: Status and research needs. A.M. Gaffney


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


11:45 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
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 LiNi_{0.5}Mn_{1.5}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


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 GEC
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 CO$_{2}$ to chemicals and fuels. Y. Sun

8:55 ENFL 18. Developing efficient heterogeneous catalysts for the conversion of CO$_{2}$ to value-added products. S. Raveendran

9:20 ENFL 19. Direct CO$_{2}$ hydrogenation into olefins and aromatics with high selectivity. P. Gao, C. Yang, S. Li, Y. Sun

9:40 ENFL 20. Activation and hydrogenation of CO$_{2}$ over iron-based bimetallic catalysts: Insight from DFT. H. Wang, X. Nie, X. Guo, C. Song

10:00 ENFL 21. CO$_{2}$ conversion to MeOH-DME fuels: Catalytic and technological aspects. G. Bonura, C. Cannilla, A. Mezzapica, L. Frusteri, F. Frusteri
10:20 Intermission.

10:35 ENFL 22. Catalytic conversion of CO2 into high value-added chemicals. X. Guo, C. Song


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


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


9:55 Intermission.

10:05 ENFL 29. Selective electrocatalytic reduction and oxidation of small organic molecules. M. Koper


11:20 ENFL 31. Immobilized polymeric electrocatalysts for redox organic reactions. Y. Sun

11:55 Concluding Remarks.

Section E
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


Symposium in Honor of Chuck Peden’s Research Career: Catalysis for Energy & the Environment

Sponsored by CATL, Cosponsored by ENFL, ENVIR, I&EC and PHYS
Data Science for Catalysis Research

Sponsored by CATL, Cosponsored by CINF, 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, ENVIR, 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

3:50 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


2:45 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
CO2 Conversion to Carbonates

Cosponsored by CATL, COMP and GECO
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


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 a,w-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


Hydrogen Evolution Reaction

Y. Sun, H. Wang, Organizers
Y. Yang, Organizer, Presiding
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


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 Ni$_3$S$_2$ 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. Correra

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


2:25 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

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


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.


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
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


2:45 Intermission.

3:00 ENFL 92. Pb-less perovskite solar cells. M. Wang, X. Gong, X. Shai


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 azadipyrrromethene-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

2:05 ENFL 98. PEM CO2 electrolysis for fuels. S. Ma, E. Cave, N. Flanders, K. Kuhl


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


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
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. Veser

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/CeO$_2$ catalysts: Mechanistic distinctions between supported single atoms and nanoparticles. R.M. Rioux, M.J. Janik, L. Wang, S. Deo


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/lz. 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
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


9:35 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


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


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

9:50 Intermission.


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


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 NiCoOₓHᵧ 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
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


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


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
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


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

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


9:35 Intermission.

9:50 ENFL 156. Mixed cerium oxides as reactive materials for thermochemical water splitting. H. Hagelin-Weaver, S.J. Roberts


11:10 ENFL 159. High-performance TiO$_2$ 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 CO$_2$ 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 CO$_2$ photoreduction by H$_2$O. H.M. Frei

8:35 ENFL 161. Unveiling active sites of CO$_2$ 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 CO$_2$ reduction by Mn(α-diimine)(CO)$_3^-$ catalysts. V. Blasczak, M.E. McKinnon, D.C. Grills, M. Ertem, J.J. Rochford

Unofficial Technical Program draft as of 2/19/2019
11:00 ENFL 166. Improvement of Co porphyrin CO$_2$ electroreduction activity via its covalent immobilization on the surface of carbon cloth electrodes. A. Marianov, Y. Jiang


11:40 ENFL 168. 2D ultrathin nanosheets for photocatalytic CO$_2$ 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 CO$_2$ issues by chemical conversion and by reducing CO$_2$ emission. J.G. Chen


9:50 Intermission.


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
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

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
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


2:45 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.


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 GECOC
H. Lin, R. Motkuri, Organizers
Y. H. Hu, S. Kawi, Organizers, Presiding
J. J. Spivey, K. Tomishige, Presiding

1:00 Introductory Remarks.


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/Al₂O₃ core-shell catalyst. T. Le, J. Kim, E. Park


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
4:25 ENFL 203. Recycling mechanism of lattice oxygen over VOₓ/ CeO₂(111) in the ethylbenzene oxidative dehydrogenation with CO₂. **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 CO₂-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 CO₂ to fuels. **J. Rosenthal**


2:35 ENFL 207. Structure sensitivity and structural dynamics of metal nanomaterials for CO₂ electrocatalysis. **Y. Li, D. Kim, P. Yang**


3:15 Intermission.

3:25 ENFL 209. Electrochemical synthesis of ammonia via nitrogen reduction using N₂ and H₂O under ambient conditions. **G. Wu**


Section E

Orange County Convention Center
West Hall B4 - Theater 16
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.


1:35 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. Vuppaladadiyam, M. Zhao

2:45 ENFL 216. Isolation of endophytic fungus Hypoxylon sp. BS15 producing volatile organic compounds (VOCs) with fuel potential and epigenetically altering VOC production over time. Y. Wang, J. Harper

3:05 Intermission.


4:00 ENFL 219. Exploring the hybrid conversion of lignin into biodiesel. Z. Shang, M.B. Foston


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 222. Two-dimensional materials design for photocatalytic water splitting from a theoretical perspective. J. Yang


2:35 Intermission.


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


2:45 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
**4:10 ENFL 235.** Effects of dopants and pressure on the stability and optoelectronic properties 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.**


**1:30 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**

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


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
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


TUESDAY MORNING
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.** CO\(_2\) capture over molecular basket sorbents: Why fumed silica is better? **X. Wang**, C. Song


9:45 Intermission.

10:00 **ENFL 258.** Heterogeneous single-atom catalysts for efficient CO\(_2\) 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 CO\(_2\) as a renewable carbon source. **A. Dibenedetto**

10:50 **ENFL 260.** Cu\(_2\)O-based electrodes for photocatalytic CO\(_2\) 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.

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
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


9:55 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


10:55 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
9:10 ENFL 273. Electrochemical conversion of CO$_2$ to formic acid under reduced CO$_2$ concentration. H. Yang, J. Kaczur, R. Masel

9:30 ENFL 274. Effect of CO$_2$ concentration on the electrolytic conversion of CO$_2$ to CO. Z. Liu, H. Yang, S.D. Sajjad, J. Kaczur, R. Masel

9:50 Intermission.

10:05 ENFL 275. Scalable electro-reduction of CO$_2$ to CO with a single atom nickel doped porous carbon electrocatalyst. H. Jeong, U. Sim, K. Nam


11:05 ENFL 278. Tuning the metal surface electronic state for effective CO$_2$ reduction. Z. Wang

11:25 ENFL 279. Chemical versatility of [FeFe]-hydrogenase models: Distinctive activity of [μ-C$_6$H$_4$-1,2-(κ$^2$-S)$_2$][Fe$_2$(CO)$_6$] for electrocatalytic CO$_2$ reduction. M. Cheng

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.


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
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


9:25 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.


10:40 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


Section F
Simulations of Materials & Processes for Energy Applications

Y. Liu, D. Lu, Y. Ping, B. Wood, Organizers
H. Zhuang, Organizer, Presiding

8:00 Introductory Remarks.


9:05 ENFL 298. Computational studies of CO\textsubscript{2} 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

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. Lisa, C. Mukarakate, S. Kim


10:10 Intermission.


11:00 ENFL 307. Acid catalyzed production of 1,3-butadiene from biomass derived tetrahydrofuran. O. Abdelrahman, P. Dauenhauer


Section H

Orange County Convention Center
West Hall B4 - Theater 19

Sustainable Energy Conversion via Innovative Electro catalysis & Photocatalysis

Electrocatalysts for Chemical Conversion

Y. Cheng, F. Jiao, Y. Shao, G. Wu, Organizers
O. Y. Gutierrez, A. J. Karkamkar, Presiding

8:00 Introductory Remarks.


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


B.A. Rohr, S. Blair, S. Mezzavilla, J. Kibsgaard, P. Vesborg, M. Cargnello, S. Bent, T.F. Jaramillo, J.K. Nørskov, I. Chorkendorff


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
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 TiO$_2$-A induces formation of Ni/anatase TiO$_2$ 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
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

**Section C**

Orange County Convention Center  
West Hall B4 - Theater 14

**Carbon Dioxide Conversion & Utilization**

**Photo, Electro & Plasma Catalysis**

Cosponsored by CATL, COMP and GECOC  
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 CO$_2$. L. He, X. He, **K. Chen**

1:30 **ENFL 337.** New surface engineering strategy to promote photocatalytic CO$_2$ reduction by TiO$_2$ 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 CO$_2$ into CO over silver-zirconium oxide. H. Zhang, T. Itoi, T. Konishi, **Y. Izumi**


2:30 **ENFL 340.** Overview and outlook on CO$_2$ 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 CsPbBr$_3$ nanorods and their use in selective photocatalytic hydrogenation of CO$_2$. **S. Kumar**, I. Poli, M. Isaacs, M. Regue, S. Eslava


3:45 **ENFL 343.** CO$_2$ 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 CO$_2$ and CH$_4$ reforming processes using additives and scavengers. **R. Snoeckx**, M. Cha

4:25 **ENFL 345.** Plasma-driven hydrogenation of CO$_2$ to methanol at atmospheric pressure and room temperature. L. Wang, Y. Wang, **X. Tu**

Section D
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. N₆ 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

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
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


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**


4:45 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 IrO$_2$(110) surfaces. **A.R. Asthagiri**, M. Kim, J.F. Weaver

1:35 ENFL 359. CH$_4$ 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. CO$_2$ hydrogenation over cubic and hexagonal In$_2$O$_3$ 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**
Emerging Materials for Renewable Energy

Z. Li, D. Liu, Organizers
M. Hu, M. Lu, S. Nair, Organizers, Presiding

1:00 Introductory Remarks.


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@Ni12P8/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.
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.


1:30 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


3:40 Intermission.

3:50 ENFL 386. Reversible hydrogen uptake/release over sodium phenoxide-cyclohexanolate pair. \textbf{T. He}, T. Autrey, P. Chen

4:10 ENFL 387. Thermodynamics and kinetics of formic acid as a H\textsubscript{2} carrier. \textbf{A.J. Karkamkar}

4:30 ENFL 388. Ammonia as an efficient CO\textsubscript{x}-free hydrogen carrier: Fundamentals and applications. \textbf{Y. Jo}, J. Cha, C. Lee, H. Jeong, J. Han, S. Nam, C. Yoon

\textbf{Elucidation of Mechanisms & Kinetics on Surfaces}

\textbf{Catalysis on Metal Interfaces with Metal Oxides}

Sponsored by CATL, Cosponsored by ENFL, ENVR, INOR and PHYS

\textbf{Exploring the Frontiers of Chemistry through NASA Research}

\textbf{Living There: Science for the Future of Manned Space Exploration}

Sponsored by COMSCI, Cosponsored by ANYL, BIOL\textsuperscript{‡}, BIOT, CELL, COLL, ENFL\textsuperscript{‡}, I&EC\textsuperscript{‡}, INOR\textsuperscript{‡}, NUCL\textsuperscript{‡}, PHYS\textsuperscript{‡}, PMSE\textsuperscript{‡} and POLY\textsuperscript{‡}

\textbf{Well-Defined Materials for Heterogeneous Catalysis: Synthesis, Characterization, & Performance Studies}

\textbf{Synthesis & Performance}

Sponsored by CATL, Cosponsored by ENFL

\textbf{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 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
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 TiO$_2$ 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 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 CO$_2$ 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 CO$_2$ to CO. H. Jeong, M. Balamurugan, U. Sim, K. Nam

ENFL 412. Pd@Cu as catalysts for CO$_2$ reduction reaction probing by *in-situ* XAS. S. Chen

ENFL 413. Decorated carbon nanotube/carbon nanosheet architecture enables improved CO$_2$ electroreduction. F. Pan, Y. Li

ENFL 414. CO$_2$ photoreduction by porous TiO$_2$ 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 417. Constructing high-efficiency MoO$_3$-polyimide hybrid photocatalyst based on strong interfacial interaction. C. Ma, H. Zhu, Y. Wang, Z. Zou
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 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 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 444. Effects of promoters on SBA-15 supported iron catalysts for high temperature fischer tropsch synthesis. S. Seby, D. Weber, B. Joseph, J. Kuhn


ENFL 446. Porous liquid covalent organic frameworks. R.E. Mow, M.B. Martinez, T. Gennett, W.A. Brahnecker

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 hydrotreating. 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 LiₓTiO₃-coating on the structure and the electrochemical properties of LiNi₀.₅Mn₀.₅O₂ 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
ENFL 455. Effect of methanol on style I methane hydrate decomposition. X. Sun, G. Zhou, G. Lu


ENFL 457. Fabrication and ionic transportation characterization of Biological ion channel array. j. kim, j. jung, i. kang, K. Choi


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


9:45 Intermission.

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


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


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
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 sorption 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


9:50 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


11:05 ENFL 487. Benzimidazoles as recyclable metal-free hydrides for CO2 reduction to formate. C. Lim, J.T. Hynes, K. Glusac, C. Musgrave


Section D
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


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 single 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

Energy Materials in Fuel Conversion & Utilization

L. Fan, L. Qin, Organizers, Presiding

8:00 Introductory Remarks.
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


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


9:35 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

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


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
Advanced Electrocatatst 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


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

11:05 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 fromic 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
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


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


11:40 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
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, ENV 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 La$_2$O$_3$ catalysts: A density functional theory study. Z. Wang, X. Gong

1:30 ENFL 536. Developing A$_2$B$_2$O$_7$ 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/MoO$_2$. Y. Wang, Y. Wang, S. Wang, Q. Zhao, C. Hu

2:20 ENFL 538. High-temperature and pressure CH$_4$ partial oxidation catalysis over Ce- and Rh-promoted Ba$_{0.75}$NiAl$_{10}$O$_{19-\delta}$ 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/ZrO$_2$ 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
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


2:55 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


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


2:25 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.


4:00 ENFL 561. Surface-Enhanced Raman Scattering (SERS) composite nanoparticles for dipicolinic acid detection. S. Chang, E. Shen, H. Ow, W. Wang


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
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


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


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 CO\textsubscript{2} 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
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


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


2:35 Intermission.

2:50 ENFL 582. Oxygen off-stoichiometry and defect entropies in solar thermochemical water splitting materials. C. Wolverton


3:50 ENFL 584. Properties of interfaces in all-solid-state rechargeable alkali-ion batteries. S. Ong
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 SO_3 to SO_2 in the HyS process for thermochemical generation of H_2 and O_2 from H_2O. 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 CO_2 utilization and biorefinery. H. Lin

2:25 ENFL 588. From chemistry to interfaces and back. A. Ulman

2:50 Intermission.


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 H_2S from CO_2-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
1:00 Introductory Remarks.


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-O$_2$ 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-MnO$_2$ for water oxidation in acidic electrolyte for more than 6000 hours. H. Han

3:15 Intermission.

3:20 ENFL 598. Towards understanding the electrified RuO$_2$ 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
1:45 ENFL 605. Novel low temperature thermochemical heat storage system. A. Dwivedi, M.C. Rajagopal, S. Ganguly, B. Sharma, N. Rajagopalan, S. Sinha


2:25 Intermission.


3:00 ENFL 608. Assessment of the performance of density functionals for hydrogen storage in sorbents. S. Veccham Krishna Prasad, M.P. Head-Gordon


3:40 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


4:35 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
Chemical Catalysis for Bioenergy Consortium: Addressing Deactivation during Biomass Conversion

Sponsored by CATL, Cosponsored by ENFL, ENVIR 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
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 Li$_4$Ti$_5$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


8:45 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


9:45 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.
8:05 ENFL 630. Flexible C-C bonded network polymers for high-density methane storage. C.T. Yavuz, V. Rozyyev, D. Thirion


9:35 Intermission.


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


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


9:45 Intermission.


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


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


11:45 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, B. Wood, Organizers
H. Zhuang, Organizer, Presiding

8:00 Introductory Remarks.

8:05 ENFL 651. Understanding pseudocapacitive energy storage. D. Jiang


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


10:50 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


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
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 SnO$_2$. 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
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


9:15 ENVR 4. Determine mechanistic causes for antagonism in PAH mixture degradation in mycobacterium species. X. Liu


9:55 Intermission.

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


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.


8:40 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


10:00 Intermission.


11:35 ENV R 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.


9:15 ENV R 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 ENV R 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 ENV R 25. I'm just a simple chemist: The environmental mass spectrometry contributions of Professor Ronald Atlee Hites. E.T. Furlong, R. Jaffe, D. Swackhammer


11:20 ENV R 27. Everything I ever needed to know about PAHs I learned from Ron Hites. S. Simonich


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

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


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.


10:40 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


11:40 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
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 CS\textsubscript{2} 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 photophysic 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


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
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.


10:40 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


11:55 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
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.


5:15 Concluding Remarks.

Section B

Science & the Perception of Climate Change

S. O. Obare, Organizer
E. Schoffers, Organizer, Presiding

1:30 Introductory Remarks.

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


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


2:35 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
3:35 ENV 78. Don’t call it a spec(k). E.M. Ulrich


4:15 ENV 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 ENV 81. Nanomaterial-Driven Electrochemistry as a Water Treatment and Sensing Tool. D. Jassby, A.K. Mulchandani

1:50 ENV 82. Nanoscale structures for enabling and enhancing membrane processes at the water-energy nexus. S. Lin

2:10 ENV 83. Investigating the Food Safety Implications of Two Broadly Applied Nano-agrichemicals. X. Ma

2:30 ENV 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 ENV 85. Potential application of few layered black phosphorus in water treatment. Q. Zhao, S. Zhang, X. Zhang, B. Xing

3:10 ENV 86. Withdrawn

3:30 Intermission.

3:50 ENV 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 ENV 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 ENV 89. Electrochemical CO conversion to valuable chemicals. F. Jiao

4:50 ENV 90. High-performance nanomaterials for the recovery of nitrogen and phosphorus nutrients. M. Manto, C. Wang

5:10 ENV 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

Unofficial Technical Program draft as of 2/19/2019
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


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


4:30 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
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


2:40 **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**
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


9:55 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


11:50 Concluding Remarks.

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
8:45 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


9:50 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


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.


9:45 ENV R 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 ENV R 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 ENV R 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 ENV R 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


11:40 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 ENV R 132. Plasctics increasing chemical contamination in ocean and coast. H. Kimukai, H. Sato, K. Koizumi, K. Takatama, S. Chung, M. Nishimura, Y. Kodera, K. Saido

8:30 ENV R 133. Chemical Mechanisms and Toxicological Effects of Microplastics in the Aqueous Environment. C. Sayes


9:50 Intermission.

10:05 ENV R 137. Reliably quantifying microplastics within a wastewater matrix. T.R. Mayo, B. Sturm, E.F. Peltier

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.


9:45 ENVR 143. Degradation of strobin 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


11:40 ENVR 148. Aquatic Photochemistry of a Fragrance Ingredient and its Use in Environmental Persistence Assessment. J. Lin, V. Hewins, M. Emberger, S. Gimeno
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**


9:35 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.


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
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.


1:30 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 caroliana 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.


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.


2:25 Intermission.


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


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
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


1:45 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
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.


3:30 ENVR 184. Photocatalytic reduction of gaseous carbon dioxide by cuprous oxide/graphitic carbon nitride composite photocatalyst. P. Chang, I. Tseng


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 benzotri fluorides. A. Manfrin, G.J. Getzinger, A. Hänggli, K.P. McNeill


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


Technical Program

2:45 Intermission.


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


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


Unofficial Technical Program draft as of 2/19/2019
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

**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

**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

**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**
Section A

Orange County Convention Center
West Hall C

Sci-Mix

S. O. Obare, Organizer

8:00 - 10:00


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 ENV R 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


9:15 ENV R 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 ENV R 207. Levels, tissue distribution and health risk assessment of organochlorine pesticides associated with Pomadasys Commersonnii and Mugil Cephalus from selected estuaries in Eastern Cape Province, South Africa. C. Olisah, O.O. Okoh, A. Okoh

9:55 Intermission.

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.


9:15 ENVR 215. Beyond legacy PFAS: Models to inform assessment across structural classes and species. **W. Cheng, M. Khazaee, C. Ng**


9:55 Intermission.


10:30 ENVR 218. Towards the Virtual Bioprofiling of PFAS Derivatives. **D. Fourches**


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.


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


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, 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


9:20 ENVR 231. FTO-TiO₂ photoelectrocatalytic degradation of triphenyltin chloride coupled to photoelectro-Fenton. H. Olvera-Vargas, X. Jianxiong, O. Lefebvre


10:00 Intermission.


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


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.

9:30 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


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.


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.

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


9:15 ENVR 252. Development of a bioelectrochemical system for simultaneous energy and nutrient recovery from wastewater treatment. C. Dykstra


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


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.


1:25 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 y-hexachlorocyclohexane versus hexachlorobenzene in an acidified ethanol using ball-milled ZVMg. A.M. Garbou, J.A. Gomez, C. Yestrebsky


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.
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 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


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 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
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<th>ENVR 278.</th>
<th>Withdrawn</th>
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<td><strong>Applications &amp; Implications of Nanomaterials &amp; Their Toxic Effects</strong></td>
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<td>4:00 - 6:00</td>
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<td><strong>ENVR 279.</strong> Environmental exposures to titanium dioxide engineered. <strong>M. Baalousha</strong></td>
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<td><strong>ENVR 280.</strong> Selective oxidation of hydroxymethylfurfural to furandicarboxylic acid using air and chitosan-derived porous nitrogen-enriched carbonaceous carbon nitride catalyst. <strong>S. Verma, R.S. Varma, M. Nadagouda</strong></td>
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<td><strong>ENVR 281.</strong> C-H activation and oxidative cyanation of amines using protuberant lychee-like goethite. <strong>S. Verma, R.S. Varma, M. Nadagouda</strong></td>
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<td><strong>ENVR 282.</strong> Quantification of TiO₂ engineered nanoparticles in natural soils. <strong>J. Wang, S. Mohanty, M. Baalousha</strong></td>
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<td><strong>ENVR 284.</strong> Enhanced immobilization of U(VI) using a new type of FeS-modified Fe⁰ core-shell particles. <strong>J. Duan, D. Zhao</strong></td>
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<td><strong>ENVR 286.</strong> Cobalt oxyhydroxide: a novel and highly efficient peroxymonosulfate activator for degradation of 2,4-chlorophenol in water. <strong>C. Lyu, Y. Lyu, T. Xi, X. Li</strong></td>
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<td><strong>ENVR 287.</strong> High fluorescence carbon dots from kappa-carrageenan for fluorescence imaging, chemical and metal ion sensor applications. <strong>M. Sinoy, M.G. de Luna, P. Paoprasert</strong></td>
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<td><strong>ENVR 288.</strong> VOC emissions from carbon nanotube composites used in 3D printing. <strong>P. Potter, S.R. Al-Abed, D. Lay, S.M. Lomnicki</strong></td>
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<td><strong>ENVR 289.</strong> Exposure of hepatocellular carcinoma (HEP-G2) to CdSTe quantum dots. <strong>A. Ponton, L. Alamo-Nole</strong></td>
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<td><strong>ENVR 290.</strong> Comparative study of methods for the synthesis of silica nanoparticles from sugarcane waste ash. <strong>S. Rovani, D.A. Fungaro, F.B. Carvalho, J.J. Santos</strong></td>
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<td><strong>ENVR 291.</strong> Development of a chemi-assay battery for nanoparticle biotransformation. <strong>M. George, C.M. Sayes</strong></td>
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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 293. Disinfection byproducts formation in UV/chlorine process for micro-polluted water treatment. X. Zhang


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 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
ENVR 301. Surveying faradaic electrode materials for efficient electrochemical water desalination. V. Pothanamkandathil, C. Gorski


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 308. Water-Energy Nexus: Electrochemical Removal of Silica from Alternative Cooling Water Sources. L. Valentino, Y.J. Lin

ENVR 309. Withdrawn


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 Metallolpolymer 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


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
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 17β-estradiol in sewage impacted rivers at environmentally relevant concentrations. **M. Carolan**, A. Romig, C. Hutchinson, D.R. Griffith


Section A
Orange County Convention Center
West Hall C

Contributions of a Simple Chemist: How Professor Ronald Atlee Hites Changed Environmental Chemistry


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
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 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 341. Enhanced membrane distillation using nanomaterial based membranes for organic solvent separation from their aqueous mixtures. O. Gupta, S. Roy, S. Mitra

**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.** Roteonone 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 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
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 La$_{1-x}$K$_x$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 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 La$_{0.9}$Ce$_{0.1}$Co$_{0.8}$Fe$_{0.2}$/ 3DOM Al$_2$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

ENVR 368. Effect of cation doping on reversible CO$_2$ 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 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 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 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
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 Sr\(^{2+}\) 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 389. Adsorption studies of the treatment of palm oil mill effluent (POME), using powdered defatted *Moringa oleifera* seed. J.E. Osazuwa


ENVR 391. Controlled release of persulfate and Fe\(^{2+}\) ions for contaminant treatment. P. Pham, R. Federico-Perez, Z. Xue


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@TiO\(_2\) 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
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 402. Simultaneous purification of PM and NOx 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 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 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 415. Adsorption of small polarisable molecules (CCl4 CHCl3) on Starbon® materials. A.S. Aljameel, V. Budarin


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


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 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 429. UV/nitrilotriacetic 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
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 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
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 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


Section A
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-MgFe$_2$O$_4$ 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/H$_2$O$_2$ 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-H$_2$O$_2$ 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
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 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 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-Sporing, C. Pazzi, F.M. Akgun, C. Mayack, R. Broadrup, A. Macherone


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


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


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
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 484. Effect of magnesium uptake by Oriza Sativa from organic and inorganic fertilizer fields -comparative study. V. Retnaswamy


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 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 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. Occurrence 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
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. Zaretzky, N.N. Ferguson, A.B. Dichiara, R.E. Rogers


2:40 ENVR 504. Selective removal of iodide from water using reduced graphene oxide aerogel functionalized with Cu$_2$O/Cu. J. Li, X. Liu, J.S. Zheng

3:00 Intermission.


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


4:55 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
2:00 ENVR 511. Mesoporous TiO$_2$-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 CH$_3$SH oxidation on self-stabilized indirect Z-scheme g-C$_3$N$_4$/I$^3$BiOI. C. He, L. Hu, Y. Huang


3:00 Intermission.


4:05 ENVR 516. Highly effective heterogeneous activation of peroxymonosulfate by Cu-doped LaFeO$_3$ 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


2:20 Intermission.

2:30 ENVR 521. Nanomaterials: Not the next asbestos. M. Wiesner

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


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


2:50 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
4:20 Concluding Remarks.

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.


1:45 ENVR 534. Biocatalytic degradation of parabens mediated by cell surface displayed cutinase. B. Zhu, N. Wei


2:55 Intermission.


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


4:45 Concluding Remarks.

Elucidation of Mechanisms & Kinetics on Surfaces
Catalysis on Metal Interfaces with Metal Oxides
Sponsored by CATL, Cosponsored by ENFL, ENVR, INOR and PHYS

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 B-D - Theater 9

Current Status of Environmental Research on Water Contaminants

S. Ahuja, B. G. Loganathan, Organizers, Presiding

8:30 Introductory Remarks.


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


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.


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


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


11:40 Closing Remarks.
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


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


10:35 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


11:55 Concluding Remarks.

Section D
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-TiO$_2$ composite reactive electrochemical membranes. S. Almassi, Z. Li, W. Xu, C. Pu, T. Zeng, B.P. Chaplin


9:35 ENVR 574. TiO$_2$ 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 TiO$_2$ nanotube electrodes with different morphologies. A. Ahmadi, T. Wu

10:55 ENVR 577. Modeling of effect of electrodeposition parameters of a graphite/PbO$_2$ anode on 2,4-dinitrophenol removal efficiency: Comparison between RSM and ANN. P. Mandal, A.K. Gupta, B.K. Dubey


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
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


9:45 Intermission.

10:05 ENVR 584. Transformation of 1,1,1,3,8,10,10,10-octa chlorodecane in air phase: promoted by phytogenic 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 micropol lutants 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


11:45 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


9:05 ENV R 591. Advanced manufacturing of hierarchical multifunctional foams for environmenttal and energy applications. K. Sierros, I. Pecora, M.T. Arango


9:45 ENV R 593. Opportunities for Expanding Membrane Functionality Through Additive Manufacturing. W.A. Phillip

10:05 Intermission.


11:00 ENV R 596. Scalable 3D printed hydrogel-based biosensors for environmental applications. A.S. Finny, A. Othman, F. Mustafa, E. Andreescu

11:20 ENV R 597. Emissions and control of particulate matter and volatile organic compounds from desktop three-dimensional (3D) printers. P. Azimi, B. Stephens

11:40 ENV R 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.


8:55 ENV R 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


10:10 Intermission.


11:05 ENVR 605. Absolute rate constant measurements for hydrated electron reductive destruction of aqueous perfluoroalkyl species in water. L. Twight, S.P. Mezyk


11:45 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
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


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


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.

1:35 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. NO$_2$ adsorption by recycled concrete aggregates and its application to control corrosion in steel reinforced concrete. S. Patel, E. Ariyachandra, A. Orlov, S. Peethamparan


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 characterization and microbial community analyses. D. Deng


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


2:55 ENVR 629. Sequential electrochemical and biological treatment train for chloronitrobenzene-contaminated water. N. Pica, S. Amiri, A. Hanson, T.B. Hofstetter, J. Blotevogel
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


3:55 Intermission.


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


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.


2:05 ENVR 637. Bioelectrochemical denitrification: Limitations and scale up. C. Castro, K. Taha, D. Yeh


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
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


4:45 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.


2:35 ENVR 649. Challenges and methodologies in creating highly curated databases and libraries for the EPA ENTACT study. T. Anumol

2:55 Intermission.


3:35 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


4:15 Panel Discussion.
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


3:40 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


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
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


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.


3:40 ENVR 669. Reactive electrochemical membrane (REM) for the oxidation of perfluoroalkyl compounds. B.P. Chaplin, H. Le


4:20 ENVR 671. Transformation of 6:2 fluorotelomer sulfonate by activated peroxymonosulfate at conditions representative of in situ chemical oxidation. Y. Zhang, J. Liu, S. Ghoshal


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
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


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
11:10 ENV 681. Red tide on the West Florida Shelf – an overview of developing technologies for mitigation. **V. Lovko**


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 ENV 683. Principal components analysis for green process development. **K.C. Caflin**, E. Gauthier


9:20 ENV 687. Role of ferrate in the valorization of biomass residues. S. Tulaphol, S. Yu, **W. Den**, N. Grisdanurak


10:00 Intermission.

10:15 ENV 689. Trapping of electromagnetic waves in shielding materials fabricated through core@shell approach. **S. Srivastava**

10:35 ENV 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 ENV 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


11:35 Concluding Remarks.

Section C
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


9:55 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. Boby

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
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


9:55 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


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


11:40 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.
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


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. Miksovska, 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
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


11:40 FLUO 8. Fluorine effects in asymmetric hydrogen atom transfer reactions. D. Cahard

SUNDAY AFTERNOON
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


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.


3:50 FLUO 14. Selectivity of different amine/HF reagents for synthesis of functionalized organic fluorine compounds. G. Haufe


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
FLUO 18. Recent topics in fluorine chemistry at Central Glass. H. Kobayashi


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


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.


11:40 FLUO 27. New strategies in fluoroalkylselenolations. T. Billard

MONDAY AFTERNOON

Section A
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. Vicic, Presiding


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
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


10:15 Intermission.


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


Section B

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.

9:05 GEOC 11. Transport of alkaline earth metals in natural and synthetic produced water through porous media. Z. Ye, V. Prigiobbe


10:15 Intermission.


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


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
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.


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


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$_2$O$_3$-water interface structure and reactivity. A. Abbaspour Tamijani, W. Marquardt, S.E. Mason


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

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


3:20 Intermission.


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
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


8:45 GEOC 37. Colloidal transport of hexavalent chromium in groundwater. M. Bhattacharya, A. Singh


Section A

Orange County Convention Center
Room W311G

General Geochemistry

N. Kabengi, Organizer, Presiding

10:00 Introductory Remarks.


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
Cosponsored by PROF†
A. Anbar, S. N. Kerisit, Organizers, Presiding

8:30 Introductory Remarks.


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


11:00 Intermission.

11:05 GEOC 51. Hydrothermal solar system: Enceladus as an example of Everett Shock’s legacy. C. Glein


11:45 GEOC 53. Hydrogen dependent carbon reduction: The physiology of the last universal common ancestor, Luca. W. Martin


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

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


4:40 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
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.

TUESDAY 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

8:30 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


9:55 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.


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


Section B

Orange County Convention Center
Room W311F

Planetary & Meteoritic Chemistry

Cosponsored by ANYL and PHYS
S. Singletery, 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.
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

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.


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


3:45 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. Humberston, 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


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
2:50 GEOC 85. Calculation of kinetic rate constants by high-level \textit{ab initio} quantum chemical methods for astrochemistry and planetary sciences. \textbf{S.R. Barua}, P. Romani

3:05 GEOC 86. Search for self-sustaining chemical systems capable of Darwinian evolution. \textbf{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. \textbf{A. Anbar}


4:35 GEOC 89. Density functional theory modeling of C and H isotopic fractionation of adsorbed organic compounds. \textbf{J.D. Kubicki}, A. Fox, J. Boettger, H. Watts, K. Freeman

4:50 GEOC 90. Study chirality of amino acids with density functional theory. \textbf{D. Kao}, S.D. Domagal-Goldman

\textbf{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

\textbf{Carbon Dioxide Conversion & Utilization}

\textbf{Photo, Electro & Plasma Catalysis}

Sponsored by ENFL, Cosponsored by CATL, COMP and GEOC

\textbf{WEDNESDAY MORNING}

Section A

Orange County Convention Center
Room W311G

\textbf{Chemical Transport & Remediation in Mining Legacy Sites}


8:00 Introductory Remarks.

8:05 GEOC 91. Geochemical and mineralogical characterization of legacy mine tailings to develop remediation strategies. \textbf{C. Ptacek}, D. Blowes, J. Bain, M. Moncur
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


Section A

Orange County Convention Center
Room W311G


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


10:45 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


12:00 GEOC 100. Theoretical study on the reaction mechanisms of most stable Si$_4$C$_4$ cluster formation from Si$_2$C$_2$ 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
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 H$_2$O structure and mobility in controlling reactivity in adsorbed H$_2$O films. J. Loring, Q. Miller, R. Placencia-Gomez, E.S. Ilton, O. Qafoku, C.J. Thompson, D.A. Dixon, K. Rosso


9:45 GEOC 104. Withdrawn

10:15 Intermission.


Section C

Orange County Convention Center
Room W311H

Mineral Crystallization, Aggregation & Dissolution

C. Pearce, Z. Shen, X. Zhang, Organizers, Presiding

8:30 Introductory Remarks .


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


10:15 Intermission.


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


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.


5:00 GEOC 120. Impact of arsenic on microbial metal reduction. S. Owings, G. McNamee, J. Beckler, M. Taillefert


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


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
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


2:45 Intermission.


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


4:45 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
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 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
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


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
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 154. Suite of geochemical and spatial analogues for planetary life detection. C.M. Novak


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

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


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


9:25 GEOC 166. Effects of F- for OH- substitution on clay hydrophobicity and the intercalation of H$_2$O 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$_2$O-CO$_2$ and H$_2$O-CO$_2$-CH$_4$ mixtures in montmorillonite clay interlayers. Q. Rao, Y. Leng

10:15 Intermission.


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


2:50 Intermission.

3:00 GEOC 174. Prediction of barium and strontium concentrations in produced water using major ion concentrations. M. Veisi, D. Whittermore, 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


4:00 GEOC 177. Thermodynamics of nanoparticles: Organics interaction. L. Wu, A. Navrotsky, X. Guo
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


9:50 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
Archaeological Chemistry

Metals & Related Metallic Compounds

M. Orna, S. C. Rasmussen, Organizers, Presiding

1:00 Introductory Remarks.


3:10 Intermission.


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

9:45 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.


11:00 HIST 17. Metabolomics analysis and its application to biomolecular archaeology of wine. K. Duffy, P. van Dommelen, U. Sommer, H. Loney


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


3:10 Intermission.

3:25 HIST 22. Color as trace evidence in archaeological materials science and forensic investigations. I. Kakoulli

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**
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


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
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


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


9:05 I&EC 4. CO\textsubscript{2} separation by crystallization of guanidinium carbonates. R. Custelcean, N.J. Williams, K. Garrabrant, C. Seipp, F. Brethome


9:45 Intermission.

10:00 I&EC 6. Hybrid membranes for CO\textsubscript{2} 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


11:40 I&EC 10. Functionalized mesoporous materials for separation and other applications. J. Liu
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


9:30 Intermission.


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


2:10 I&EC 17. Meta-organic frameworks for artificial photosynthesis. W. Lin


3:20 Intermission.

3:35 I&EC 20. CO oxidation on single atom Pt1/CeO2. Y. Wang


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.


5:05 Concluding Remarks.
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


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


10:45 I&EC 36. Microscopic view of observable trends in reactor performance during the hydrodeoxygenation of carboxylic acids. J. Gopeesingh, J. Bond

11:05 Intermission.
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


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


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

Sponsored by CATL, Cosponsored by ENFL, ENVR, I&EC and PHYS
Industrial Innovations in Polymer Science
Sponsored by POLY, Cosponsored by I&EC

Celebrating 50 Years of ExxonMobil's Corporate Strategic Research Laboratories: A View Forward from a Retrospective
Sponsored by ENFL, Cosponsored by CATL and I&EC

Celebrating 50 Years of ExxonMobil's Corporate Strategic Research Laboratories: A View Forward from a Retrospective
Sponsored by ENFL, Cosponsored by CATL and I&EC

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 SnS$_2$ and MoS$_2$ for enhanced CO$_2$ 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
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


4:50 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


3:05 I&EC 58. Ethylene Oxide catalyst and process technology development. S.S. Dhingra

3:30 Intermission.


4:10 I&EC 60. Industrial problem solving using advanced analytical techniques and expertise. W.V. Konze


5:00 Concluding Remarks.

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium
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

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

Industrial Innovations in Polymer Science

Sponsored by POLY, Cosponsored by I&EC

Celebrating 50 Years of ExxonMobil's Corporate Strategic Research Laboratories: A View Forward from a Retrospective

Sponsored by ENFL, Cosponsored by CATL and I&EC

Critical Materials: Rare Earth Elements

T. E. Albrecht-Schmitt, Organizer
G. A. Fugate, Organizer, Presiding
M. R. Healy, Presiding

TUESDAY MORNING

Section A

Orange County Convention Center
Room W224E
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


9:05 Intermission.

9:20 I&EC 65. Accelerated development of substitutes for rare-earth permanent magnets. T. Lograsso


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


11:55 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
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


9:40 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

Sponsored by CELL, Cosponsored by ANYL and I&EC

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

Sponsored by CHED, Cosponsored by COLL, I&EC, ORGN², PHYS, POLY and PRES

Light-Driven Chemistry: Photoelectrochemistry & Photocatalysis

Sponsored by CATL, Cosponsored by COLL, ENFL, I&EC, INOR and PHYS
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


2:35 Intermission.


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


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


3:10 Intermission.


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


3:10 Intermission.


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

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‡

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
Light-Driven Chemistry: Photoelectrochemistry & Photocatalysis
Sponsored by CATL, Cosponsored by COLL, ENFL, I&EC, INOR and PHYS

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 PdCeOₓ 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. Dolzhnikov, 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. Sangasaeng, N. Sirimungkalakul, T. Sornchamni, Y. Boonyongmaneerat, S. Jongpatriwut
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 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.
I&EC 129. Electro catalytic oxidation of a surrogate for methane. S. Liu


I&EC 131. Fundamental studies of Metal-Organic Frameworks and their application in CO₂ capture. S.C. Weston


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.


8:45 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
10:25 Intermission.


11:05 I&EC 142. Chemistry of actinyl (VI) ions in alkaline solution. R. Wilson


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


8:50 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
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


2:30 Intermission


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


5:25 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
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.


3:35 I&EC 165. Preparation of organo-silica sol-gel monoliths using "single-pot" approach for applications in capillary liquid chromatography. Z. Zajlickova

4:00 Intermission.

4:20 I&EC 166. Recent progress in understanding ionic liquid-based metal ion extraction systems. M.L. Dietz


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. Dolzhnikov, 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


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.


10:55 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


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
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 Cua protein from Thermus thermophilus. L.M. Hunsicker Wang, T. Devlin, C. Hofman, Z. Acevedo, K. Kohler


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
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


10:50 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


9:50 Intermission.

10:05 INOR 11. Using noncovalent interactions to control molecular magnetism and (photo)reactivity. M.P. Shores


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
8:30 Introductory Remarks.


9:00 INOR 15. Excited-state proton-coupled electron transfer using inorganic and organic complexes. E.R. Young, A.N. Oldacre


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


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.


9:45 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.

11:00 INOR 27. Investigations in low coordinate iron chemistry. G.M. George, D. Pokhriyal, S.P. Heins, S.N. MacMillan, P.T. Wolczanski


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 Yb₃Rh₄Sn₁₃ structure type. **J. Chan**

9:00 INOR 31. Synthesis, crystal structures and physical properties of the quaternary solid solutions Ca₁₄₋ₓREₓMSb₁₁ (RE = La–Nd, Sm, Gd; M = Zn, Cd). **S. Baranets**, S.S. Bobev


9:40 INOR 33. Identifying an unanticipated origin of strength in Mo₂BC. A. Mansouri Tehrani, A. Lim, **J. Brgoch**

10:10 Intermission.

10:40 INOR 34. Hydride route to complex intermetallics. G. Bhaskar, T. Cox, V. Gvozdetskyi, **Y.V. Zaikina**


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**
S. Marinescu, J. Y. Yang, Organizers
V. Thoi, Organizer, Presiding


9:00 INOR 39. Probing sulfur redox chemistry in supramolecular frameworks for energy storage applications. A. Baumann, D. Burns, V. Thoi


10:00 Intermission.


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 peroxodihyrdom(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

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


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. CO$_2$ insertion into C–H bonds for carboxylic acid synthesis. D.J. Xiao, E. Chant, A. Yau, M. Kanan


9:30 INOR 58. Structural dynamics of bismuth cathodes during the electrochemical reduction of CO$_2$ 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


11:25 INOR 63. Doping effect on structures and properties of metal oxide semiconductor nanomaterials. Z.J. Li, A. Riley, S. hosseini, T.S. Zubkov

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. Mikovska, K. Kavallieratos


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


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
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


10:40 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
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


2:10 INOR 85. Mechanistic studies of alkene aziridination with a dinuclear silver catalyst. C. Mak, M.G. Campbell

2:30 Intermission.


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
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


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


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


2:45 INOR 101. Exploring non-covalent interactions for energy storage and water purification. N. Elgrishi

3:10 Intermission.


3:50 INOR 103. Thermodynamic considerations for hydrogenation of CO₂: factors that limit catalyst performance. C.T. Saouma
4:15 INOR 104. Heterometallic polyoxovanadate clusters as redox-reservoirs for multielectron small molecule activation. E.M. Matson


Section D

Orange County Convention Center
Room W224C

ACS Award in Organometallic Chemistry: Symposium in Honor of Alan S. Goldman

M. Brookhart, Organizer, Presiding
F. Hasanayn, Presiding

1:30 INOR 106. Tandem C-H activation and N-N activation during conversion of arenes and N\textsubscript{2} 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 \( \pi \) character of M-alkyl \( \sigma \)-bond in \( d^0 \)metal alkyl complexes. O.G. Eisenstein, C. Raynaud, R.A. Andersen, C. Gordon, C. Coperet


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. Hultzsch, L. Homberg, N. Hofmann


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
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. Roccanova, 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

3:00 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


2:30 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
3:30 Intermission.


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


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

Biinorganic 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


2:25 INOR 133. Copper(I)-dioxygen derived complexes; formation, stabilization and reactivity. K.D. Karlin


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


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
5:10 INOR 569. Tungsten oxo alkoxide precursors for the deposition of WOₓ 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


2:50 INOR 144. From molecular magnets to tons of plutonium. A. Schake

3:10 Intermission.


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


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
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*

2:35 **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*

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**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, ENVIR, INOR and PHYS

**SUNDAY EVENING**

Section K

Orange County Convention Center
West Hall C
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 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
INOR 180. Ab initio computational thermochemistry of SF₅OOX (X=H, F an Cl). J.A. Martinez, G.P. Pieffet, V.P. Loretta, C. Buendia


INOR 184. Study of tri-t-butyl tin hydride complexes of transition metals towards activation of small molecules. S. Etezadi


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


Bioinorganic Chemistry: DNA, RNA & Inorganic Drugs

INOR 193. Dinuclear platinum(II) complex with switchable near-infrared emission as a probe of nuclease activity. M. Gabr, F. Pigge


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 199. BODIPY optical probes for pH-responsive imaging. P.B. Tsitovich, B.N. Animasaun, J. Jeouty, M. Henary

Section K

Bioinorganic Chemistry: Proteins & Enzymes & Model Systems

INOR 200. Biomimetics of [Fe-Fe]-hydrogenase: Catalysts for proton reduction. C.A. Mebi


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 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 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


Section K

Orange County Convention Center
West Hall C

Coordination Chemistry: Characterization & Applications

A. Larsen, Organizer

5:30 - 7:30


INOR 216. Functionalization of azamacrocycles by appendage attachment of molecules with known antioxidant properties. T.M. Schwartz, K.N. Green


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 borenium ions. J.D. Culpepper, S.R. Daly, K. Lee


INOR 223. First-row transition metal complexes supported by a redox-active NNP-type pincer ligand and their application to electrocatalytic CO\textsubscript{2} reduction. K. Talukdar, A. Issa, J.W. Jurss

Section K

Orange County Convention Center
West Hall C


L. J. Murray, Organizer

5:30 - 7:30

INOR 224. Design and synthesis of WO\textsubscript{2}L\textsubscript{2} precursors for chemical vapor deposition of WO\textsubscript{x} films. X. Su, P. Panariti, L. McElwee-White

INOR 225. Influence of photochemistry of (η\textsuperscript{3}-allyl)Ru(CO)\textsubscript{3}X precursors on photoassisted chemical vapor deposition. O.M. Hawkins, C.R. Brewer, N.C. Sheehan, B. Salazar, A.V. Walker, L. McElwee-White


INOR 227. Synthesis and evaluation of fluorinated tungsten (VI) oxo-alkoxide complexes as precursors for the chemical vapor deposition of WO\textsubscript{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\textsubscript{3}N\textsubscript{y} films. T. Kim, M.M. Nolan, L. McElwee-White
Section K

Orange County Convention Center
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* (*Dd*HydAB). *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
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 240. Ambient bi-stable reversible crystalline-crystalline phase transition in two-dimensional gete flake. F. Zhou, L. Gan


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 Mudiyanselage, S. Huang


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
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 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 nitrile 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 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. Vijjamarri, 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 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 Ca₁₄₋ₓREₓMSb₁₁ (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. Poeppelmeier

INOR 267. In situ diffraction studies on the structure evolution of perovskite La₁₋ₓSrₓCoO₃₋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 Cu₅Sn₂O₇ (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 Fe₅Se₆ trapped in a non-centrosymmetric framework of metal chalcogenide. C. Weng, C. Yang, J. Jang, K. Hsu


INOR 272. Tunable molecular fluorescence in multivariate metal organic frameworks. W. Newsome, F.J. Uribe-Romo


Section K
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 279. Effect of pH on the reduction potential of cytochrome c2 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 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 286. Impact of Cu(I) on RING finger domain structure. I. Eckart-Frank, K.E. Splan


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

INOR 290. Characterization of PnpC1C2, a “type II” hydroquinone ring-cleaving dioxygenase. M.C. Maker, T.E. Machonkin


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 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 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


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 308. TCNE attachment to iron dinitrosyl complexes containing bis(diphenylphosphine) derivatives: potential as anti-tumor agents. D.A. Velarrde, R. Bourland, L. Li


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 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
INOR 319. Redox Active Al(III) complexes: Electron donating ligands to improve charge transfer. A. Smith, A. Arnold, L.A. Berben


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

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 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. Eitrheim
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(II) 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 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 phosphate ligands for CO₂ reduction. N. Walker, B.J. Bellott

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 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 germoles. C. Lucy, J.L. Mullin, C.M. Prudente, H. Tracy


INOR 353. Synthesis and DFT calculations of Cu₄(I)₄(SbR₃)₄ cuboids with near-IR thermoluminescence. S.A. Shubert-Zuleta, L. Taylor, M.J. Rose


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 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 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 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 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.
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


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

Organometalics and Catalysis
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 proazaphosphatrane complexes. M. Johnson

2:30 Intermission.


3:05 INOR 380. Hydroamination reactions catalyzed by [Au2(μ-Cl)(μ-bis(phosphino)ferrocene)][BArF24]. N. Wamser, C. Nataro


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


2:45 INOR 385. Coordination chemistry of +3 actinides. S.A. Kozimor

3:10 Intermission.


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


3:10 Intermission.


4:40 INOR 397. Ph-dependent optical bandgaps in cdse quantum dots. E.A. Weiss

Section D
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


2:30 INOR 401. Iridium PCP complexes: The importance of steric effects. D.M. Heinekey, T. Lekich, L.M. Guard

2:50 Intermission.


3:45 INOR 404. Empirical microkinetic modeling of enantioselective hydroformylation. C.R. Landis, A. Brezny


Section E

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

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.


4:20 INOR 412. Designing oxide perovskites that break corner sharing toward realizing polar materials. A.M. Fry


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


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.


3:45 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
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.


2:00 INOR 422. Small molecule and biometal adjuvants for oncolytic immunotherapy. J. Diallo


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-Ramirez, 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
1:30 INOR 430. MOF design to applications: Impact of pore system control on gas separations. M. Eddaoudi


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


3:10 Intermission.


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: Supramoleculsar chemistry meets magnetism. K.R. Dunbar


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

3:15 Intermission.

3:30 INOR 444. Novel low-dimensional tin halide compounds: structures, properties and perspective applications. M. Kovalenko


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 t12C2T (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


4:05 INOR 454. Insights on the thermal and chemical stability of V2CTx MXene under different environments. R.K. Thakur, C.A. Carrero
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


TUESDAY MORNING

Section A
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


9:45 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


Section B

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. Agbeworvi

9:25 INOR 462. Understanding itinerant magnetism of CuFe2-xCoxGe2 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
10:10 Intermission.


10:50 INOR 465. Tuning the effective dimensionality of triangular-based magnetic lattices by control of stoichiometry. V.O. Garlea


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.


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.
11:05 INOR 472. Small molecule activation with manganese(I) and (II) complexes. D.C. Lacy

11:30 Discussion.


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


10:10 Intermission.

10:30 INOR 477. Mechanism of nitrogen fixation by nitrogenase. B.M. Hoffman


Section E

Orange County Convention Center
Room W221C


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
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


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.


8:30 INOR 493. Synthesis of ureas by oxovanadium(v)-catalyzed carbon dioxide activation. T. Moriuchi

8:55 INOR 494. V-catalysed bromination of tetrapyrrolyc 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. Altat, 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 phosphaalkenes-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
8:30 INOR 501. Multivariate zirconium MOFs for tuneable redox activity. G. Pour, F.J. Uribe-Romo


9:10 INOR 503. Hierarchically porous zirconium metal-organic framework: facile synthesis, characterization and applications. Q. Zhang


10:10 Intermission.


10:45 INOR 507. Synthesis and characterization of materials for proton conduction studies. P.O. Adelani


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.


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

9:50 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


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


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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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

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


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 colloidally-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 La₀.₄Ce₀.₆Co₂P₂. 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
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.


2:30 Discussion.


3:00 Discussion.

3:05 Intermission.


3:50 Discussion.


4:20 Discussion.


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
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.


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


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
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. Lattturner

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


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$_x$F$_{(4+2x)}$. 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


4:25 INOR 562. First principles investigation of metal-insulator transitions in rare earth nickelates induced by chemical doping. P. Yoo, S. Yao, P. Liao


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

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


3:15 Intermission.


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 phosphate 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
1:30 INOR 574. Comparison of structure, properties, and electrocatalytic activity of phosphorus-rich metal phosphides. E.G. Gillan, A. Flores, M.D. Lovander


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


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. Yb₂₋ₓAₓCdSb₂ (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


5:10 INOR 584. Cerium/copper flux synthesis of new cerium borocarbides. M.B. Hertz, S. Lattumper, 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.

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


1:50 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


2:30 INOR 594. New architectures in the chemistry of polyNHCs: Synthesis and coordination. D. Tapu


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

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'-biazulenic core. M.V. Barybin

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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 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-SiO$_2$ 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
INOR 607. Investigation of structure-property relationship in a family of uranyl tetrahalides paired with substituted methyl-pyridinium cations. N. Byrne, R.G. Surbella, C.L. Cahill


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 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 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 624. Surface alteration of aluminum alloy: Graphene protection and corrosion test. B. Baruah

INOR 626. Pyridinethiolate heterobimetallic precursors to 10-14 binary intermetallics. C. Daniels, J. Vela


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 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. Elsiddieg

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
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 644. Ternary pentagonal-bipyramidal oxovanadium(V) complexes containing five- and six-membered chelate rings: Syntheses, structures and properties. A.K. Srivastava, S. Ghosh


INOR 649. Synthesis and characterization of dinitrosyl iron complexes using pyrazole-derived ligands. M. Le, L. Li


INOR 651. Primary amine pendant arms useful for conjugation of cross-bridged tetraazamacrocycles to other bioactive groups. E.M. Allbritton, M.R. Koper, F. Okorocha, T.J. Hubin


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. Efiong

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. Oreilly, 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 658. Synthesis of multimetallic clusters of lithium and 1st row transition metals with 2,6-bis(tert-butylidimethylsilylamino)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 phenanthroline and azolate ligands. A. Kolek, R. Kidwell, R. Jawaid, V. Nesterov, M. Omari


Section K

Orange County Convention Center
West Hall C

Electrochemistry

N. S. Radu, Organizer

5:30 - 7:30


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


Section K
Environmental & Energy-Related Inorganic Chemistry

S. A. Koch, Organizer

5:30 - 7:30


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 680. Withdrawn

Section K

Inorganic Catalysts

S. A. Koch, Organizer
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 689. Withdrawn

INOR 690. Intramolecular C–H functionalization followed by a [2n+2n]-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 699. Zinc complexes of tetradeutate 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. Resende, 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 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 709. Stark effect in various lanthanide and actinide complexes. J. Campbell


INOR 713. Influence of phosphorus substituents on homoleptic lanthanide and actinide phosphinodiboranate structures. R. Harrison, S.R. Daly

INOR 715. Lanthanum dialkyl and monoalkyl phosphates as precursors for lanthanum phosphates. M. Albqmi, A.W. Apblett


INOR 718. Synthesis and spectroscopic studies of porphyrinate ytterbium (III) complexes. E. Micheli, H. He

INOR 719. Novel Modifications of UC\textsubscript{6} and UB\textsubscript{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[\text{Ni(SiHMe\textsubscript{2})\textsubscript{2}}\textsubscript{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 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. Petrukhina, A.Y. Rogachev
INOR 729. Cyanoxime derivatives of main group V elements. K. Pinks, N. Gerasimchuk


INOR 731. Berylliumcarboxylates, their formation and structural diversity. M. Müller, M.R. Buchner


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 737. Solution calorimetric studies of N₂O₅ 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


Section K
Organometallic Chemistry: New Ligand Platforms

N. S. Radu, Organizer

5:30 - 7:30


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 748. Synthesis, characterization and reactivity of bifunctional transition-metal complexes containing hydride-relay functionality. N. Devi, C.M. Zall


INOR 750. Synthesis of multidentate ligands with a pyrrole-derived backbone and the reactivity of resultant organometallic complexes. M.N. Cosio


Section K

Organometallic Chemistry: Synthesis & Characterization

N. S. Radu, Organizer

5:30 - 7:30

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 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 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 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


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 AAk₂SnQ₄X. K. Murphy, B.J. Bellott


INOR 778. Incommensurate crystal structures of doped rhenium silicides: Promising thermoelectric properties. V. Decocq, F. Wang

INOR 780. Structural and photoluminescence characterization of RE\textsuperscript{3+}-substituted Ba\textsubscript{2}SrGaO\textsubscript{4}F via microwave synthesis. R. Green, V. Pierre

INOR 781. Structural and photoluminescence characterization of the RE\textsuperscript{3+}-substituted hexagonal anti-perovskite Na\textsubscript{2}CaV\textsubscript{3}O\textsubscript{4}F. R. Green, T. Kelly

INOR 782. Electronic and structural \textit{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, \textit{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. Marschilok, K.J. Takeuchi, E.S. Takeuchi

WEDNESDAY MORNING

Section A

Orange County Convention Center
Room W221A

Inorganic Catalysts

S. A. Koch, \textit{Organizer}
A. Bengali, J. W. Jurss, \textit{Presiding}

8:30 INOR 784. Base metal-catalyzed, additive-free C–O bond cleavage of β-O-4 lignin model compounds. O. Brown


9:30 INOR 787. Mechanistic study for the reduction of CO$_2$ to CO using M[bpyMe(ImMe)](CO)$_3$Cl$^+$ 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


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


10:15 Intermission.


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.


9:30 Discussion.


10:00 Discussion.

10:05 Intermission.


10:50 Discussion.


11:20 Discussion.


11:50 Discussion.

Section D
**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.


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.


10:55 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.

**Francis P. Garvan_John M.Olin Medal-Olin Medal: Symposium in Honor of Lisa McElwee-White**

L. J. Murray, Organizer, Presiding


10:00 Intermission.
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


11:45 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


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 CeIV. 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.


11:00 INOR 824. Scorpionate-supported cobalt(II) borohydride complexes. A.M. Aboelenen, J.L. Petersen, M.P. Jensen


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


10:10 Intermission.


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 manich-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
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


10:10 INOR 842. Mechanistic spectroscopic analysis of carbonate synthesis from CO$_2$ and epoxides using aminebis(phenolate) complexes. C.M. Kozak, K. Ni, K. Devaine-Pressing


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 MoS$_2$ nanosheets for hydrogen generation. E. Miller

9:00 INOR 847. Single atomic vacancy catalysis. M. Chhowalla
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


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
Activation of Light (C1-C4) Hydrocarbons: Theory & Experiments

Sponsored by CATL, Cosponsored by ENFL, ENVR, INOR and PHYS

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

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 oxidation of N₂ or N₂O 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.


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
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**


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**


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

2:10 INOR 874. Influence of organic bridging groups on the mechanical properties of organosilica materials. D.A. Loy, K.M. Frederick


2:50 Intermission.


3:25 INOR 877. Preparation of functional zirconium phosphates by stepwise interlayer and surface modification. E. Cruz, B.M. Mosby


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


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
3:45 INOR 886. Genetically engineered peptides used in MOF synthesis. S. Lymperopoulou, 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


Section E
Orange County Convention Center
Room W221C

Environmental & Energy-Related Inorganic Chemistry

S. A. Koch, Organizer
A. W. Apblett, I. Chakraborty, Presiding


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. Raithel, T. Kim, T. Hamann


Section F
Orange County Convention Center
Room W224D

Chemistry of Materials - Synthesis & Properties
C. G. Lugmair, *Organizer*
A. B. Martinson, *Presiding*


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. Prodingier**, M.A. Derewinski, J.A. Lercher


Section G

Orange County Convention Center
Room W221D

**Organometallic Chemistry: Catalysis**

N. S. Radu, *Organizer*
O. Ozerov, *Presiding*


2:10 INOR 907. Withdrawn
2:30 INOR 908. Studies of mechanism of dehydrogenative borylation of terminal alkynes by (PNP)Ir complexes. O. Ozerov, B.J. Foley, J. Zhou


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


2:30 INOR 918. Some novel metal complexes of mixed carboxylates-nitrogen containing lewis bases. J.A. Obaleyé, A.A. Ajibola


3:10 Intermission.

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 fuctionalization by multimetallic uranium complexes. M. Mazzanti


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


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 ^{19}\text{F} magnetic resonance imaging: sensors for biomarkers and chemical environments. E.L. Que

4:00 INOR 932. Oligotetrapyrrrole complexes as efficient photochemotherapeutic agents with remarkably high phototoxicity indices. J. Rosenthal, A. Potocny, M. Martin

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**

Sponsored by CATL, Cosponsored by ENFL, ENVR, INOR and PHYS

**Innovative Chemistry & Materials for Electrochemical Energy Storage**

**Advanced Materials & Synthesis**

Sponsored by ENFL, Cosponsored by CATL, INOR and PMSE

**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

**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

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


10:10 Intermission.


10:45 INOR 942. Subcellular compartment targeting manipulated by porous coordination cages for cancer nanotherapy. **Y. Fang**


11:25 INOR 944. Copper sulfide nanocrystals for plasmon-enhanced multiphoton optical absorption. **A.R. Tao**


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


8:55 INOR 947. Ligand-induced tuning of the ground state spin of Ce$_3$Mn$_8$ 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**


10:05 Intermission.
10:20 INOR 950. Controlled growth of Mn₁₂ single-molecule magnet polymers and oligomers. C. Lampropoulos


Section C

Orange County Convention Center
Room W224A

Coordination Chemistry: Synthesis & Characterization

A. Larsen, Organizer
E. R. Trivedi, Presiding


8:50 INOR 956. Withdrawn


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

Section D

Orange County Convention Center
Room W224C

Electrochemistry

N. S. Radu, Organizer
A. Paolella, Presiding

8:30 INOR 964. Withdrawn


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. Zaghib

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.


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


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


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


10:40 INOR 984. In-silico inorganic spectroscopy using the local spectroscopy data initiative (LSDI). S. Dwaraknath, S.E. Hayes, S. Ong, K. Persson
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


8:50 INOR 987. Enhancing the optical properties of semiconducting 2D materials by plasmonic nanoparticle 2D arrays. M.A. Mahmoud


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.


10:45 INOR 992. DNA-gold bioconjugate with outstanding resistance to nuclease degradation. S. Panickar, A. Mohamed

11:05 INOR 993. Environment sensitive photosresponse of spontaneously partially oxidized 2D transition metal carbides (MXenes). V. Mochalin, S. Chertopalov


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
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


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


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

9:30 INOR 1008. Polymer-assisted solution strategy: from thin films to patterns. G. Zou

9:50 INOR 1009. Electrocatalytic CO\textsubscript{2} 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


11:10 INOR 1012. Withdrawn

11:30 INOR 1013. Rhenium complexes with second coordination sphere functionality for electrocatalytic CO\textsubscript{2} 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 deceptorless 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


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
10:50 INOR 1021. Hydrogenation knölker 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


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.


10:40 INOR 1029. Improving the luminescence of Ln³⁺ (Ln = Eu, Tb, Eu₃Tb₁ 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

Sponsored by CATL, Cosponsored by ENFL, ENVRL and INOR

Elucidation of Mechanisms & Kinetics on Surfaces

Sponsored by CATL, Cosponsored by ENFL, ENVRL, INOR and PHYS

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 TeMo$_6$O$_{24}$$^{6-}$ in aqueous solution. E.M. Villa, G.M. Kuhl


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


3:10 Intermission.


3:40 INOR 1037. Exploring electronic communication between metal centers facilitated by non-innocent ligands. C. Bell, K. Clark, C. Moore
4:00 INOR 1038. Synthesis, isolation, and comparative studies on the transition metal diselenodiphenylphosphinate complexes, M(Se₂PPh₂)₃ (M = V, Cr). J.L. Brown

4:20 INOR 1039. Synthesis and characterization of pyrazolate supported Cr₃⁻(μ₃-O) cores. J.M. Lopez, R. Raptis


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 1042. Control of the speed of a light-induced spin transition through mesoscale core-shell architecture. D.R. Talham


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 1047. Assessing the magnetic properties of low-coordinate iron(II) complexes supported by β-diketiminate 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 Ce⁴⁺. S. Das Gupta, K.A. Abboud, G. Christou
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.


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
A. Larsen, Organizer
M. Stollenz, Presiding


1:50 INOR 1061. Decoding the nuclear coordinate for ground-state recovery in iron(II) polypyridyls. S. Adelman, J.K. McCusker


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


4:40 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 N₂O₂⁻⁻ formazanate ligands. R.R. Maar, S. Barbon, J.B. Gilroy
1:50 INOR 1071. Supramolecular chemistry and chirality of tris(pyridyl) aluminate ligands. **R. Garcia-Rodriguez**

2:10 INOR 1072. Withdrawn


2:50 Intermission.

3:00 INOR 1074. Interesting excited-state behavior in borafluorene derivatives. **J. Cassidy**


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−π and M−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 steric s 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 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
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 1089. Polyarylated boranes exhibit electrochomism 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


3:30 Intermission.

3:50 INOR 1096. Withdrawn

4:10 INOR 1097. Withdrawn
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<th>Time</th>
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<td>4:30</td>
<td>INOR</td>
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<tr>
<td>4:50</td>
<td>INOR</td>
<td>Manganese and iron tetraazamacrocyclic monomers, dimers, and trimers</td>
<td>(oh my!). K.N. Green, T.J. Hubin, H.M. Johnston, S.M. Brewer</td>
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<td>5:10</td>
<td>INOR</td>
<td>Insights into the design of synthetic analogues of metalloenzymes</td>
<td>T.J. Paul, G. Sharma, V. Jayasinghe-Arachchige, Q. Hu, R. Prabhakar</td>
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<td>INOR</td>
<td>Insights into the design of synthetic analogues of metalloenzymes</td>
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<td>1:30</td>
<td>INOR</td>
<td>Oxygen atom transfer from nitrogen oxides for applications in organic</td>
<td>L. Geary</td>
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<td>2:10</td>
<td>INOR</td>
<td>Exploring redox catalysis with well-defined dinuclear silver</td>
<td>M.G. Campbell</td>
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<td>2:30</td>
<td>INOR</td>
<td>Tuning the catalytic activity/selectivity of water-soluble bimetallic</td>
<td>D. Bouzouita, S. Tricard, L. Martinez-Prieto, L. Guy, B. Chaudret</td>
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<td>2:50</td>
<td>INOR</td>
<td>Reactivity and catalytic properties of substituted η⁴-cyclopentadiene</td>
<td>Y. Peng, D. Lionetti, J. Douglas, V. Day, J.D. Blakemore</td>
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<td>3:10</td>
<td>INOR</td>
<td>CO₂ hydrogenation to formate via a Co(-1/1) cycle featuring two stable</td>
<td>M.V. Vollmer, J. Ye, C.C. Lu, J.C. Linehan, L. Gagliardi</td>
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<td>3:30</td>
<td>INOR</td>
<td>Molecular iron complexes as catalysts for CO₂/epoxide coupling and</td>
<td>C.M. Kozak, F.M. Kerton, K.A. Andrea, E.D. Butler, T.S. Anderson</td>
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<td>3:50</td>
<td>INOR</td>
<td>Hydrogenation catalysis with [Co, Rh] and [Co, Ir] heterobimetallic</td>
<td>A. Kumar, V. Day, J.D. Blakemore</td>
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<td>4:30</td>
<td>INOR</td>
<td>Rare earth metal catalyzed intermolecular hydroamination of alkenes.</td>
<td>K. Hultzsch, J.B. Soltys, L. Schickhofer</td>
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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


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


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

Chemistry of Materials - Metal Organic Frameworks

C. G. Lugmair, Organizer
E. D. Bloch, Y. Fang, Presiding

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


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


3:10 Intermission.


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


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
8:30 Introductory Remarks.


9:05 MEDI 2. Small molecule ectonucleotidase inhibitors for the immunotherapy of cancer. **C.E. Muller**


10:35 Intermission.


11:20 MEDI 6. Antiviral innate immunity through small molecules for protection against RNA viruses. **M. Gale**


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**

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 PI4KIIIβ inhibitors as immunosuppressive agents for the prolongation of allogeneic organ engraftment. J. Reuberson


Drug Discovery: Informatics Approaches

Sponsored by CINF, Cosponsored by MEDI

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

Section A

Orange County Convention Center
Room W414AB

General Orals

J. B. Schwarz, Organizer, Presiding


2:45 MEDI 22. Geopharmaceuticals: New drug scaffolds from Baltic amber. E.A. Ambrose, C. McDermott


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, Organizer, Presiding
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

Sponsored by CARB, Cosponsored by CELL, MEDI, ORGN and PROF

Isabell Award

Sponsored by CARB, Cosponsored by CELL, MEDI, ORGN and PROF

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
General Posters

J. B. Schwarz, Organizer

7:00 - 9:00


MEDI 34. Using small molecule adjuvants to combat antibiotic resistant bacteria in cystic fibrosis. V.B. Hubble, C. Melander


MEDI 36. Quinazoline derivatives as potential tubulin polymerization inhibitors. F. Herrera-Vázquez, R. Aguayo-Ortiz, L. Dominguez, F. Hernández-Luis


MEDI 38. Identification of novel PPAR α/γ dual agonist by in silico screening and molecular dynamics simulations. V. Nath, V. Kumar


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

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 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 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. Petruncio, 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 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**

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 66. Aurora-A inhibitor alisertib potentiates VEGFR inhibitors in glioblastoma cell lines. K. Smith, C. Mifsud, C. Zumbar, N. Lehman


MEDI 69. Regioselective alkylation, arylation, and heteroarylation of 3-substituted pyrazoles. A. Bao, A. Huang


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-tetradhydro-1H-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 77. PPE51-mutation effect the sensitivity of Tubercle bacilli to selected thio-sugars. Z.J. Witczak, M. Korycka-Machala, A. Brzostek, P. Borowka, D. Strapagiel, J. Dziadek


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 gabonesis 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 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 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
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 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 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 110. Discovery and characterization of peptide inhibitors of RsmC function. D.D. To, K. GC, S. Abeyesirigunawardena


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 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 130. Optimizing the anti-proliferative activity of CJ-15,208 in prostate cancer cells. R. Pescatore, 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 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 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 148. Identifying of the molecular target for the potent antimicrobial agent TI-1-100 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 153. Inhibition of Dengue virus protease by chemical constituents of a clove: From food ingredient to medicine. M. Saeed


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 158. Multiple quantitative structure-activity relationships (QSARs) analysis for γ-secretase inhibitors. V. Patil, N. Masand


MEDI 162. Discovery of novel toll-like receptor 7 antagonists. S. Jiang, H. Chen, H.H. Yin

MEDI 163. Green synthetic approach to access thiazetidin-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 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 176. Anthrax antitoxin lead optimization via bioisosteric replacement and other in silico strategies. C. McDermott, E.A. Ambrose


MEDI 178. Evolution of commercially available compounds for HTS. D. Volochnyuk, S. Ryabukhin, Y. Moroz


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
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 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 186. Catalytic allylic oxidation of cyclic enamides and 3,4_dihydro_2H_pyrans by TBHP. **R. Humeidi, Y. Yu, M. Doyle**


MEDI 188. BD2-selective BET inhibition induces cell death in pediatric tumor cell lines. **P.J. Slavish, N. Martinez, A. Shelat**


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 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. Reddavide, 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 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 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


Metal-Mediated Reactions & Syntheses
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


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


9:40 MEDI 220. Developing peptides and peptidomimetics as potential treatments for substance abuse. J.V. Aldrich, J.P. McLaughlin
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
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


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
Section A

Orange County Convention Center
West Hall C

Sci-Mix

J. B. Schwarz, Organizer

8:00 - 10:00


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


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
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\textsuperscript{G12C}. A.L. Gill


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. Kalguutkar


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


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
E. F. DiMauro, Organizer, Presiding

8:30 Introductory Remarks.


9:25 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


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


11:25 MEDI 265. Selective FKBP51 inhibitors enabled by transient pocket binding. F. Hausch

Section C

Orange County Convention Center
Room W414AB
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


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 KRASG12C for the treatment of solid tumors. V. Cee


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


3:30 MEDI 281. 2NDEP highlights allosteric activation of the α7 nicotinic acetylcholine receptor. A. Gulsevin, C. Stokes, R.L. Papke, M. Quadri, N. Horenstein


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
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


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

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 296. Saturated bioisosteres of benzene with improved solubility. P. Mykhailiuk, V. Levterov, O.O. Stepaniuk


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 301. Design, synthesis, and evaluation of biological properties of new 5-cyanopyrimidine-based compounds. A.S. Bunev, D. Khochenkov, Y. Khochenkova, E. Stepanova


MEDI 303. 4-Amino-5- (tiazol-2-il) 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 309. Medicinal chemistry and chemical biology approach in order to design and synthesize of TBK1/ IKK-ε small molecules inhibitors. A. Assadieskandar, C. Zhang

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. Latisis, C. Suarez, K. Norris, A. Vulcan, 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 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-HT1A 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 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

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 331. Synthesis of novel functionally selective and long-acting muscarinic antagonists. L. Mesa, C. Martin, J. Boulos


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 339. Synthesis, optimization, and analysis of hexavalent sulfoglycodendrimers as anti-viral agents. C. Vierra, K.D. McReynolds


MEDI 341. 2-Amino-quinolin-4(1H)-ones as novel anti-coronavirus agents. C. Park, J. Song, J. Lee, J. Lee, S. Kim, H. Kim


MEDI 343. Design, synthesis, and biological evaluations of next-generation taxoids, bearing m-OCF₃and 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
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 347. Studies toward an amide core for zampanolide mimics as potential anti-prostate cancer agents. M. Gonzalez, G. Chen, Q. Chen


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 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 360. Synthesis of small molecules for protein control. E. Bray, C. Alvarez, J. Leahy, M.W. White


MEDI 364. Conformational constraint of aromatic residues of the kappa opioid receptor antagonist arodyln using ring closing metathesis. S.A. Gisemba, J.V. Aldrich, T. Murray


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 377. Heterocycle libraries based on natural anti-imflammatories. B. Maki

MEDI 378. New tools for targeting the asialoglycoprotein receptor. N.L. Snyder, A. Strasser, N. Fendler


MEDI 380. In silico models for predicting metabolism by Flavin-Containing Monoxygenases (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


Asymmetric Reactions & Syntheses

Sponsored by ORGN, Cosponsored by MEDI‡

CH Activation

Sponsored by ORGN, Cosponsored by MEDI‡

Heterocycles & Aromatics

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Peptides, Proteins & Amino Acids
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.


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


2:40 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.


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


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


2:55 NUCL 19. Understanding the polymorphism of $A_4[(\text{UO}_2)_3(\text{PO}_4)_2\text{O}_4]$ ($A=$alkali metals) uranyl phosphate framework structures using density functional theory. V. Kocevski, T. Besmann

3:15 Intermission.


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

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


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


11:40 NUCL 32. Actinide chemistry at the most fundamental and comprehensible level: Gas-phase reactions. J.K. Gibson

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

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 W330C

Glenn T. Seaborg Award for Nuclear Chemistry: Symposium in Honor of Thomas E. Albrecht-Schmitt
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


2:40 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 $^{99}$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

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 W330C

Glenn T. Seaborg Award for Nuclear Chemistry: Symposium in Honor of Thomas E. Albrecht-Schmitt

K. N. Raymond, Organizer
D. E. Hobart, Presiding
8:00 NUCL 43. Review of synthesis, spectroscopy, and structural characterization of the intrinsic Pu(IV) colloidal polymer. D.L. Clark, D.E. Hobart


8:40 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.


10:40 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 leaching behavior of Tc. W.W. Lukens


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

TUESDAY AFTERNOON

Section A

Orange County Convention Center
Room W330C

Young Investigators in Nuclear & Radiochemistry
1:15 Introductory Remarks.


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


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


3:55 Intermission.

4:15 NUCL 63. Spectroscopic studies of novel N-donor ligand metal ion complexation. K. Lawson, J.D. Carrick, C.A. Hawkins


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
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


9:30 Intermission.


10:30 NUCL 73. Oxygen isotope fractionation in the processing of uranium oxides relevant to the nuclear fuel cycle. M. Klosterman, L.W. McDonald
10:50 Intermission.


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


1:50 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


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


THURSDAY MORNING

Section A

Orange County Convention Center
Room W231B

General Topics in Nuclear Chemistry & Technology

J. Shafer, Organizer, Presiding

8:20 Introductory Remarks.


9:20 NUCL 87. Explorations of high-pressure behavior of lanthanide and actinide complexes. E. Warzecha, T.E. Albrecht-Schmitt


10:20 Intermission.


11:00 NUCL 91. Functional hybrid molecules for the visualization of cancer: Dimeric BBN$_{7}$-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


11:40 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
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


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


3:10 Intermission.


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. Bonraisain, M. Mokili, F. Haddad, G. Montavon

4:10 NUCL 102. Chemistry of the strong force. G.L. Smith


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


9:00 ORGN 4. Sustainable p-hydroxycinnamic acids synthesis through proline-mediated Knoevenagel reaction. C. Peyrot, A. Peru, L. Mouterde, F. Allais


10:00 ORGN 7. Unusual products from the thionation of bicyclic ketones. T. Nguyen, J.D. Williams


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

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


9:40 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


10:40 ORGN 19. Synthetic utility of boracarboxylated styrene derivatives. T.M. Perrone, B.V. Popp


Section C
Orange County Convention Center
Room W230C

CH Activation

S. M. Silverman, Organizer
K. Olsen, Presiding

8:40 ORGN 22. Reactivity of hypercoordinated iodanes in C-H functionalization. A. Stirling

9:00 ORGN 23. Newly discovered ruthenium Formato 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. Kenttämaa


10:00 ORGN 26. Selective synthesis of mono-functionalized naphthalenediimides by copper-catalyzed C-H activation. J.J. Reczek


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


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
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. Diarenoidacenes 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


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

Wolfson 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
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-trialkysilyl-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


3:20 ORGN 50. Direct substitution of alcohols to form new C-X and C-C bonds. L. Geary


4:00 ORGN 52. Recent advances in nickel-catalyzed amide C–N bond activation. J.E. Dander, N.K. Garg


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
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 phospha-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


3:40 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


2:00 ORGN 67. δ C–H (hetero)arylation via Cu-catalyzed radical relay. Z. Zhang, L.M. Stateman, D.A. Nagib
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


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\textsubscript{sp3}-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
ACS Award for Encouraging Disadvantaged Students into Careers in the Chemical Sciences

K. N. Maloney, Organizer
D. E. Figueroa, Presiding

1:00 Introductory Remarks.


1:40 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
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-acyloxy carbamates and azidoformates as metallanitrene and mettloradical precursors. I. Roccoi, 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 91. Method development of air-free techniques with samarium diiodide. G. Rojas


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 98. Quinoline-oxazoline ligand synthesis for bimetallic catalysis. A. Noonikara Poyil

ORGN 100. Supramolecular ensemble of PBI derivative and metal NPs: Potential application in various organic transformations. G. Singh, V. Bhalla


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 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 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 alkylithium 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 daistereoselective synthesis of (Z)-trisubstituted alkenes containing phenyl and (1,3-dioxan-2ylethul) moieties via organoboranes. N.G. Bhat

ORGN 113. Highly daistereoselective 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
ORGN 114. Mild intramolecular ring opening of oxetanes. L. DeRatt, S.D. Kuduk


ORGN 116. Mild and efficient synthesis of amides from acid chlorides and amines using Cs$_2$CO$_3$ & TBAI. J. Champ, 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 122. New frontiers in Castagnoli–Cushman reaction. S. Ryabukhin, D. Volochnyuk, M. Adamovskiy, 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 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 iminoidane reagents. C.L. Makitalo, S. Larson, G. Rohde, V. Nemykin, A. Saito, V.V. Zhdankin, A. Yoshimura

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. Martin-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 137. Synthesis of indolizidines from L-pyroglutamic acid using the Ireland–Claisen rearrangement and ring-closing metathesis. D. Essayan, J. Cannon


ORGN 139. Development of a reductive enyne Cope rearrangement for synthesis of allenyl malonates. K. White, S. Scott, A.J. Grenning


ORGN 141. Simple, tunable synthetic routes to cannabinoid natural product analogues. P.V. Navaratne, 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, fischerinolides, hapalonomide H, and ambiguous 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 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
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 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 158. Direct acyl amide synthesis from carboxylic acids using N-haloimide reagents. C.D. Irving, S. Walker, M. Gasonoo, S. Laulhe


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 regiospecific 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

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 175. Microwave-assisted sustainable entry to 6H-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 180. One-step synthesis of biflavones mediated by peroxynitrite 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
Photoredox Chemistry

E. C. McLaughlin, Organizer

5:30 - 7:30


MONDAY MORNING

Section A

Orange County Convention Center
Room W230A

New Reactions & Methodology

S. M. Silverman, Organizer
C. Yeung, Presiding


8:40 ORGN 191. Impact of increased CO₂ pressure on substrate scope and boracarboxylation reaction efficiency. S.W. Knowiden, B.V. Popp

9:00 ORGN 192. Decarboxylative amination of redox-active esters using diazirines. P.P. Chandrachud, J.M. Lopchuk


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

10:40 ORGN 197. Palladium-catalyzed imine formation from acetylenes and anilines. M. Mihelac, J. Kosmrlj, M. Gazvoda


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 tetraradicals. 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


9:35 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


10:50 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
Biologically Related Molecules & Processes

S. M. Silverman, Organizer
S. Choi, Presiding


9:00 ORGN 211. Total synthesis of 9-CD$_3$:9-cis-retinal for studying vision. M. Navidi, s. yadav, A.V. Struts, M.F. Brown, N. Nesnas


9:40 ORGN 213. Kinetic dearomatization strategy for an expedient biomimetic route to the Bielschowskysin skeleton. P.D. Scesa, S. Roche, L.M. West


10:40 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


Section D

Innovative Green Chemistry: Striving toward Zero Waste API Manufacturing

Financially supported by Green Chemistry Institute
G. R. Humphrey, K. M. Maloney, Organizers, Presiding
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


10:45 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
## New Reactions & Methodology

S. M. Silverman, **Organizer**  
J. McCabe Dunn, **Presiding**

<table>
<thead>
<tr>
<th>Time</th>
<th>Session Title</th>
<th>Presenters</th>
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<tbody>
<tr>
<td>1:00</td>
<td><strong>ORGN 227.</strong> C-H arylation via Cu-catalyzed radical relay.</td>
<td>L.M. Stateman, Z. Zhang, D. Nagib</td>
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<tr>
<td>1:40</td>
<td><strong>ORGN 229.</strong> Controlled α-halogenation of alkyl sulfones using reagent-solvent halogen bonding.</td>
<td>C. Poteat, V. Lindsay</td>
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<td>2:00</td>
<td><strong>ORGN 230.</strong> Water mediated benzyne reactions using aryldiazodioxaboroles.</td>
<td>A. Yoshimura, J. Fuchs, G. Rohde, V. Nemykin, A. Saito, M. Yusubov, V.V. Zhdankin</td>
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<td>2:20</td>
<td><strong>ORGN 231.</strong> Palladium-catalyzed dearomative syn-1,4-oxyamination and carboamination.</td>
<td>C. Tang, M. Okumura, Y. Zhu, D. Sarlah</td>
</tr>
<tr>
<td>2:40</td>
<td><strong>ORGN 232.</strong> Harnessing the reactivity of strained heterocyclic allenes.</td>
<td>M. Yamano, N.K. Garg</td>
</tr>
<tr>
<td>3:00</td>
<td><strong>ORGN 233.</strong> HFIP and the development of an interrupted Schmidt reaction.</td>
<td>J. Aube, M. Charaschanya, K. Li, H. Motiwala</td>
</tr>
<tr>
<td>3:20</td>
<td><strong>ORGN 234.</strong> Reductive ketyl radical couplings via atom transfer catalysis.</td>
<td>S.M. Rafferty, J. Rutherford, D. Nagib</td>
</tr>
<tr>
<td>4:00</td>
<td><strong>ORGN 236.</strong> Gold-catalyzed oxidative coupling of alkynes toward the synthesis of cyclic conjugated diynes and its application on polymer post-functionalization.</td>
<td>J. Wei, X. Ye, X. Shi</td>
</tr>
<tr>
<td>4:20</td>
<td><strong>ORGN 237.</strong> Synergistic, Au-Fe-catalyzed, directed aldol reaction.</td>
<td>t. yuan, X. Shi</td>
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<td>4:40</td>
<td><strong>ORGN 238.</strong> Catalytic enantioselective approaches to allenes.</td>
<td>S. Ma</td>
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### Section B

Orange County Convention Center  
Room W230B

### Physical Organic Chemistry: Calculations, Mechanisms, Photochemistry & High-Energy Species

S. M. Silverman, **Organizer**  
M. Jaramillo, **Presiding**

<table>
<thead>
<tr>
<th>Time</th>
<th>Session Title</th>
<th>Presenters</th>
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<tbody>
<tr>
<td>1:00</td>
<td><strong>ORGN 239.</strong> Fundamental studies of the singlet oxygenation of melanin model compounds: Reaction products and pathways.</td>
<td>M. Jaramillo, K.E. O'Shea</td>
</tr>
</tbody>
</table>

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-pi interactions and reaction selectivity. S.L. Wiskur

2:40 ORGN 243. Computational mechanistic study of a P₄-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. Satakar


3:55 ORGN 246. Copper-catalyzed difunctionalization of alkenes with boron and CO₂: 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
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


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**


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\textsubscript{N}1 and S\textsubscript{N}2 reactions. **G.C. Fu**
3:05 ORGN 264. Chrial H-bond donor/Lewis acid cooperativity. E.N. Jacobsen


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


TUESDAY MORNING

Section A

Orange County Convention Center
Room W230A

Molecular Recognition & Self-Assembly

S. M. Silverman, Organizer
J. Jung, Presiding


9:00 ORGN 268. Can self-assembly into wormlike micelles occur in polar solvents at sub-zero temperatures? N. Agrawal, S.R. Raghavan


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


10:40 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


11:40 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


10:00 ORGN 283. Thioenamide synthesis inspired by peptide macrocycles. J.A. Lutz, C.M. Taylor

10:20 ORGN 284. Aerobic oxidation of N-phenylglycinyl peptides for catalyst-free oxime ligations. Q. Guthrie, C. Proulx


11:00 ORGN 286. Structural revision and total synthesis of the bacterial siderophore madurastatin C1. M.J. Hall


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


8:40 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


9:40 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

10:40 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. Cliff, 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.


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


11:55 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
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 nanohoops. 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.


10:55 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


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


4:40 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 Mo(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**


2:40 ORGN 326. Copper-catalyzed synthesis of sterically encumbered allenylboronic acids using B₂(OH)₄ as boron source. **J. Zhao**, S. Jonker, **D.N. Meyer**, G. Schulz, C. Tran, L. Eriksson, K.J. Szabo
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


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 dipyrrromethene 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


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]quinolizine 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


3:40 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
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


3:50 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
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. Brash, 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 350.** New small, rigid nitrooxide 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 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 356.** Synthesis of 4-(methylsulfanyl)benzyl and 3-pyridylmethyl glucosinolate via the nitronate pathway. M.A. Anderson, E. Ronning, A.A. Snyder, S. Fisher, J.R. Mays

ORGN 358. Flavins as enophiles in ene reactions and catalysts for retro-ene reactions. **A.W. Jensen**


ORGN 360. Effect of selenium nutrition, temperature, and photoperiod on gibberellic acid accumulation in spinach plants. **A. Malkawi**, C. True, A. Bailey


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 369. Development and synthesis of conjugated cyclic diyne as a novel alpha-helix structure constraining strategy. **X. Li**


ORGN 373. Synthesis of the enantiomers of the environmental contaminant diethylhexylphthalate (DEHP) and its metabolites. **D. Oldham**, L. Harris, C. Amurrio, K. Bempong

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 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

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 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 392. Phytoceutical 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**


Section A
Materials, Devices & Switches

E. C. McLaughlin, Organizer

5:30 - 7:30


**ORGN 398.** Synthesis and electronic properties of alkylated spirobifluorene derivatives. R. Kundu


**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
Orange County Convention Center
West Hall C

Molecular Recognition & Self-Assembly

E. C. McLaughlin, Organizer

5:30 - 7:30


ORGN 411. Photochemical assisted synthesis of interlocked organic molecules. V. Ramalingam, M. Pattabiraman

ORGN 412. Supramolecular catalysis. S. Teng, X. Shi


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 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 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

ORG 425. Self-assembly of tetraphenylethylene-based dimer with tunable fluorescence. Y. Yan, G. Yin, X. Li

ORG 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

ORG 427. Spontaneous resolution of an octahedral supramolecular cage. R. Ni, C. Xu, X. Li

ORG 428. Effects of small molecules that selectively bind to phosphatidylglycerol(PG). B. Seelam, D. Burns

ORG 429. Synthesis of small bis-phenolic ether scaffold cationic molecule that binds to phosphatidylglycerol at the membrane interface. K. Donavalli, D. Burns

ORG 430. Developing a basket-shaped host molecule based on calix[4]arene featuring urea groups for volatile guest molecules. V. Lokugama Widanelage

ORG 431. Synthesis and characterization of N-acetyl-glucosamine-based macrocycles by SN2 reactions. S. Adhikari, A. Chen, G. Wang

ORG 432. Tightly-knit dual hydrogen bonding for fluorescence turn-on detection of cyanide: Evolving design principles and synthetic implementations. H. Park, D. Lee


ORG 434. Self-assembly of supramolecular pentagonal prisms. B. Song, H. Wang, M. Wang, X. Li


ORG 436. Effect of electron demand on sensing behavior of carbazolopyridinophanes. G. Abban, A.B. Brown


ORG 441. Functional thin films on plastic surfaces for applications in bacterial biosensor. E. Hjelvik, A. Anderson, H. Mukundan

ORG 442. Design and synthesis of an enlarged M8L6−metallocubes for encapsulation of nanocrystals. E. Tiernan, J.D. Thoburn

ORG 443. Construction of nano-tube via terephthalic acid linked G-octamer. M. Liu, X. Shi
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 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 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 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
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. Iptycenyl effect: Primary vs. secondary stereoelectronic bias of bridged bicyclic molecular skeleton. H. Kim, T. Kang, D. Lee


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 465. Generation of solid-state, efficient emitters based on 6-membered ring Excited State Intramolecular Proton Transfer (ESPIT) 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

10:00 ORGN 471. Hypervalency aided route to 3,3,3-trifluoropropenylated heterocycles, 1,2-diamines and N-aryl-2-(trifluoromethyl)aziridines. Á. Méaszáros, A. Székely, F. Béke, Á. Tóth, J. Csenki, A. Stirling, Z. Novák


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


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


9:00 ORGN 479. Early process route to fungicide DAS-087. N. Choy, F. Li, G.T. Whiteker


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

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


8:40 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**


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


Section D
**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


9:00 ORGN 500. Studies toward total synthesis of enantiopure hydnocarpin D. P.S. Rajaram, A.S. Rivera, Q. Chen


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. Verhoeest, 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
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


1:20 ORGN 512. Room temperature cross-coupling of unactivated arenes and nitriles via photoinitiation of π-conjugated triazenes. A. Bugarin


2:00 ORGN 514. Development of strategies for the application of eliminative cross-coupling to polyfunctional alkene targets. S. Tanpure, P.R. Blakemore


3:00 ORGN 517. Base-catalyzed stereospecific isomerization of electron-deficient allylic halides. S. Martinez Erro, V. García-Vázquez, A. Sanz-Marcos, 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
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


2:40 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 Eu(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
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


4:00 ORGN 543. C-N cross-coupling via photoexcitation of nickel-amine complexes. C. Lim, M. Kudisch, B. Liu, G. Miyake


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


1:20 ORGN 547. Development of increased spontaneous nucleation rates for continuous crystallization processes of organic molecules in solution. B. Rimez, R. Debuyschère, B. Scheid

2:00 ORGN 549. Boosting electrochemical transformations by using continuous flow. T. Noel


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


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 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 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
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 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 568. Total synthesis of (+)-DMDP and (+)-hyacinthacine A2. Y. Jung, S. Park, J. Jung, Y. Kim


ORGN 570. Stereoselective multicomponent couplings of conjugated aldehydes. H. Bauer, S. Luesse


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 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 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 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*CoIII-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 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
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 595. Cycloaddition reactions of vinyl-dihydroisoquinolines for the synthesis of complex alkaloids. A.N. Specht, G. Moura-Lets

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 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 603. Development of an asymmetric zinc phthalocyanine as a NIR fluorescent probe for EGFR. G. Ducharme, E.E. Nesterov


ORGN 605. Microwave-promoted synthesis of 2,4-diamido-5-aminooxazoles. J.S. Benner, A. Purohit, A. Cottingham, 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 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 619. Synthesis and metalation of internally alkylated porphyrinoids. T.D. Lash, A.N. Latham


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 623. Oxone as an effective reagent for 2-(alkylthio)pyrimidine oxidation. A.S. Bunev

ORGN 624. Progress towards the synthesis and chemistry of 2-sulfobenzoypiaziridines. C. Mitzel, S.M. Bonser
ORGN 625. Mild and efficient synthesis of phosphane-carbodithioates 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 LiBH₄ and CH₃I: 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 634. Synthesis of functionalized y-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 637. Site-selective chemical protein modification via Umpolung catalysis. L.M. Gooch, M. Fascione
ORGN 638. New evidence for the mechanism of Strecker synthesis with ketones as substrates. W. Li, X. Song, I.J. Posey, A. Mondie


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 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


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 cyclopropenone-containing sesquiterpenoid. I.W. Gilbert, K.P. Reber

ORGN 652. Total synthesis of (R)-dihydroresorcyldie via Pd enolate ring closure. K. Haney
**TECHNICAL PROGRAM**


**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. Yearly, 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 661.** Synthetic studies toward the 4-alkylidene proline natural products eleganline 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-pyridynecarboxaldehyde. **H. Arcure**, Z.J. Witczak, R. Bielski, D.E. Mencer

**ORGN 664.** Total synthesis of tuberatolide B. **K. Maurent**, A. Corbu, S. Arseniyadis

**ORGN 665.** Progress towards the stereoselective total synthesis of scytophyycin 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. Nieborowska-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**
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


10:00 ORGN 677. Cycloaddition of vinylcyclopropanes through energy transfer photocatalysis. D. Chen, G. Miyake

10:20 ORGN 678. Hydrofunctionalization of diene. X. Yang


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 bioavailability. H.M. Patel, M.G. Sharma

Section B
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


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


Section C

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


9:00 ORGN 694. Enhancing pyromellitic diimide electron acceptor ability through cationic core functionalization. D.D. Cao


10:00 ORGN 697. Synthesis and polymerization of diynes containing thiocyanate and thiophene end-groups en route towards polydiacetylenes. R. DeCicco


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
8:35 PHYS 2. Structural characterization of an engineered adenovirus vector with cryoEM, de novo structure prediction, and molecular dynamics. P. Stewart, C. Emerson


9:30 PHYS 4. Hybrid approaches to reveal structure and dynamics of large biological complexes from single molecule experiments. F. Tama

10:05 Intermission.


11:00 PHYS 6. Refining conformational ensembles using vibrational probe group data and frequency simulations. C.H. Londergan, R.J. Xu, C. Fu


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


10:05 Intermission.


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


10:15 Intermission.


11:30 PHYS 23. Thermodynamics and kinetics of heterogeneously nucleated calcium carbonate on quartz. Y. Jun, Q. Li

Section D
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


9:45 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


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
8:45 PHYS 33. What we can learn from exact embedding potentials of model systems. Y. Oueis, A. Wasserman


9:45 Intermission.


11:05 PHYS 37. Embedded correlated wavefunction methods based on DFT embedding with a unique embedding potential. X. Zhang, J.P. Martirez, 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


9:55 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
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.


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
Elucidation of Mechanisms & Kinetics on Surfaces

Mechanisms on Surfaces: C-C Coupling, C-H & C-O Bond Maniupulations

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

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


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

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.


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

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
2:00 PHYS 65. Energetics of formation and disordering in RE$_3$TaO$_7$ 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.


4:35 PHYS 71. He irradiation-induced structural degradation, interfacial phenomena, and energetic evolution for defect-fluorite Gd$_2$Zr$_2$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$_2$O$_5$ 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


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
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


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.


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
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 nanoconfinment 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


3:30 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

**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*
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


Materials & Techniques to Advance Redox Flow Batteries

Expanding Techniques & Environments

F. Brushett, S. A. Odom, Organizers
J. R. McKone, Presiding

8:30 Introductory Remarks.


9:15 PHYS 108. What is the right way to measure flow battery kinetics? J.R. McKone, T.V. Sawant


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.
10:30 PHYS 111. Electrolytes to expand the range of options for flow batteries. T. Zawodzinski, K. Lou


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


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
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


10:00 Intermission.

10:20 PHYS 125. Coherent ultrafast photoinduced coupled electronic-nuclear dynamics in dense manifolds of electronic states in molecules. F. Remacle


11:20 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
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.


10:35 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

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
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. Kisela, 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. Clampalini, J. Li, V.G. Sakai, M. Tyagi, H.M. O'Neill, Q. Zhang, S. Capaccioli, K. Ngai, L. Hong


3:35 Intermission.


4:30 PHYS 150. Integrative modeling of biomolecular assembly structures and pathways. A. Sali

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.


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
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


2:45 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


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. Staue 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
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 ABO₃ 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


4:55 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
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


2:50 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.


4:05 PHYS 187. Sum frequency generation of Li-ion battery solvents and electrolyte on amorphous silicon. R.L. Sacci, B. Doughty, 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

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.
3:20 PHYS 193. Composing and decomposing quantum chemistry software: Adventures with the Psi4 ecosystem. L.A. Burns


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
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, ENVIR and PHYS

MONDAY EVENING

Section A

Orange County Convention Center
West Hall C

Sci-Mix

A. B. McCoy, Organizer

8:00 - 10:00


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

9:30 PHYS 198. Multiscale simulations of amyloid formation and conversion. U. Hansmann

10:05 Intermission.


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


8:30 PHYS 203. Super-resolution study of nuclear structure and dynamics. Y. Sun


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
Frontiers in Vibrational Spectroscopy: Experiments & Theory

Tracking Chemical Reactivity via Vibrations

E. Garand, R. Steele, *Organizers*
S. Luber, *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


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


Section D

Modeling Dynamics in Dense Manifolds of Electronic States

Materials & Surfaces

Cosponsored by COMP
B. G. Levine, P. Slavicek, *Organizers*
B. M. Rubenstein, *Presiding*
8:00 PHYS 218. Nonadiabatic dynamics in noble metal nanoclusters. C.M. Aikens, R.D. Senanayake, P. Pandeya, O. Hull


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


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


9:50 Intermission.
10:00 PHYS 229. Probing ensemble effects on the selective conversion of CO$_2$ 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


11:00 PHYS 231. Thermochemistry of multi principal element alloys. **S. Hayun**, A. Navrotsky


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.


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**


Section G

Orange County Convention Center
Valencia Ballroom B-D - Theater 7

**Sustainable Software for Computational Molecular Science**

**High-Performance & Massively-Parallel Chemistry**
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**


9:50 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.


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**


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
Kinetic Modeling
Sponsored by CATL, Cosponsored by ENFL, ENVIR, 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
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
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, ORGN², 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.


10:40 PHYS 255. Morphology and thermal properties of polymer films by slow deposition. R.D. Priestley

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


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

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

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.


10:25 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
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(MeIm)2. **W. Chen**, N. Ross, N. Greaves


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**


11:00 PHYS 284. Calculation of electric fields for better catalyst design. **V. Vaissier**


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
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


9:35 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.


10:55 PHYS 291. Solvent embedding and molecular response properties. T. Crawford


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


9:50 Intermission.

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**


**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
Producing Equilibrium Amorphous Packings

Making & Transforming Stable Glasses

Cosponsored by COLL and PMSE
Z. Fakhraai, D. Sussman, Organizers
K. K. Mandadapu, Presiding


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.

4:30 PHYS 310. H-atom product channel in the ultraviolet photodissociation of the thiomethoxy radical (CH$_3$S) via the B$_2^\text{A}_2$ state. G. Sun, X. Zheng, Y. Song, J. Zhang

4:50 PHYS 311. Singlet fission in perylenediimide 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


3:00 Intermission.

3:15 PHYS 315. Electronic and vibrational information on "solution species" from cryogenic ion spectroscopy. J. Weber


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
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


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.


3:55 PHYS 324. Solvation structure and Li ion transport in molten Li salt solvate electrolytes. K. Ueno, K. Dokko, M. Watanabe


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

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


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


2:35 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
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*


2:00 PHYS 342. QM/MM in Amber: The past, the present, the future. *A.W. Goetz*


2:40 Intermission.

3:00 PHYS 344. Efficient and sustainable software for many-body molecular dynamics. *M. Riera Riambau*, D.G. Smith, F. Paesani


**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**
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 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 359. Multiple bonds between boron and metal atom: Matrix isolation infrared spectrometry and theoretical calculations of FBMF$_2$ (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 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 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
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 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 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 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 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
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 400. Effect of strain on graphene functionalization dynamics. R.M. Brinn, K.Z. Rinaldi, A. Crowther


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 CH$_3$I Rydberg states with spin-orbit coupling. C. Huang, H. Hao, B.M. Rubenstein


PHYS 409. Mass-selected soft-landing of Au$_6$(PPh$_3$)$_2^{2+}$ 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
PHYS 413. Automatic active space selection for multiconfiguration pair-density functional theory. J. Bao, S. Dong, L. Gagliardi, D.G. Truhlar


PHYS 416. Probing the rotational spectra of methyl-substituted piperidines. E. Johnson, S.T. Shipman


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 423. Withdrawn

PHYS 424. Determining the pH of frozen and annealed solutions using infrared spectroscopy. C. English, R.R. Michelsen


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
| 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 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. Brancalone, 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 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 methylanthracene fluorescence quenching by dimethylaniline. Y. Yan, S. Marshall, B.H. Milosavljevic |
| 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 |
PHYS 449. Computational electronic structure investigations of the photophysics of Cr and group 13 bis(4'-aryltetpyridyl) 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 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 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 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

PHYS 468. Radiation-induced reduction of (TPQ-2)^3+. M. Cover, B.H. Milosavljevic


PHYS 470. Computational studies of the pathways for the reaction of hydroxyl (OH) with ketene. C. Leung, P. Marshall

PHYS 471. Withdrawn


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 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 491. Segmental $^{13}$C-labeling and Raman microspectroscopy of α-synuclein amyloid formation. J.D. Flynn, Z. Jiang, J.C. Lee


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 acidichromism. 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 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 502. Projected site-occupation embedding theory (P-SOET). B. Senjean, E. Fromager
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 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


8:40 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.
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•H₂O 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
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/H$_2$O 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


11:15 PHYS 531. Quantum calculations of vibrational dynamics of the proton and H$_2$ 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. Subasinghege 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
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**


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**


10:00 Intermission.
10:15 PHYS 545. Pore chemistry and size control in anion-pillared hybrid porous materials for highly efficient gas separation. H. Xing


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


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
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


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


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


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


10:55 PHYS 567. Active feedback tracking of single viruses and fluorophores in solution. S. Hou, J. Exell, X. Lang, K. Welsher


**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.


3:30 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
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


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.
3:20 PHYS 584. Infrared spectroscopy hemibonded clusters of H$_2$S. 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


2:10 PHYS 589. Interfacial water at graphene oxide surface: Ordered or disordered? V. Subasinghege 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


3:45 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
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.


4:45 PHYS 603. Insights into the role of counterions on polyelectrolyte-modified nanopore accessibility. E. Gonzalez Solveyra, L. Silles, 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
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 simplectic 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


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


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
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-EI, S. A. Sydlik, Organizers, Presiding

8:10 Introductory Remarks.


8:45 POLY 2. Programming macromolecules to encode functions. V. Percec


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
8:00 Introductory Remarks.

8:05 POLY 8. Densely grafted polymers by ATRP. K. Matyjaszewski


9:50 Intermission.


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 acetics. Y. Guillaneuf


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
10:20 Intermission.

10:35 POLY 20. Extraction, synthesis, and characterization of biopolymers from plant waste. S. Shen, J.A. Thomas, S.A. Miller


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


9:20 POLY 27. Spectroscopic characterization of modified polyethyleneimine. J.D. Mizvesky, R. Wodzinski, M.R. Elshaer


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

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 sulfanyl 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 thermosts 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


9:40 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


10:40 POLY 40. Moisture adsorption of the benzoxazine-based thermostet 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
Rosen Centre Hotel
Salon 21

Poly(2-oxazoline)s & Polypeptoids

R. Hoogenboom, H. Schlaad, R. N. Zuckermann, Organizer
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


9:35 Intermission.

9:50 POLY 45. Amplification of protein detection signal using poly(2-methyl-2-oxazoline) based mixed brushes with switchable properties. Y. Wang


10:50 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, Organizer
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
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


9:40 Intermission.

10:00 POLY 53. Polymer prodrug nanocarriers for anticancer therapy. J. Nicolas


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


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-El, S. A. Sydlak, 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[1,2-4,5-b'] and Naphtho[2,1-b:6,5-b'] chalcogenophenes. M. Jeffries-El, C. Gott, E. Muller, A. Brown

2:30 Intermission.

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


1:30 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.


4:00 POLY 71. Crystallizable α-olefin molecular bottlebrushes: Microstructure evolution during extensional deformation. C.R. Lopez-Barron


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*

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


1:40 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 CO\textsubscript{2} 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
3:20 POLY 84. Chemical recyclability of polar vinyl polymers derived from renewable methylene butyrolactones. **R.A. Gilsdorf, E.Y. Chen**


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**


4:40 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. Geubele, 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**
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


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


2:35 POLY 103. Polyanhydrides from radical-mediated thiol-ene polymerizations: From synthesis to drug delivery. D.A. Shipp

2:55 Intermission.


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


8:35 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


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
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


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


9:45 POLY 135. Improving mechanical properties of fatty acid-derived thermoplastic elastomers by incorporating a transient network. W. Ding, M.L. Robertson
10:10 Intermission.


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.


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


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
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


10:35 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


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
8:55 POLY 155. Redox-responsive PEGylated macrophotosensitizer nanoparticles for enhanced near-infrared imaging-guided photodynamic therapy. L. Yan


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


11:35 POLY 162. Effects of protonation and salt concentration on the structure of polyethyleneimine (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, ENV, 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
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.


3:45 POLY 170. Design of high-precision polymers by multistep synthesis. J. Lutz


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
1:00 POLY 173. Precise control over structure and properties in brush polymers. R.H. Grubbs


2:15 POLY 175. Alkyl wedge-type polymer architectures and their applications as photonic crystals. B. Boyle, G. Miyake


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


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

3:40 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


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


2:55 Intermission.


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
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


2:35 Intermission.


3:35 POLY 199. Sustainable plastics: Using polymer stabilizers to yield recyclable polyolefins. K.M. Knauer, R.E. King


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


2:50 Intermission.
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


4:25 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


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


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
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


8:50 POLY 219. Collages of arts and science. G.R. Newkome


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. OReilly

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


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


Section C
Rosen Centre Hotel
Salon 19

Transport in Polymer Membranes

Flow Batteries & Alkaline Fuel Cells
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


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


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
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


9:45 POLY 247. Macromolecular engineering through metal-free ring-opening metathesis polymerization. P. Lu, A.J. Boydston

10:10 Intermission.


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


Section F
Rosen Centre Hotel
Salon 21

Undergraduate Research in Polymer Science
S. E. Morgan, Organizer
S. Nazarenko, Presiding

8:00 Introductory Remarks.


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


10:45 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
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


9:00 POLY 269. Intracellular delivery of biomolecules via freeze concentration using polyampholyte nanocarriers. K. Matsumura, S. Ahmed


9:40 Intermission.


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. Vergaelen, B. Monnery, C. Vervaet, R. Hoogenboom


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

Sponsored by MPPG, Cosponsored by COLL‡, INOR‡, PMSE‡ and POLY‡

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

Sponsored by CHED, Cosponsored by COLL, I&EC, ORGN², 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


3:55 POLY 282. Modeling the rheological behavior of sulfonated polystyrene ionomers. R.A. Weiss, C. Huang


4:45 POLY 284. New resorbable materials and inks are needed if additive manufacturing will really change medicine. M. Becker

Section B
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


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


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

Transport in Polymer Membranes

Gas Separation

Cosponsored by PMSE‡
M. D. Dadmun, C. M. Stafford, Organizers
T. Saito, Organizer, Presiding
Z. P. Smith, Presiding
1:00 POLY 294. Enhancing CO$_2$/N$_2$ 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 CO$_2$-philic polymers for high flux CO$_2$ separation. T. Hong, P. Cao, B. Li, S. Zhao, A.P. Sokolov, T. Saito


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 CO$_2$/N$_2$ separation properties. **H. Lin**


4:00 POLY 301. Synthesis and characterization of polyimides containing bulky ethyl substituents for propylene/propane separation. **S. Yoo**, H. Park


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


1:25 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

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


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; Anasys 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**


Section F
Rosen Centre Hotel
Salon 21

**Undergraduate Research in Polymer Science**
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**


1:45 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**


2:30 POLY 320. Synthesis of di- and trisalicylide monomers for ring-opening polymerization. **M. Maday, M.D. Scholten**

2:45 Intermission.


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‡
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

Dispersity 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 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 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 tripod 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
POLY 330. Oriented block copolymer domains in fibers. Z. Zhou


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 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

POLY 343. Biod advantaged hydrophobic nylon-6,6 copolymers. S. Abdolmohammadi, N. Hernandez, J. Tessonnier, E.W. Cochran


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 346. Polycarbonate/polypeptide hybrid copolymers for soft tissue adhesives. J. Wilson, A. Heise


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 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 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 368. Development of a cheap, efficient and stable “click” platform to access complex polymer architectures. S. Bailey, J. Read de Alaniz, E. Discekici


POLY 370. Synthesizing macromonomers for brush polymers via anionic polymerization strategies. R.M. Pearson, G. Miyake


POLY 372. Analysis of various synthetic procedures to generate poly(S-r-DVB) by inverse vulcanization. A. Fistrovich, C. Jenkins
POLY 373. Effect on dispersity of end-capping in ATRP-grown surface-initiated brushes. N.H. Vy, D.H. Adamson


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 376. High-temperature polybenzoaxazine resins for aerospace applications. C.L. Crickmore, D.A. Rider


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
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


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 393. Design and development of dual-headed nanosystems: Drug delivery applications. **G. Kaur**, N. Majeti


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


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 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
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 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


Section A

Orange County Convention Center
West Hall C

Transport in Polymer Membranes

Posters

M. D. Dadmun, T. Saito, C. M. Stafford, Organizers
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 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 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 420. Improving the recyclability of PET-PE mixed waste streams. A.F. Bratton, C.J. Ellison, K.M. Miller

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 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-monoureia-3,5-bisamide polymers. K. Bone, M. Raynal


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 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 438. Thermal carbon analysis as a novel tool for examination of transparent polyimide aerogel properties. T. Berg, B. Nespor, A. Kubatova, S.L. Vivod

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 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 sustained 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 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
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.


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. Burridge, 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


Section C

Rosen Centre Hotel
Salon 19
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. Loianno, 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


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


Section D

Rosen Centre Hotel
Salon 7

Polymers & Biomimicry

Concepts in Biomimicry
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


11:00 POLY 482. Bioinspired toughening mechanism of elastomers. K. Ahn

11:25 POLY 483. Biomimetic polymer-based polymersomes as functional biomaterials. S. Lecommandoux


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
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. Bhattacharjee


9:50 Intermission.


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


Section G
General Topics: New Synthesis & Characterization of Polymers

D. Garcia, Organizer
J. Cole, J. Imbrogno, Presiding


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


10:00 POLY 502. Application of core-modified phenoxazine photocatalysts 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 photocatalysts. D. Corbin, B. McCarthy, G. Miyake

11:00 POLY 505. Radical ring-opening copolymerization of cyclic ketene acetalts with vinyl monomers. C. Lefay


WEDNESDAY AFTERNOON

Section A

Rosen Centre Hotel
Signature 2
Dispersity in Block Copolymers: Synthesis, Characterization, Modeling & the Effects on Self-Assembly

Dispersity 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. Daugs, 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


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


1:40 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

2:50 Intermission.

3:20 POLY 518. Cyclic peptide / polymer conjugates for therapeutic applications. S. Perrier


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


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
Polymers & Biomimicry

Concepts in Biomimicry

T. Williams, Organizer
A. N. Dhinojwala, Organizer, Presiding


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


Section E
Ro
sen 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


2:50 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


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. Bleam, N.D. Steese, D. Barvaliya, X. Poole, H.J. Schanz


2:40 POLY 560. Ring-opening reactions to functional polyamides and polyurethanes. K. Odelius


4:00 POLY 564. Halide rebound polymerization of twisted amides. M. Xu, L. Fu, A.M. Nicely, J. Yu, W. Gutekunst
4:20 POLY 565. Relay conjugation and chain-end functionalization of ROMP. **L. Fu**, T. ZHANG, W. Gutekunst


**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


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.


11:00 POLY 578. Lipase-polymer biohybrids. M. Kovalov, S. Averick


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
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**


Section D

Rosen Centre Hotel
Salon 7

**Polymers & Biomimicry**

**Concepts in Biomimicry**

A. N. Dhinojwala, **Organizer**
T. Williams, **Organizer, Presiding**


9:25 POLY 593. Thin films and nanoparticles with nanoscale reactive patches. D. Varadharajan, H. Turgut, H. Yabu, **G. Delaittre**


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**


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.


10:40 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
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


9:50 Intermission.


10:35 POLY 610. Fluorine containing poly-2-oxazolines as contrast agents for 19F 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


11:45 Concluding Remarks.

THURSDAY AFTERNOON

Section A
Rosen Centre Hotel
Signature 2

Dispersity in Block Copolymers: Synthesis, Characterization, Modeling & the Effects on Self-Assembly

Architectural Dispersity 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
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


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


1:20 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.


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
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


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. Gercke, 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
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<tr>
<th>Time</th>
<th>Poly</th>
<th>Title</th>
<th>Authors</th>
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<tr>
<td>1:30</td>
<td>POLY 636.</td>
<td>Micro-nanofibrillar polycaprolactone scaffolds as translatable osteoconductive grafts: An exploration of osteoblast viability, osteogenic phenotype, and innate antibacterial efficacy.</td>
<td>J.W. Moxley, P. Ghannadian, T. Webster</td>
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<td>1:50</td>
<td>POLY 637.</td>
<td>Laser pulse heating of nanocomposites to create self-cleaning superhydrophobic surfaces.</td>
<td>S.F. Bartolucci, J.A. Maurer</td>
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<td>2:10</td>
<td>POLY 638.</td>
<td>Plant-based polyphenol coatings for preparing highly active protein surfaces.</td>
<td>A.M. Sousa, T. Li, S. Varghese, P.J. Halling, K. Lau</td>
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<td>2:30</td>
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<td>Intermission.</td>
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<td>2:40</td>
<td>POLY 639.</td>
<td>Mussel-inspired polyesters with aliphatic pendant groups demonstrate the importance of hydrophobicity in wet adhesion.</td>
<td>A. Narayanan, S. Kaur, A.N. Dhinojwala, A. Joy</td>
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<td>3:10</td>
<td>POLY 640.</td>
<td>Synthesis of bioinspired polymeric adhesives for precise control of properties via well-defined crosslinking chemistry.</td>
<td>H. Chung, I. Pramudya, C. Kim</td>
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<td>3:30</td>
<td>POLY 641.</td>
<td>Fully degradable polycarbonate/polypeptide hybrid copolymer bioadhesives for soft tissue repair.</td>
<td>J. Wilson, A. Heise</td>
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<tr>
<td>3:50</td>
<td>POLY 642.</td>
<td>Synthetic biology enables production of repetitive mussel foot proteins with enhanced underwater adhesion.</td>
<td>E. Kim, F. Zhang</td>
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<td>4:10</td>
<td>POLY 643.</td>
<td>Understanding the bioadhesion of chitosan-catechol polymers.</td>
<td>A. Narkar, K. Ahn</td>
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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 |
1:40 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 |
2:40 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


4:40 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. Hofs, 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


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 Tg PSA to high Tg 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
10:20 PMSE 5. Controlling polymer backbones in ROMP using cycloalkene derivatives. **N.S. Sampson**

10:40 Intermission.


11:30 PMSE 7. Molecular design and activity of sequence-defined antimicrobial macromolecules. **C.A. Alabi**


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**


10:10 Intermission.


Section C

Rosen Centre Hotel
Salon 15
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


9:35 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


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

### PMSE 25. Strain-promoted cycloadditions for the synthesis and functionalization of polymers and nanocomposites.  
**A. Adronov, V. Kardelis, K. Li**

9:30

**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**
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.


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
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


9:30 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


10:50 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. Puretskiy, A. Boker

Innovative Chemistry & Materials for Electrochemical Energy Storage

Li-Ion & Na-Ion

Sponsored by ENFL, Cosponsored by CATL, INOR and PMSE

Unofficial Technical Program draft as of 2/19/2019
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 oligothiophenes. 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
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


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
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


2:10 PMSE 80. 3D-printed, electrically-driven soft actuators based on hydrogel-elastomer hybrids. G. Haghiashhtiani, 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

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. Triphilic pentalock copolymers with a perfluoroalkyl middle block. **J. Kressler**, D. Heinz

2:40 Intermission.


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 micrdomain geometry on reverse micelle mobility within organogels. **W.W. Walker**, K. Mineart


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**

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


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.


1:35 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


3:05 Intermission.

3:25 PMSE 104. Aggregation and coacervation of the tau peptide. J.E. Shea


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.


2:05 PMSE 110. Heavy lifting with soft materials: Layered liquid crystal elastomer actuators. T. Guin, T.J. White


2:45 PMSE 112. Shape-responsive main chain liquid crystalline epoxy elastomers. J.M. McCracken, J.D. Berrigan, T.J. White

3:05 Intermission.


3:50 PMSE 114. Photo-switchable polymer networks. S. Schlögl


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

10:00 PMSE 120. Antifouling coating strategies for antimicrobial applications. Z. Cao


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


9:10 PMSE 128. Adhesion control of human umbilical vein endothelial cells using clickable poly(2-oxazoline)-grafted biosynthesized extracellular matrix protein. A. Takasu


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

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


10:00 Intermission.


10:45 PMSE 138. Localization of nanoparticles controlled by amphiphilic block copolymer. R. Wang


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
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


Section E

Rosen Centre Hotel
Salon 24

Multicomponent Block Polymer Systems

K. Mineart, R. Riggelman, 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


10:10 Intermission.


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
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


9:30 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


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
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.


10:40 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. Grieser, 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


9:40 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


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
1:55 Introductory Remarks.

2:00 PMSE 177. Antimicrobial polymers: Key structural parameters in their performance. L. Yang


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


4:50 PMSE 184. Engineering polymeric biomaterials in the era of antimicrobial resistance. J. Haldar


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
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


3:50 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


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. Puodziukynaitė, B. Okerberg, R. Rock, C.A. Wilson, P. Votrubadrzl

**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.**

3:40 PMSE 209. Impact energy delocalization properties of carbon-based nanomaterials and nanocomposites. **J. Lee**, W. Xie


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.


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**
**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


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. Grieser, *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
2:20 PMSE 230. 3D printing of multifunctional metal oxides via a novel photopolymer system. D. Yee, M.L. Lifson, J.R. Greer


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

Innovative Chemistry & Materials for Electrochemical Energy Storage

Supercapacitors

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Interdisciplinary Chemistry for New Frontiers in Biology and Medicine

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Transport in Polymer Membranes

Block Copolymers, Morphology Control & Poly(ionic Liquids)

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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.


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.
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


9:40 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.


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

10:50 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
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.


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, 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. Winetrout, 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


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. Stryutsky, 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
<table>
<thead>
<tr>
<th>Time</th>
<th>Session</th>
<th>Title</th>
<th>Presenter(s)</th>
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<tbody>
<tr>
<td>8:40</td>
<td>PMSE 277</td>
<td>Backbone engineering of informational polypeptides.</td>
<td>S.H. Gellman</td>
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<tr>
<td>9:05</td>
<td>PMSE 278</td>
<td>New methods to introduce diverse functionality into synthetic polypeptides.</td>
<td>T.J. Deming</td>
</tr>
<tr>
<td>9:30</td>
<td>PMSE 279</td>
<td>Biomimetic membranes based on peptides and polymers.</td>
<td>W. Meier, C. Palivan</td>
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<td>9:55</td>
<td>Intermission.</td>
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<tr>
<td>10:05</td>
<td>PMSE 280</td>
<td>Sequence-controlled polypeptides: Understanding biology via coacervation.</td>
<td>S.L. Perry</td>
</tr>
<tr>
<td>10:30</td>
<td>PMSE 281</td>
<td>Designer polypeptides for enhanced RNA and helper protein co-delivery.</td>
<td>P.T. Hammond</td>
</tr>
<tr>
<td>11:20</td>
<td>PMSE 283</td>
<td>Peptide-mediated surface deposition of polymers and polymer nanoparticles.</td>
<td>H.A. Klok</td>
</tr>
<tr>
<td>11:45</td>
<td>PMSE 284</td>
<td>Chemoselective post-modifications of thermosensitive polypeptides towards bioactive self-assembled materials.</td>
<td>E.B. Garanger, M. Rosselin, Y. Xiao, S. Lecommandoux</td>
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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. Grieser, A. Guymon, S. Marco, S. Schlögl, Organizer
C. Bowman, Organizer, Presiding

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<tr>
<th>Time</th>
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<tr>
<td>8:30</td>
<td>PMSE 285</td>
<td>Photoinitiated heterogeneous radical-mediated thiol-ene polymerizations.</td>
<td>D.A. Shipp</td>
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<tr>
<td>9:20</td>
<td>PMSE 287</td>
<td>Phosphate-based crosslinked polymers from iodo-ene photopolymerization.</td>
<td>J. Sinha, B.D. Fairbanks, M. Chen, H. Song, C. Bowman</td>
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<tr>
<td>10:00</td>
<td>Intermission.</td>
<td></td>
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</tbody>
</table>
10:45 PMSE 290. Photoredox copolymerization to synthesize gradient polyesters. R. Tong

11:05 PMSE 291. Photo-Induced phase separation in dimethacrylate/diepoxide 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

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
Biomaterials Take Form
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Innovative Chemistry & Materials for Electrochemical Energy Storage
Flow Batteries
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Transport in Polymer Membranes

Flow Batteries & Alkaline Fuel Cells

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New Frontiers in Aerospace Polymers: Advances & Challenges in Experiments & Simulations

Bioinspired Materials for Aerospace Composite

Sponsored by POLY, Cosponsored by PMSE

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


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


2:40 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

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


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 copolymer peptide 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
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


2:00 PMSE 312. Crystallization of poly(3-hexylthiophene) on graphitic surfaces with different curvatures. L. Zhai, C. Shen


3:00 Intermission.


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 Pierro, 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.
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


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
1:30 PMSE 329. Structure and behavior of carbon interfaces from multiscale modeling. **B.I. Yakobson**


3:10 Intermission.


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**


1:30 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**


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**
3:45 PMSE 341. Genetically encoded biomaterials that self-assemble across multiple length scales. A. Chikoti


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


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. Braunischweig


3:00 Intermission.

3:15 PMSE 349. Photoinitiators: Reactivity, efficiency, and wavelength dependence. G. Gescheidt


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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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 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


Section A
Orange County Convention Center
West Hall C

PMSE-POLY Poster Session
General Posters/New Concepts in Polymeric Materials
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 362. Polymer chain interaction to improve the properties of flexible polyimides. A. Rivera Nicholls, M. Pellissier, Y. Perez, J. Allan Stock, J. Harmon


PMSE 364. Modifying dextran with stable boronic ester groups to produce an oxidation-sensitive, biocompatible polymer. A. Manaster, C. Batt, 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 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. Jatta, R. Tao, X. Sun, S. Dai
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. Chaisuwon

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 379. Delivery of antimicrobial polymers through coacervation to mitigate toxicity. Z. Voo, C. Alexander, J. Hedrick, Y. Yang


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 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 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 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 405. Resorcinarene-based hierarchically porous polymer networks utilized for water purification. J. Willman, D. Bozdag, 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
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 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. Hambourger, 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 424. Hierarchical open porous black PDMS membrane toward efficient solar to steam generation. K. Go, M. Gil, S. Moon, K. Lee

PMSE 426. Self-assembly behavior of drugs and proteins based on amphiphilic block copolymers. L. Jia, R. Wang


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 434. Tailoring poly(styrene-ethylene-co-butylene-co-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. Schnepper, J. Roles, J.J. Hickman


PMSE 437. Preparation and characterization of starch-brea gum films. M.A. Masuelli


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
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 454. Photosensitizing antimicrobial polymer solid-state composites for water treatment. R. Wodzinski, J.D. Mizvesky, M.R. Elshaer


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. Pichelmayr, T. Griesser


PMSE 459. LiCo$_{0.8}$Fe$_{0.2}$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
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 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 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 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 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 hybriding with exfoliated nanolayered montmorillonite. L. Xing, Y. Ke


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. HYLON, K. Matsumura


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
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 500. Dynamic control of hydrogel crosslinking through reversible sortase-mediated transpeptidation. M. Arkenberg, D. Moore, C. Lin


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
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. Kashfiopour, 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
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
Sponsored by POLY, Cosponsored by PMSE

New Frontiers in Aerospace Polymers: Advances & Challenges in Experiments & Simulations

Posters
Sponsored by POLY, Cosponsored by PMSE

Poly(2-oxazoline)s & Polypeptoids

Posters
Sponsored by POLY, Cosponsored by PMSE

Undergraduate Research in Polymer Science

Posters
Sponsored by POLY, Cosponsored by PMSE

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


9:40 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 acetal s and divinyl ether derivatives. Y. Guillaneuf


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
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.


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


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

8:40 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.


9:55 PMSE 533. Affinity of functionalized graphene and linker molecules to industrial carbon fibers. R. Sarder


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


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
**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


**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

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. Bundlemers: 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


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
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


9:40 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


10:45 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†
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


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


Section B

Rosen Centre Hotel
Salon 16

General Papers-New Concepts in Polymeric Materials

E. Harth, *Organizer*
K. Bullard, J. Jefcoat, *Presiding*


2:30 Intermission.


3:30 PMSE 582. End-on orientation of semiconducting polymer chains and its applications to organic solar cells. **K. Tajima**


Section C

Rosen Centre Hotel
Salon 15

Hybrid Functional Materials from Controlled Assembly of Polymer & Inorganic Nanoparticles

Polymer Film & its Applications
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


3:45 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
2:10 PMSE 595. Stimuli responsive microscale architectures: Two-photon lithography with shape memory polymers. L. Navrazhnykh, J.R. Greer

2:30 Intermission.


3:30 PMSE 598. Conjugated polymers with embedded aggregation-induced emitters. M.D. Cole, R. Holley, R. Meyer, T. Emrick


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
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


2:30 Intermission.


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


1:30 PMSE 614. Towards control of energy migration within dynamic peptide-based supramolecular materials. J.D. Tovar

2:20 PMSE 616. Fast gels and slow gels: Understanding dynamics in a bioconjugated peptide network. R.S. Tu


3:00 Intermission.


3:45 PMSE 619. Coarse-grained modeling of peptide assembly in bulk and at interfaces. M. Shell


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


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

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
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**


9:50 Intermission.

10:10 PMSE 635. Poly(phenylene oxide) based ion conducting polymers for electrochemical applications. **P. McCormack**, G. Koenig, G. Geise


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*

<table>
<thead>
<tr>
<th>Time</th>
<th>Session</th>
<th>Title</th>
<th>Authors</th>
</tr>
</thead>
<tbody>
<tr>
<td>8:30</td>
<td>PMSE 638</td>
<td>Biodegradable polymeric microspheres: Preparation and evaluation.</td>
<td>S. Harsha</td>
</tr>
<tr>
<td>9:10</td>
<td>PMSE 640</td>
<td>Alginate bio-film preparation with aloe vera and cat’s claw, and their chemical, physical, and biological characterization.</td>
<td>S. Kim, M. Elgegren, J. Nakamatsu</td>
</tr>
<tr>
<td>9:30</td>
<td>PMSE 641</td>
<td>Functionalization of self-healing polyelectrolyte multilayer films via thiol-ene click chemistry and its implication to refunctionalizable surface.</td>
<td>S. Cho, N. Zacharia</td>
</tr>
<tr>
<td>9:50</td>
<td></td>
<td>Intermission.</td>
<td></td>
</tr>
<tr>
<td>10:30</td>
<td>PMSE 643</td>
<td>Engineering of specialized 3D printer for rapid prototyping of thermoplastic materials.</td>
<td>T. Mensch, B. Boyle, G. Miyake</td>
</tr>
<tr>
<td>10:50</td>
<td>PMSE 644</td>
<td>Evaluation of large-area projection sintering time and temperature on polyamide-12.</td>
<td>T. Kaur</td>
</tr>
</tbody>
</table>

Section C

Rosen Centre Hotel
Salon 15

**General Papers-New Concepts in Polymeric Materials**

E. Harth, *Organizer*
T. W. Franklin, V. Romani, *Presiding*

<table>
<thead>
<tr>
<th>Time</th>
<th>Session</th>
<th>Title</th>
<th>Authors</th>
</tr>
</thead>
<tbody>
<tr>
<td>8:30</td>
<td>PMSE 645</td>
<td>Flow-induced crystallisation of polymers.</td>
<td>T.W. Franklin, A.J. Ryan, O. Mykhaylyk</td>
</tr>
<tr>
<td>8:50</td>
<td>PMSE 646</td>
<td>PEG-based nanocomposite hydrogels with controlled thermoresponsive gelation and hydrolytic degradation.</td>
<td>T. Maeda, M. Kitagawa, S. Koizumi, A. Hotta</td>
</tr>
<tr>
<td>9:10</td>
<td>PMSE 647</td>
<td>Soft-templated synthesis of lightweight, elastic, and conductive aerogels.</td>
<td>W. Liang, J. Fang</td>
</tr>
<tr>
<td>9:50</td>
<td></td>
<td>Intermission.</td>
<td></td>
</tr>
<tr>
<td>10:10</td>
<td>PMSE 649</td>
<td>Active polymer films from agro-sources used to extend the shelf-life of Italian salamis.</td>
<td>V. Romani, B.D. Olsen, V.G. Martins</td>
</tr>
</tbody>
</table>

Unofficial Technical Program draft as of 2/19/2019
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


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


9:50 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
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


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. Uleri, 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

10:50 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**


8:50 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**


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**

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. Kammakakam, J.E. Bara, K.E. O’Harra

9:50 Intermission.


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‡
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

Wolf from Award

Sponsored by CARB, Cosponsored by CELL, MEDI, ORGN and PROF

Issues Challenging Entrepreneurs & Start-ups

Sponsored by SCHB, Cosponsored by PROF
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.


1:55 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


2:55 Panel Discussion.

3:25 Concluding Remarks.

Hudson Award
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
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, 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


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


10:55 Introductory Remarks.


Senior Chemists’ Career Stories

Chemistry for New Frontiers
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
1:00 Introductory Remarks.

1:05 PROF 11. Supporting diversity in the classroom with open-access chemical assessments. J.R. Silverman


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
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
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
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 20. Progress toward the total synthesis of falcatin A. S.D. Mendoza, S.E. Reisman


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 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 29. Modeling the formation and fate of halogenated estrogens. C. Hutchinson, D.R. Griffith


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
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
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


2:05 SCHB 5. Best practices cyber security. R. Scherer

2:35 Intermission.

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 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
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.


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
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


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
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


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

3:55 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


9:50 Intermission.

10:05 SCHB 38. Creating the quantified skin category: An entrepreneur’s journey. R. Mehendale


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.
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
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
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
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
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


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


11:15 Discussion.

TUESDAY AFTERNOON

Section A
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


2:35 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.


4:15 COMSCI 12. Metal–organic frameworks to the rescue. O.K. Farha


5:15 Discussion.

WEDNESDAY MORNING

Emerging Frontiers in BIOT

Beyond Earth: BIOT’s Role in Space

Sponsored by BIOT, Cosponsored by COMSCI

SCC
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.
MONDAY MORNING

Excellence in Graduate Polymer Research
Biobased, Degradable & Chain-Exchange Polymers
Sponsored by POLY, Cosponsored by PRES, PROF\(^\dagger\), SOCED\(^\dagger\) and YCC\(^\dagger\)

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
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
Undergraduate Research Posters

Computational Chemistry
Sponsored by CHED, Cosponsored by COMP and SOCED

Environmental Chemistry
Sponsored by CHED, Cosponsored by ENVR and SOCED

Geochemistry
Sponsored by CHED, Cosponsored by GEOC and SOCED

Green Chemistry & Sustainability
Sponsored by CHED, Cosponsored by CEI and SOCED

Inorganic Chemistry
Sponsored by CHED, Cosponsored by INOR and SOCED

Medicinal Chemistry
Sponsored by CHED, Cosponsored by MEDI and SOCED
TECHNICAL PROGRAM

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
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‡
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
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
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


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.
1:45 WCC 12. Silanediols in enantioselective catalysis and complex molecule synthesis. A.E. Mattson


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
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*
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†
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


2:40 Intermission.

2:55 YCC 22. Harvesting solar energy for pharmaceutical production in outer space using flow chemistry.  T. Noel


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
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
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.


10:00 YCC 27. Gas-liquid interface studies by molecular beam scattering on water surfaces. C. Lee, I.A. Ramphal, D.M. Neumark


11:15 YCC 30. Vibrational spectroscopy and structure of complex atmospheric clusters. J.J. Kreinbihl, Y. Yang, C.J. Johnson


12:05 YCC 32. Calculation of the peak progression in the vibrational spectrum of HCO₃( H₂O) in the OH stretch region: application of a one-dimensional adiabatic model. B. Henderson, K.D. Jordan
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 CO$_2$ 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


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


4:00 Concluding Remarks.

Fundamentals of Chemistry Outreach Education: From Program Design to Assessment

Sponsored by CHED, Cosponsored by CCA, LSAC, SOCED and YCC