



ACS

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MEETINGS & EVENTS

AUGUST 25-29

2019

SAN DIEGO | CA

CHEMISTRY & WATER

AMERICAN CHEMICAL SOCIETY
FALL 2019 NATIONAL MEETING & EXPO

DRAFT TECHNICAL PROGRAM

as of July 10, 2019

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AGFD

DIVISION OF AGRICULTURAL AND FOOD CHEMISTRY

L. Yu and X. Fan, *Program Chairs*

SUNDAY MORNING – AGFD

SECTION A

San Diego Convention Center
Room 33B

Chemistry & Utilization of Agro-Based Materials Water in Chemistry & Agriculture

Cosponsored by AGRO

A. Biswas, S. Chang, H. Cheng, *Organizers*

M. Appell, *Organizer, Presiding*

- 8:30** Introductory Remarks.
- 8:35** **1.** Biomimetic agrobased materials for food safety. **M. Appell**, M.A. Jackson, K.O. Evans, D.L. Compton, W. Bosma
- 9:05** **2.** Developing novel catalytic coupling of phenols for efficient lignin biomass utilizations. **C. Li**
- 9:35** **3.** Assessing water quality of runoff water in irrigated rice cropping systems in Arkansas. **A.A. Adviento-Borbe**
- 10:05** Intermission.
- 10:20** **4.** Long-term persistence of polymer hydrogels in silt loam soil: Soil water retention. **R. Lentz**
- 10:50** **5.** Chitosan biopolymer particles decorated with synthetic polymer for the removal of EDCs by adsorption from water. **X. Solimando**, M.F. Cunningham, P. Champagne

SECTION B

San Diego Convention Center
Room 33A

Novel Structures from Food Biopolymers for Delivery of Bioactive Components

Y. Zhang, *Organizer*

A. Luo, Q. Wang, *Organizers, Presiding*

- 8:00** Introductory Remarks.
- 8:05** **6.** Milk fat globules: Universal delivery systems for bioactives. **N. Nitin**, M. Alshehab
- 8:35** **7.** Molecular encapsulation of bioactive compounds by starch-guest inclusion complex. **J. Guo**, **L. Kong**

- 9:05** **8.** Withdrawn
- 9:35** **9.** Novel self-assembly strategy for high efficiency delivery system based on polyphenol self-polymerization. **D. Wu**, H.S. Liang, B. Li
- 10:05** Intermission.
- 10:20** **10.** Computer-assisted design for stable porous metal-organic framework (MOF) as a carrier for curcumin delivery. **Q. Wang**
- 10:50** **11.** Octenylsuccinate hydroxypropyl phytoglycogen to enhance the solubility and *in vitro* permeation of resveratrol. **J. Chen**, Y. Yao
- 11:20** **12.** Natural fluorescent L-histidine crystals surface-functionalized with tumor-specific self-degradable hydrogels for systemic delivery of hydrophobic small molecules. R. Ravanfar, **A. Abbaspourrad**

SECTION C

San Diego Convention Center
Room 32B

Food Phenolics: From Bitterness & Astringency to Health-Promoting Properties

K. G. Lee, C. Osorio Roa, Y. Wang, *Organizers, Presiding*

- 8:00** Introductory Remarks.
- 8:05** **13.** Redox reactivity of phenolics in sweet sorghum and sugarcane. **S.M. Uchimiya**
- 8:30** **14.** Green, all-natural approach to extracting antioxidants from rosemary leaves. **S. Ginsburg**, F. Maleky
- 8:55** **15.** Polyphenols in cells: Critical examination. **J.A. Vinson**
- 9:20** **16.** Reducing phenolic compounds related to bitterness in table olives using amberite resins: Influence of pH and salt. **A.E. Mitchell**
- 9:45** Intermission.
- 10:00** **17.** Role of sour guava (*Psidium friedrichsthalianum* Nied.) fruit polyphenols on human gut microbiota. C. Cuadrado, M. Pozo-bayon, **C. Osorio Roa**
- 10:25** **18.** Physical complexation between phenolic acid and starch can modulate starch digestibility and intestinal glucose absorption from model starch food systems. **M. Li**, C. Ndiaye, S. Corbin, E.A. foegeding, M.G. Ferruzzi

- 10:50** 19. Molecular-sensory studies on key bitter and astringent compounds in hazelnuts. **A. Dunkel**, B. Singldinger, T. Hofmann
- 11:15** 20. Identification of somatosensory compounds in prunes. **S.A. Deshpande**, D.G. Peterson
- 11:40** Concluding Remarks.

SECTION D

San Diego Convention Center
Room 32A

Metals & Trace Elements in Food Safety, Health & Food Quality

Toxicology

Cosponsored by AGRO

L. Jackson, B. Redan, *Organizers, Presiding*

- 8:30** Introductory Remarks.
- 8:35** 21. Overview of USDA-FSIS heavy metals monitoring program. **L. Zipperer**
- 9:05** 22. Survey of cadmium and lead in cocoa powder and chocolate products in the U.S. market. **E. Abt**, J. Fong Sam, P.J. Gray, L.P. Robin
- 9:35** 23. Use of food processing aids in manufacturing: Potential sources of trace metal contaminants and methods for remediation. **B. Redan**
- 10:05** Intermission.
- 10:20** 24. Novel mechanism for potential adverse effects induced by foodborne titanium dioxide nanoparticles: Gut microbiota dysbiosis. X. Cao, H. Du, **H. Xiao**
- 10:50** 25. Health risks of dietary cadmium exposure in Shanghai residents, China. **G. He**, J. Yang, Y. Qing
- 11:20** 26. Withdrawn

CRISPR/Gene Editing & RNAi: Utilization for Enhanced Crop Production

Sponsored by AGRO, Cosponsored by AGFD and BIOL

SUNDAY AFTERNOON – AGFD

SECTION A

San Diego Convention Center
Room 33B

Chemistry & Utilization of Agro-Based Materials Value-Added Products from Agricultural Raw Materials

Cosponsored by AGRO

M. Appell, A. Biswas, S. Chang, H. Cheng, *Organizers*
Z. Liu, *Presiding*

- 1:30** 27. Preparation of polysaccharide-based functional soft materials using ionic liquids. **J. Kadokawa**
- 2:00** 28. Advanced biopolymers for environmental and biomedical applications. **S. Sun**
- 2:30** 29. Development of a two-step process for the production of D-tagatose from whey permeate. S. Cheng, **S. Martinez-Monteagudo**
- 3:00** 30. Novel biobased and biodegradable thermoplastic polymer. **S.D. Luebben**
- 3:30** Intermission.
- 3:45** 31. Development of new vegetable oil-based antimicrobial polymers. **K. Huang**, H. Ngo, X. Fan, R. Ashby, R. Moreau
- 4:15** 32. Modified tung oil-based fatty acid esters used as diesel additives to give improved lubricity. **Z. Liu**, J. Li, G. Knothe, B. Sharma, J. Jiang
- 4:45** 33. Effects of water addition and microwave on natural deep eutectic solvents (NADES) and their extraction properties. A.V. Gomez, A. Biswas, C.C. Tadani, **H.N. Cheng**

SECTION B

San Diego Convention Center
Room 33A

Novel Structures from Food Biopolymers for Delivery of Bioactive Components

Q. Wang, *Organizer*

A. Luo, Y. Zhang, *Organizers, Presiding*

- 1:30** 34. Novel protein-lipid composite nanoparticles as delivery systems of hydrophilic nutraceutical compounds. **L. Chen**, G. Liu, Z. Tian
- 2:00** 35. Formation and characterization of zein-oleic acid oleogels. **G.W. Padua**
- 2:30** 36. Preparation and characterization of zein and gum arabic binary nanocomplexes in aqueous ethanol. **C. Sun**, J. Song, Y. Fang
- 3:00** 37. Withdrawn
- 3:30** Intermission.
- 3:45** 38. Effects of polysaccharides incorporating into sodium caseinate-high melting point fat microparticles to the survival of probiotic bacteria during simulated gastrointestinal digestion and storage. **H. Liu**, S. Nie, J. Gong, S.W. Cui, F. Zhong, Q. Wang
- 4:15** 39. Synthesis and characterization of alkylated caseinate, and its structure-curcumin loading property relationship in water. **Y. Zhang**, F. Yao, L. Jie, L. Yu
- 4:45** 40. Development of cereal prolamin based nanoparticles as oral drug delivery system. **Y. Zhang**

SECTION C
San Diego Convention Center
Room 32B

Food Bioactives: Chemistry & Health Effects

Cosponsored by AGRO

F. Shahidi, C. Udenigwe, *Organizers, Presiding*

- 1:30** Introductory Remarks.
- 1:35** **41.** Multidisciplinary strategy for the investigation of legume derived multifunctional peptides. **C. Lammi**, R. Pugliese, C. Bollati, G. Aiello, A. Arnoldi
- 2:05** **42.** Effect of whey peptides on metabolism and insulin signaling in muscle and fat cells. **K. D'Souza**, A. Mercer, H. Mawhinney, T. Pulinilkunnil, **C. Udenigwe**, P.C. Kienesberger
- 2:35** **43.** Functionality and bioactivity of edible bioplastics derived from yellow pea proteins. **C. Acquah**, E. Di Stefano, Y. Zhang, M. Dube, C. Udenigwe
- 3:05** Intermission.
- 3:20** **44.** Role of plastin structure in biomolecular interactions of peptides. **I.D. Nwachukwu**, S. Yao, C. Acquah, C. Udenigwe
- 3:50** **45.** Impact of dietary γ -glutamylvaline (EV) against TNF- α induced inflammatory response in adipocytes via the activation of CaSR and PPAR- γ pathways. **Y. Mine**
- 4:20** **46.** Bioactive peptides in cured meats and its health relevance. **F. Toldra**, M. Gallego, M. Aristoy, M. Reig, L. Mora

SECTION D
San Diego Convention Center
Room 32A

Metals & Trace Elements in Food Safety, Health & Food Quality

Food Quality and Safety

Cosponsored by AGRO

L. Jackson, B. Redan, *Organizers, Presiding*

- 1:30** **47.** Transition metals: Multifaceted catalysts of lipid oxidation and degradation of food quality. **K.M. Schaich**
- 2:00** **48.** Role of iron in meat pigment and quality. **F. Shahidi**
- 2:30** **49.** Effects of copper-based fungicides on Pennsylvania hop quality. **B. Chrisfield**, B. Gugino, H. Hopfer, R. Elias
- 3:00** Intermission.
- 3:15** **50.** Heavy metal speciation in agricultural soils. **S.M. Uchimiya**

- 3:45** **51.** Fate of silver nanoparticles in lettuce wash water as impacted by chlorine and organic matter. **G. Gunathilaka**, J. He, H. Li, W. Zhang, E. Ryser
- 4:15** **52.** Interaction of leafy vegetable romaine lettuce (*Lactuca sativa L. var. Longifolia*) with coexisting of ZnO nanoparticles and divalent heavy metals (Cd and Pb) with and their in planta accumulation. **H. Sharifan**, J. Moore

SECTION E
San Diego Convention Center
Room 31C

Agnes Rimando Memorial International Student Symposium

Biomedical & Biochemical Research

Cosponsored by AGRO

B. Gao, R. Tardugno, M. H. Tunick, *Organizers*
M. Granvogl, *Organizer, Presiding*

- 1:30** Introductory Remarks.
- 1:35** **53.** Procyanidin B2 attenuates metabolic syndrome by promoting TFEB nuclear translocation and restoring redox status. **H. Su**, W. Chen
- 1:55** **54.** Withdrawn
- 2:15** **55.** Identification of a human gut bacterial strain with anti-inflammatory and anti-cancer properties. **Y. Sun**, E. Zhao, M. Gu, H. Xiao
- 2:35** **56.** Gut microbiota-mediated protective effects of whole strawberry against colonic inflammation. **Y. Han**, H. Xiao
- 2:55** Intermission.
- 3:10** **57.** Anti-inflammatory and anti-cancer effects of free and bound polyphenols from *Laminaria japonica*, a widely consumed seaweed. **Y. Gao**, L. Yi, Y. Yang, Y. Han, H. Xiao
- 3:30** **58.** Absorption and metabolism of curcumin in different type of nanoemulsion. **H. Luo**, **Z. Li**, D. McClements, E.A. Decker, H. Xiao
- 3:50** **59.** Piceatannol protects human retinal pigment epithelial cells against hydrogen peroxide mediated oxidative stress and apoptosis through PI3K/Akt signaling pathway. **Y. Hao**, Z. Wang, J. Liu, J. Wang
- 4:10** **60.** Dietary intake of king oyster mushroom (*Pleurotus eryngii*) ameliorated dextran sulfate sodium-induced colitis in mice. **H. Du**, B. Yuan, Y. Han, M. Gu, Q. Hu, H. Xiao

Agrochemical Residue & Metabolism Chemistry

Sponsored by AGRO, Cosponsored by AGFD

SECTION A
San Diego Convention Center
TBD

General PostersL. Yu, *Organizer***5:30 - 7:30**

- 61.** Plasticizer di-(2-ethylhexyl) phthalate (DEHP) in vegetables and fruits. **X. Cao**
- 62.** Espresso from first principles: Route to highly reproducible cup quality. **C.H. Hendon**
- 63.** Effect of organic selenium supplementation in cattle on mozzarella cheese quality and antioxidant activity. Z. Liu, Y. Xiao, J. Liu, **D. Ren**
- 64.** Enzyme inhibition, antioxidant, and insecticidal activities of flavonoids and fixed oil from *Albizia zygia* (J. F. Macbr). **G.K. Oloyede**, M.S. Alli, M. Lateef
- 65.** Potential evaluation of *Ganoderma formosanum* extract against PM_{2.5}-induced ROS generation. **S. Chen**, Y. Chan, K. Cheng
- 66.** Screening of yeasts from fruits for grape wine production. **L. Tien-Han**, Y. Lai, K. Cheng
- 67.** Chemical compositions of commercial chrysanthemum tea samples and their anti-inflammatory and antioxidant properties. **L. Yanfang**, P. Yang, Y. Luo, B. Gao, J. Sun, W. Lu, J. Liu, P. Chen, Y. Zhang, L. Yu
- 68.** Immobilized of laccase for ginkgolic acid degradation. **H. Chen**, K. Cheng, Y. Ting
- 69.** Evaluation of *Ganoderma formosanum* extract against PM_{2.5}-induced ROS generation and cell damage. **Y. Hsu**, Y. Chan, K. Cheng
- 70.** Insulin regulates the expression and translocation of GLUT8 to increase glucose uptake in bovine mammary epithelial cells. Y. Li, W. Dai, Q. Wang, J. Liu, **H. Liu**
- 71.** Trans-10, cis-12 conjugated linoleic acid reduced the activity of nSREBP1 in bovine mammary epithelial cells via altering SCAP and INSIG1 expression. **H. Shi**, D. Tai, C. Wang, J. Liu, H. Liu
- 72.** Study on fatty acid profile, flavour, and quality of mozzarella cheese made from a high omega-3 milk produced by lactating cow fed with flaxseeds diet. **D. Ren**, C. Wang, C. Liu, X. Wang, J. Liu, M. He, H. Wang
- 73.** Evaluation of the phytochemical and fatty acids compositions of *Vernonia amygdalina*, *Ocimum gratissimum* and *Telfairia occidentalis* leaves. P.B. Ayoola, **O.O. Onawumi**
- 74.** Effect of ethylene content in EVOH films on

activation energies of diffusion of organic migrants and polymer modeling parameters. **J.L. Koontz**, Y.S. Song, A. Sarang

75. Immobilization of reporter bacteriophage PP01 on electrospun PHB fibers for *Escherichia coli* O157:H7 detection. **S. Chen**, M. Harrison, D. Sauvageau, A. Elias

76. Identification of aroma compounds in frozen surimi made from silver carp (*Hypophthalmichthys molitrix*) by normal phase chromatography fractionation and gas chromatography/olfactometry. **Y. An**, Y.L. Qian, S. Xiong, M.C. Qian

77. Uptake of cadmium and arsenic by radishes grown in bat guano amended soil and remediation using modified natural zeolites. **s. carrillo**, S. Crawford

78. Development of a biocontrol agent using rice husk biochar with *Bacillus* sp. IA. **T. Ano**, S. Ebe, T. Ohike, M. Okanami

79. Comparing tomato seed flour and oil as potential value-added products. **E.R. Bailoni**, U. Choe, Y. Li, B. Gao, L. Yu

80. Study on fatty acid profile, flavor, and quality of mozzarella cheese made from high omega-3 milk produced by lactating cows fed with flaxseeds diet. **D. Ren**, C. Wang, C. Liu, X. Wang, J. Liu, **M. He**, **H. Wang**

81. Enhanced bacterial cellulose production using response surface methodology for *Komactobacter intermedius*. **C. Chou**, K. Cheng

82. Bakkenolides and caffeoylquinic acids from the aerial portion of *Pestisites japonicas* and their bacterial neuraminidase inhibition. **H. Woo**, H. Cho, Y. Oh, Y. Kim, **D. Kim**

83. Effective application of anode solution in microbial fuel cell to agriculture. **Y. FUKUMOTO**, S. Ebe, T. Ohike, M. Okanami, T. Ano

84. Isolation of anticancer constituents from *Cucumis prophetarum* var. prophetarum through bioassay-guided fractionation. **A. Alsayari**

85. Interactions between casein and sodium phosphate salts in processed cheese using surface-enhanced Raman spectroscopy. **A.P. Barth**, Y. Qu, C.B. Karaziack, W.H. Viotto, L. He

86. Pectin extraction from lemon peels and characterization. **A. Rukhadze**, **S. Mestvirishvili**, N. Kokiashvili

87. Hazard characterization of commercial products of dark brown sugar in Taiwan using fluorescence spectroscopy. Y. Lin, G. Yen, **J. Lin**

88. California elderberries: Model for the utilization of hedgerow crops as a source of value-added compounds for improving agricultural sustainability. **K. Uhl**, S. Brodt, K. Fyhrie, A.E. Mitchell

- 89.** Chemical composition of cold-pressed blackberry seed flour and its free radical scavenging and anti-inflammatory capacities. **U. Choe**, Y. Li, B. Gao, J. Sun, P. Chen, L. Yu
- 90.** Triterpenoids from *Acanthopanax trifoliatus* attenuate inflammation in macrophage cells and tetradecanoylphorbolacetate-treated mice. M. Chen, Y. Qin, H. Ma, X. Zheng, R. Zhou, S. Sun, Y. Huang, Q. Duan, P. Wu, X. Xu, W. Liu, Z. Sheng, K. Zhang, **D. Li**
- 91.** Acid-triggered gastric-floating emulsion gel for sustained release. X. Liu, L. Wang, H.S. Liang, J. Li, B. Li
- 92.** Metabolic profiling of leaf secondary metabolites in Japanese citrus cultivars under stress conditions. **T. Matsukawa**, S. Kajiyama
- 93.** Antioxidant activities and constituents of leaves and fruits of a Japanese persimmon (Fudegaki). **M. Yasuda-Torii**, M. Inuzuka, K. Furuhashi, A. Nagata
- 94.** Comparison of volatile compounds in garlic extracts according to different extraction methods. **E. Jang**, S. Lee, Z. Shim, M. Jeon, D. Lee, Y. Kim
- 95.** Relationships between protein composition and texture of tofu made from soybeans planted in three locations. R. Chen, **S.K. Chang**, A. Gillen, P. Chen, B. Zhang, Y. Zhang
- 96.** Characterization of food additive silica nanoparticles in commercial products. **S. Choi**
- 97.** Charge-switchable starch magnetic microparticles for highly effective separation of a broad range of bacteria. **K. Luo**, K. Jeong, S. You, H. Adra, J. Ryu, Y. Kim
- 98.** Alpha-hederin nanopore for single-molecule detection. **K. Jeong**, K. Luo, Y. Kim
- 99.** Solid-state fermentation for development of functional *Chenopodium formosanum* product. T. Chien, H. Chen, **K. Cheng**
- 100.** Nutritional analysis and study of shiitake mushrooms focusing on the dietary fiber content. **J. Lee**, J. An, S. Kim, D. Seo
- 101.** Significant 19 amino acid analysis using three eggs and determination of LOD and LOQ. **S. Kim**, D. Seo, J. Lee
- 102.** Comparison of mineral contents in raw and boiled poultry eggs by ICP-OES and ICP-MS. **D. Seo**, S. Kim, J. Park, S. Kim, J. Lee
- 103.** Analysis of chemical diversity in *Lilium japonicum* population using floral scent composition. **M. Fujisawa**, T. Matsukawa, T. Akino, S. Arai, Y. Takikawa, S. Kajiyama
- 104.** Purification and identification of a putative sperm chemoattractant in the liverwort *Marchantia polymorpha* L. **Y. Yamasaki**, M. Takemura, T. Matsukawa, K. Yamato, S. Kajiyama
- 105.** Withdrawn
- 106.** Protein engineering of recombinant α -D-glucose isomerase from *Actinotalea fermentans* ATCC 43279 to alter its thermostability. **T. Fang**, Y. Liou
- 107.** Paper-based radial flow immunoassay for the detection of *Escherichia coli* O157:H7 using surface-engineered gold nanoparticles. **J. Ryu**, K. Luo, I. seol, K. Jeong, H. Adra, Y. Kim
- 108.** Molecular self-assembly of chitosan/starch-based nanoparticles for drug delivery system. **H. Adra**, K. Luo, D. Lee, K. Jeong, J. Ryu, Y. Kim
- 109.** Withdrawn
- 110.** Bio-based antioxidants for lubricant additives. **Y. Cao**, K.E. Uhrich
- 111.** Difference in the aroma profiles of mealworm (*Tenebrio molitor*) according to cooking methods. H. Seo, D. Kim, **I. Cho**
- 112.** Accumulation of P3HB by *Methylocystis parvus* MK using methane gas produced from anaerobic digestion of rice straw. **M. Kim**, B. Kim, Y. Choi, K. Nam
- 113.** Studying plant-insect interactions with solid phase microextraction: Screening for airborne volatile emissions response of soybeans to the soybean aphid, *Aphis glycines* Matsumura (Hemiptera: Aphididae). **L. Cai**, J.A. Koziel, M.E. O'Neal
- 114.** Metabolic profiling of secondary metabolites in phorbol ester containing and deficient *Jatropha curcas* seeds. **K. Matsukubo**, T. Matsukawa, S. Kajiyama
- 115.** Comparative transcription and experimental analysis of photosensitive and non-photosensitive eggplant to identify genes involved in dark regulated anthocyanin biosynthesis. **Y. Liu**, H. Chen, Y. He
- 116.** Volatile sulfur compounds exudated from roots of garlic plants and their activities toward the germination of spore of fungus *Sclerotium cepivorum*. **Y.L. Qian**, M.C. Qian, J. Dung
- 117.** Identification of volatile compounds of blended coffee bean and application of principal components analysis. **Y. Lee**, **H. Kim**, D. Hong, J. Yu
- 118.** Aroma characterization of oolong teas using ITEX dynamic headspace and SPME arrow coupled with gas chromatography-mass spectrometry. Y. Lin, W. Chang, S. Li, M. Pan, C. Ho, **C.Y. Lo**
- 119.** Newly recognized phosphine resistance mechanisms in the rice weevil, *Sitophilus oryzae*. **K. Kim**, H. Jeon, S. Lee
- 120.** Noble biomarkers in *Eisenia fetida* induced by CuO nanoparticles. **H. Jeon**, K. Kim, S. Lee
- 121.** Green energy generation in a metal-organic framework implemented in electrochemical

- reactors and microbial fuel cells. **H. Jeon**, K. Kim, S. Lee
- 122.** Saudiarabicain A–E, macrocyclic diterpenoids from *Euphorbia saudiarabica*. **A.J. Bin Muhsinah**, Y. Liu, N. DaSilva, A. Alsayari, N.P. Seeram
- 123.** Extraction and biological evaluation of polysaccharides from Niudali (*Millettia speciosa* champ.) roots. **X. Tang**, Y. Lu, D. Li, N.P. Seeram, H. Ma
- 124.** Effects of particle size on protein extraction from catfish by-products. **Y. Zhang**, S.K. Chang
- 125.** Ochratoxin A analysis in wine and grape juice using LC-fluorescence detection with nanosponge solid phase extraction clean-up. **M. Appell**, K.O. Evans, M.A. Jackson, D.L. Compton
- 126.** Phospholipid quantitation in whey matrices by HILIC chemistry UPLC-ELSD: Industry developed, validated, and applied method for determining phospholipid composition. **Q. Ferraris**, J. Hale, E. Teigland, A. Rao, M.C. Qian
- 127.** Differentiation of commercial vanilla extracts by volatile and non-volatile chemical profiles employing GC-MS and UPLC-UV-ESI-QTOF-MS: A market basket authenticity study. **J. Godshaw**, R. Rucker
- 128.** Sustainable conformational modification of soy proteins by physical and chemical treatments. **J. Zou**, N.T. Nguyen, G. Sun
- 129.** Differential proliferation of bacterial species under varying poised potentials and its functional implications in bioelectrochemical denitrification. **T. Brandon**, A. Cummings, X. Wang, B. Stamps, D. Jiang
- 130.** Atmospheric cold plasma promoted mung bean sprouting and the content of bioactive components. **Y. Chou**, Y. Ting, J. Wu, K. Cheng
- 131.** Long-term impact of mushroom derived β -glucan on obesity and gut microflora in mice fed with high fat diet. **M. Cho**, M. Karthika, Y. Kim
- 132.** Comparison of the adhesive performance of water- and alkali-soluble cottonseed protein. **Z. He**, H. Cheng
- 133.** Detection of *Vibrio parahaemolyticus* in marine foods based on denatured bubble-mediated isothermal nucleic acid amplification. X. Zhao, C. Yan, **C. Ma**
- 134.** Characterization of cadmium absorption and translocation in amaranth affected by iron deficiency. **H. Fan**, R. Zou, L. Wang
- 135.** Exploration of the compositional changes of Californian Hass and Gem avocados throughout the season and its effect on avocado flavor. **B. Hausch**, D.M. Obenland, M. Arpaia
- 136.** Implications of the acid/base profile of food chemicals. **M.G. Santibanez-Moran**, M. Rico-Hidalgo, D. Manallack, J.L. Medina-Franco
- 137.** Comparative study of safety, nutrition and flavor of aronia berry (*Aronia melanocarpa*) grown in the United States. **X. Xie**, T. Yi, W. Fang, C. Xu
- 138.** Acylated glucose for integrated pest management in greenhouse production of tomatoes. H.M. Payne, D. Payne, B. Liedl, **M.W. Fultz**
- 139.** Phenolic compound profile and physiological activities of fermented blueberries. **S.K. Cho**, J. Ryu
- 140.** Removal of dilute ethylene using repetitive cycles of adsorption and plasma-catalytic oxidation over Pd/ZSM-5 catalyst. S. Kim, **Y. Mok**
- 141.** Linear and non-linear calibration approaches for the rapid quantification of marine oil omega-3 supplements using vibrational spectroscopy. **S. Karunathilaka**, B. Yakes, S. Choi, L. Brückner, Z. Ellsworth, M.M. Mossoba
- 142.** Efficient engineering of T4 bacteriophage via CRISPR-Cas9. **M.M. Duong**, S.R. Nugen
- 143.** Protein oxidation in food: Focus on individual structures. P. Richter, **M. Hellwig**
- 144.** Identification of predominant contributors to off-odors in thermally processed muskmelon juice using multidimensional gas chromatography techniques and comparative aroma extract dilution analysis. **X. Pang**, K.R. Cadwallader, F. Kong
- 145.** Plant and dairy protein and their covalent interactions with flavor. **V. Anantharamkrishnan**, G.A. Reineccius
- 146.** Effect of thermal sterilization on the aroma profile of Lychee (*Litchi chinensis* Sonn.) juice. **K. An**, Y. Xu, M.C. Qian
- 147.** Fondness for ethanol: Influence of host tree chemistry on fungiculture by ambrosia beetles. **C. Ranger**, P. Biedermann, V. Phuntumart, G. Beligala, S. Ghosh, R. Mueller, P. Schultz, M. Reding, J. Benz
- 148.** Differences in lipid content of young and aged Pinot Noir wines and their impacts on wine mouthfeel perception. **Q. Phan**, E. Tomasino
- 149.** Identifying hyperstable proteins in legumes: Implications for food allergy and intolerance, and GMOs. **W. Colon**, J. Thibeault, K. Xia
- 150.** Analysis of fungicides by liquid chromatography-mass spectrometry. **R. Raina-Fulton**, A. Mohamad, A. Behdarvandan
- 151.** Chemical composition of a red sorghum variety (Ji Liang No.1) and its antioxidant and anti-inflammatory properties. **Y. Zhang**, M. Li, H. Gao, B. Wang, T. Xu, B. Gao, L. Yu
- 152.** Establishment of a stable human small intestinal and colonic microbiota in an *in vitro* cultivar: Form vs. function and response to oxygen. **J. Firrman**, P. Tomasula, L. Liu
- 153.** Chemical compositions and antioxidant properties of cold-pressed edible seed flours. **Z. Song**, L. Yanfang, B. Gao, L. Yu

154. Sensory properties and consumer acceptance of mushroom-egg white blends. **X. Du**, J. Sissons, A. Muniz, M. Shanks

155. Novel metal–organic frameworks for encapsulating curcumin to achieve controlled release. **Q. Wang**, **P. Ma**

156. Effect of fragmentation degree on sensory and texture attributes of cooked rice. **Z. Wang**, H. Su, X. Bi, M. Zhang

157. Gypenosides prevent obesity and insulin resistance in C57BL/6J mice by improving thermogenesis in association with alleviating gut dysbiosis. **J. Liu**, L. Yanfang, P. Yang, L. Yu

158. Triacylglycerols composition analysis of olive oils by ultra-performance convergence chromatography combined with mass spectrometry. **Y. Luo**, B. Gao, L. Yu

159. Analysis of triacylglycerol, sterol, and tocopherol compositions of oils from 8 different berry seeds by ultra-performance convergence chromatography–quadrupole time-of-flight mass spectrometry. **B. Gao**, Y. Luo, F. Yuan, Y. Zhang, L. Yu

Novel Structures from Food Biopolymers for Delivery of Bioactive Components

A. Luo, Q. Wang, Y. Zhang, *Organizers, Presiding*

8:00 **166.** Lignin and hemicelluloses isolated from the largest bamboo species: *Dendrocalamus sinicus*. **Z. Shi**, C. Wu, G. Xu, J. Zhang, M. Dong, C. Liu, **Z. Guo**

8:30 **167.** Formation of coacervated Pickering emulsions: Effect of the interactions between protein and polysaccharide. **Y. Yuan**, M. Li, S. He

9:00 **168.** Development of phospholipid-based pterostilbene nanoemulsion system: Preparation, storage stability, and oral bioavailability. **Y. Ting**, F. Sun, Y. Chou

9:30 **169.** Industrially scalable complex coacervation process for microencapsulation: Robust protection and effective delivery. **Y. Tang**, H.B. Scher, T. Jeoh
Intermission.

10:00 **170.** Development of GI-stable lipid–polymer hybrid nanoparticles for potential oral delivery of astaxanthin. **Y. Luo**, T. Wang

10:45 **171.** Enhanced stability and bioaccessibility of resveratrol infused in grape skin powder. **R. Rai**, N. Nitin

11:15 **172.** Cellulose-coated emulsions with multilayered structure for microencapsulation. **Y. Cohen**, S. Napso, D. Rein

11:45 Concluding Remarks.

SECTION C

San Diego Convention Center
Room 32B

Food Bioactives: Chemistry & Health Effects

Cosponsored by AGRO

F. Shahidi, C. Udenigwe, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 **173.** Antidiabetic and anti-inflammatory potential of isolated compounds from bitter melon: *In vitro* and *in silico* approaches. S. Shivanagoudra, W. Perera, J. Perez, G. Athrey, Y. Sun, C. Wu, G.K. Jayaprakasha, **B. Patil**

9:05 **174.** Phytochemical screening and antioxidant activities of *Irvingia gabonensis* and its effect on alloxan induced diabetes rats. **O.E. Ogunjinmi**, M.O. Abdulganeey, I.A. Salaudeen,

9:35 **175.** Wheatscan: Unraveling the causes for wheat sensitivities. **D. Pronin**, K. Scherf

10:05 Intermission.

MONDAY MORNING – AGFD

SECTION A

San Diego Convention Center
Room 33B

Chemistry & Utilization of Agro-Based Materials

Agro-Based Fibers & Textiles

Cosponsored by AGRO

M. Appell, A. Biswas, H. Cheng, *Organizers*

S. Chang, *Organizer, Presiding*

8:30 **160.** Gating infrared radiation in a textile. **Y. Wang**

9:00 **161.** Value-added uses for raw cotton and cotton by-products. **A.F. Bopp**, V. Edwards, B.D. Condon

9:30 **162.** Novel technologies development for the value added cotton fabrics. **S. Chang**, B.D. Condon, J. Smith

10:00 Intermission.

10:15 **163.** Preparation and evaluation of composites comprising polypropylene and cotton gin trash. **M.J. Miri**, J.B. Francis, S.M. Demyttenaere, N.A. Alharbi, C. Ge, R.K. Hailstone, H.N. Cheng

10:45 **164.** Imaging of cotton fiber maturity using an infrared focal plane array detector. **M. Santiago**

11:15 **165.** Variation in the level of metals on raw, scoured, and bleached varietal cotton samples produced in different locations. **C.A. Fortier**, C.D. Delhom, M.K. Dowd

- 10:20 176.** Chemistry of psilocetin: Prodrug of psilocin. **D.R. Manke, A.R. Chadeayne**
- 10:50 177.** Cytotoxic and antioxidant activity from Andean mashua (*Tropaeolum tuberosum* R. & P.) extract against prostate (DU-145) and human breast (MCF-7) cancer cell lines. **I. Best, J. Arenas, J. Iglesias, O. Reategui Arevalo, J. Arcos**
- 11:20 178.** Amination as a novel metabolic pathway of myricetin in mice. **S. Zhang, R. Wang, Y. Zhao, F. Tareq, S. Sang**

SECTION D

San Diego Convention Center
Room 32A

Metals & Trace Elements in Food Safety, Health & Food Quality

Health & Nutrition

Cosponsored by AGRO

L. Jackson, B. Redan, *Organizers, Presiding*

- 8:30 179.** Changes in the elemental profiles of grapes and wines from the vineyard through processing. **C.K. Tanabe, J. Nelson, H. Hopfer, S.E. Ebeler**
- 9:00 180.** Iron and zinc fortification of cheddar cheese. **Z. Ustunol, A. Arce, O. Kahraman**
- 9:30 181.** Calcium absorption and metabolism is influenced by age, sex, race, bioactive constituents, and the gut microbiome. **C.M. Weaver**
- 10:00** Intermission.
- 10:15 182.** NCOA4-mediated ferritinophagy: Linking cellular iron storage with systemic iron homeostasis and inflammation. **M. Ryu, C.A. Guggisberg, E.F. Bengson**
- 10:45 183.** Dietary phosphorus in human health: Cause for concern?. **K.M. Hill Gallant**
- 11:15 184.** Manganese-induced neurotoxicity: Lessons from worms to human neonates. **M. Aschner**

SECTION E

San Diego Convention Center
Room 31C

Chemistry of Aged Beer & Spirits

Cosponsored by YCC

N. O. Flynn, B. Schneider, *Organizers, Presiding*

- 8:00** Introductory Remarks.
- 8:05 185.** Key note address: The ageing of beer and spirits. **C. Bamforth**
- 8:35 186.** Barrel-aged compounds associated with the brewing process. **B. Schneider, N.O. Flynn**
- 8:55 187.** Rapid wood aging in beer. **R.R. Wilson, R.J. Ordonez, E.G. Theisen, M.D. Mosher**

- 9:15 188.** Barrel-aged compounds commonly associated with barrel substrate. **J. Welbaum**
- 9:35 189.** Age-induced haze formation in beer. **B. Baechler, A. Dunkel, T. Hofmann**
- 9:55** Panel Discussion.
- 10:05** Intermission.
- 10:10 190.** History and chemistry of tequila. **C.E. Hobbs**
- 10:30 191.** Effect of oak spiral aging on beer IBU, dissolved oxygen, SRM, and ABV. **N.O. Flynn**
- 10:50 192.** In-line detection of diacetyl throughout fermentation in brewing beer. **A. Campanella, M.D. Mosher**
- 11:10 193.** Impact of water constituents on taste/mouthfeel properties of distilled spirits. **Z. Wang, K.R. Cadwallader**
- 11:30 194.** Nanoscience of bourbon: Self-assembled micro-webs of colloids from whiskey droplet evaporation as unique identifiers of bourbon whiskeys. **S. Islam, O.D. Velev, S.J. Williams**
- 11:50** Panel Discussion.

Agrochemical Residue & Metabolism Chemistry

Sponsored by AGRO, Cosponsored by AGFD

2019 ACS International Award for Research in Agrochemicals: Advances in the Physiology & Biochemistry of Insect Control

Sponsored by AGRO, Cosponsored by AGFD, BIOL, MEDI, POLY and PROF

MONDAY AFTERNOON – AGFD

SECTION A

San Diego Convention Center
Room 33B

Chemistry & Utilization of Agro-Based Materials Improved Utilization of Agricultural Raw Materials

Cosponsored by AGRO

M. Appell, A. Biswas, H. Cheng, *Organizers*
S. Chang, *Organizer, Presiding*

- 1:30 195.** Bioproduct development toward zero waste agricultural processing. **W.J. Orts, G.H. Tonoli, L.F. Torres, B. Chiou, D.F. Wood, T. Williams, G. Glenn**
- 2:00 196.** Functional properties of pulse flours affected by processing. **M. Singh**
- 2:30 197.** Variability of the chemical composition in the *Abies* species. **J. Kim, S. Lim, C. Lee**
- 3:00 198.** Diabetes is an environmental risk factor: Chemistry, biochemistry, and structural

characterization via MALDI-TOFMS of target molecules found in bitter melon peel potentially useful for fighting macro- and micro-vascular complications as well as blindness in diabetic patients. **B. Dayal**, A. Kulkarni, G.S. Hall

3:30 Intermission.

3:45 **199.** Phosphorus flame retardants from crop plant phenolic acids. **B.A. Howell**, E.A. Ostrander, K. Oberdorfer

4:15 **200.** Experimental design for the extraction of phenolics from *Mentha arvensis* L. using green extraction media. Z. Naseem, **M. Zahid**, M.A. Hanif, M. Shahid, T. Hussain

4:45 **201.** Computer-aided agrochemistry: Overview of modelling possibilities at the molecular level. **B. Horta**

SECTION B

San Diego Convention Center
Room 33A

Nanotechnology Applications for Food & Agriculture

Cosponsored by AGRO

T. V. Duncan, *Organizer*

S. Nam, B. Park, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 **202.** Rapid paper tests for detection of pathogenic *Vibrios* in aquaculture. C. Rodriguez-Quijada, B. Leonardo, C. Lyons, S. Quinn, M. Tlusty, M. Shiaris, **K. Hamad-Schifferli**

2:00 **203.** Withdrawn

2:25 **204.** High-throughput Shiga toxin detection using immune-sensing technology with surface plasmon resonance imaging. **B. Park**, J. Chen, X. He

2:50 Intermission.

3:05 **205.** Macromolecular therapies in treatment of citrus greening. **V.A. Piunova**, J. Hedrick, N. Haiminen

3:30 **206.** Preparation of starch graft copolymers and grafted starch nanoparticles via nitroxide mediated polymerization. J.C. Cazotti, A.T. Fritz, O. Garcia-Valdez, N.M. Smeets, **M.F. Cunningham**

3:55 Concluding Remarks.

SECTION C

San Diego Convention Center
Room 32B

Food Bioactives: Chemistry & Health Effects

Cosponsored by AGRO

F. Shahidi, C. Udenigwe, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 **207.** Omega-3 oils and lipophenols as important food bioactives. **F. Shahidi**

2:05 **208.** Canola oil: Important source of omega-3 fatty acids, but also an oil with flavor challenges. **M. Granvogl**, K. Matheis

2:35 **209.** Effects of honey extracted polyphenols on serum antioxidant capacity and metabolic phenotype. **H. Zhao**

3:05 **210.** Effect of growing conditions on the digestibility and anti-oxidant activity of the Nebraskan Great Northern dry edible bean (*Phaseolus vulgaris*). **K. Majumder**

3:35 Intermission.

3:50 **211.** Protective effect of wheat alkylresorcinols against hydrogen peroxide-induced oxidative stress in ARPE-19 cells. **J. Liu**, Y. Hao, Z. Wang, J. Wang

4:20 **212.** Nucleophilic chemistry of tea polyphenols. **W. Hung**, C. Ho

4:50 **213.** Aqueous extracts of vegetable leaf-fortified bread reduce blood pressure and heart rate when orally administered to spontaneously hypertensive rats. A.M. Alashi, K. Taiwo, D. Oyedele, O. Adebooye, **R. Aluko**

SECTION D

San Diego Convention Center
Room 32A

Metals & Trace Elements in Food Safety, Health & Food Quality

Analytical Methods of Metals & Trace Elements

Cosponsored by AGRO

L. Jackson, B. Redan, *Organizers, Presiding*

1:30 **214.** Status update on methods for arsenic speciation at FDA. **S. Conklin**

2:00 **215.** Two-year study of elemental differences in pinot noir wines from different neighborhoods within one AVA. **C.K. Tanabe**, **J. Nelson**, **S.E. Ebeler**, **H. Hopfer**

2:30 **216.** Selective and sensitive determination of bromate in bread by IC-MS. **M. Aggrawal**, J.S. Rohrer

3:00 Intermission.

3:15 **217.** Rapid detection of engineered nanomaterials in environmental and food matrices using surface-enhanced Raman spectroscopy. **L. He**

3:45 **218.** Iodine, bromine, and arsenic speciation analysis in infant formulas. **J. Nelson**, L. Pacquette, C.K. Tanabe, S. Dong, M. Yamanda

4:15 Concluding Remarks.

SECTION E

San Diego Convention Center

Room 31C

Agnes Rimando Memorial International Student Symposium

Cosponsored by AGRO

B. Gao, M. Granvogl, M. H. Tunick, *Organizers*

R. Tardugno, *Organizer, Presiding*

- 1:30** **219.** Comparison of aroma compounds in fresh-water and salt-water frozen surimi. **Y. An**, Y.L. Qian, S. Xiong, M.C. Qian
- 1:50** **220.** Elucidation of the molecular background of smoky and hammy off-flavors in cocoa. **D. Fuellemann**, M. Steinhaus
- 2:10** **221.** Thermally induced generation of desirable aroma-active and undesirable toxicologically relevant compounds from glucosinolates. **C. Schury**, T. Hofmann, M. Granvogl
- 2:30** **222.** Fatty acid profiles of neutral and polar whey lipids determined by ionic liquid stationary phase gas chromatography. **Q. Ferraris**, M.C. Qian
- 2:50** Intermission.
- 3:05** **223.** Discovery of novel α -amylase inhibitors from natural products with a computer-aided approach. **L. Xie**, W. Chen
- 3:25** **224.** Development of a filter-based SERS platform for total and specific bacterial detection. **S. Gao**
- 3:45** **225.** Optimization of curcumin delivery system functionality: Impact of pH, temperature, and molecular environment. **M. Kharat**, G. Zhang, D. McClements
- 4:05** **226.** Identification and characterization of curcumin-metabolizing gut bacteria. **E. Zhao**, K. Chacon-Vargas, J. Gibbons, H. Xiao

2019 ACS International Award for Research in Agrochemicals: Advances in the Physiology & Biochemistry of Insect Control

Sponsored by AGRO, Cosponsored by AGFD, BIOL, MEDI and PROF

Challenges & Opportunities Facing Early Career Scientists: Early Career Scientist Symposium

Sponsored by AGRO, Cosponsored by AGFD and BIOL

MONDAY EVENING – AGFD

SECTION A

San Diego Convention Center

TBD

Sci-Mix

L. Yu, *Organizer*

8:00 - 10:00

54, 61, 63, 65, 68, 74, 75, 76, 79, 80, 82, 83, 87, 88, 131, 133, 136, 138. See Previous Listings.
346. See Subsequent Listings.

TUESDAY MORNING – AGFD

SECTION A

San Diego Convention Center

Room 33B

Chemistry & Utilization of Agro-Based Materials Nanoscience & Related Materials

Cosponsored by AGRO

M. Appell, A. Biswas, S. Chang, H. Cheng, *Organizers*

C. Sabliov, *Presiding*

- 8:30** **227.** Biopapers, a novel barrier and active electrospun fiber based materials concept. K. Figueroa-Lopez, A. Cherpinski, B. Melendez, M. Pardo-Figuerez, C. Prieto, S. Torres-Giner, **J. Lagaron**
- 9:00** **228.** Development of functional materials by utilizing bioresource polymers. **J. Li**
- 9:30** **229.** Pesticide-loaded cationic zein nanoparticle as a control agent against soybean looper. **C. Sabliov**, S. Navarro, C.E. Astete, J. Davis
- 10:00** **230.** Seed priming with nanomaterials from agro-industrial byproducts modulate the growth and metabolome of onion seedlings. J. Semper, P. Acharya, **G.K. Jayaprakasha**, B. Patil
- 10:30** **231.** Therapeutic nanoparticles penetrate leaves and deliver nutrients to agricultural crops improving tomato yields. **A. Schroeder**
- 11:00** **232.** Cellulose nanocrystals confined to polymer microgels. **S. Lee**, E. Reichmanis, J. Park, M. Srinivasarao

SECTION B
San Diego Convention Center
Room 33A

Nanotechnology Applications for Food & Agriculture

Cosponsored by AGRO

T. V. Duncan, *Organizer*

S. Nam, B. Park, *Organizers, Presiding*

- 8:30** Introductory Remarks.
- 8:35** **233.** Tuning aesthetic and mechanical properties of oleogels via formulation of enzyme-enabled stereoisomeric molecular gelators. M. Samateh, S.S. Sagiri, R. Sanni, **G. John**
- 9:00** **234.** Reclaiming phosphorus from secondary treated municipal wastewater with engineered biochar. **Y. Zheng**, B. Gao
- 9:25** **235.** Behavior of nanosilver anchored inside cotton fiber in laundering water. **S. Nam**, M.B. Hillyer, B.D. Condon, M. Reynolds
- 9:50** Intermission.
- 10:05** **236.** Biomineralization-mimetic shape-adjustable growth of pristine and ultrahigh-load metal-organic frameworks on inert glass fibers to prepare hybrid membranes for collecting hazards in water/organic solvents. **Q. Zhang**, Z. Li, H. Dai, L. Zhang, Y. Fu, Y. Li
- 10:30** **237.** Continuous flow formulations by fast nanoprecipitation and in silico structure determination of selected agrochemical active ingredients. **Á. Bódis**, F. Somodi, T. Bihari, F. Darvas
- 10:55** Concluding Remarks.

SECTION C
San Diego Convention Center
Room 32B

Nutrition, Diet, Functional Foods in Health

W. Chen, Y. Ito, M. Kobori, L. Liu, D. Ren, *Organizers, Presiding*

- 8:00** Introductory Remarks.
- 8:05** **238.** Diet and microbiota during adulthood in health and disease. **G. Wu**
- 8:40** **239.** Antioxidative properties of dietary quercetin in plasma and tissues in diet-induced obese mice and aged mice. **M. Kobori**
- 9:00** **240.** Current research in intestinal microbiota, synbiotics, and obesity-related disease. **H. Kim**, K. Seo, D. Kim, W.H. Yokoyama
- 9:20** **241.** Epicatechin reverses aging-induced skeletal muscle dysfunction and prolongs lifespan in mice. **H. Si**, X. Wang, L. Zhang, C. Lai
- 9:40** Intermission.

- 9:50** **242.** Effects of rice with different amount of resistant starch on mice fed high-fat diet: Attenuation of adipose weight gain. **J. Wan**, Y. Wu, Q. Pham, L. Yu, M. Chen, A.M. McClung, S. Boue, W.H. Yokoyama, B. Li, T.T. Wang
- 10:10** **243.** Western diets affect hippocampus metabolism and neuropeptides through gut-microbiota-brain axis. **M. Zhang**, S. Song, G. Zhou, X. Xu, C. Li
- 10:30** **244.** Activation of AMPK/SIRT1 pathway contributes to Salvianolic acid A-conferred protection against lipotoxicity in hepatocytes and NAFLD in mice. **S. Li**, Q. Qian, N. Ying, J. Lai, L. Feng, s. Zheng, F. Jiang, Q. Ding, H. Chai, X. Dou
- 10:50** **245.** Advancing the detection of immunoreactive cereal proteins to protect sensitive individuals. **K. Scherf**

SECTION D
San Diego Convention Center
Room 32A

Agnes Rimando Memorial Symposium in honor of the Scientist & International Ambassador of Agricultural & Food Chemistry

Cosponsored by AGRO

K. Mahattanatawee, *Organizer*

J. V. Leland, W. H. Yokoyama, L. Yu, *Organizers, Presiding*

- 8:00** Introductory Remarks.
- 8:05** **246.** Agnes Rimando, a pioneer in the fate of glyphosate and its primary metabolite in plants. **J.W. Finley**, S.O. Duke
- 8:25** **247.** Amazing health benefits of pterostilbene: Beloved molecule of Dr. Agnes M. Rimando. **C. Ho**
- 8:45** **248.** Early career discovery of bioactive natural products. **M. Appell**
- 9:05** **249.** Methods for identifying and characterizing health-promoting compounds in fruit and other agricultural products: Tribute to the work of Dr. Agnes Rimando. **L. Jackson**
- 9:25** Intermission.
- 9:40** **250.** Agnes Rimando, scientist and international ambassador. **H.N. Cheng**
- 10:00** **251.** Healthy and tasteful berry fruits-from pterostilbene to raspberry ketone. **M.C. Qian**
- 10:20** **252.** Inactivation of pathogenic bacteria, fungi, and protozoa by phenolic and other natural compounds. **C. Tam**, J. Kim, C. Levin, L.W. Cheng, K. Land, M. Friedman
- 10:40** **253.** Agnes Rimando's studies of sorgoleone, a weed-fighting quinone. **S.O. Duke**, Z. Pan, F.E. Dayan, S. Baerson

- 11:00** **254.** Subcritical hydrolysis of ice-cream wastewater for value-added applications. **M. Enteshari, S. Martinez-Monteagudo**
- 11:20** Concluding Remarks.

SECTION E

San Diego Convention Center
Room 31C

ACS-AGFD Young Scientist Award

Cosponsored by PROF
K. Deibler, L. Yu, *Organizers, Presiding*

- 10:00** Introductory Remarks.
- 10:05** **255.** Biomolecular interactions between myoglobin, mitochondria, and metabolites governing fresh meat color. **R. Ramanathan**
- 10:45** Concluding Remarks.

SECTION E

San Diego Convention Center
Room 31C

USDA-ARS Sterling B. Hendricks Memorial Lectureship Symposium

Cosponsored by AGRO
M. Appell, C. Hapeman, *Organizers, Presiding*

- 11:30** Introductory Remarks.
- 11:40** **256.** Evolution and future needs of food chemistry in a changing world. **J.W. Finley**
- 12:30** Concluding Remarks.

2019 ACS International Award for Research in Agrochemicals: Advances in the Physiology & Biochemistry of Insect Control

Sponsored by AGRO, Cosponsored by AGFD, BIOL, MEDI and PROF

TUESDAY AFTERNOON – AGFD

SECTION A

San Diego Convention Center
Room 33B

Chemistry & Utilization of Agro-Based Materials Advanced Materials from Agricultural Sources

Cosponsored by AGRO
M. Appell, A. Biswas, S. Chang, H. Cheng, *Organizers*
D. L. Compton, *Presiding*

- 1:30** **257.** Utilizing the organization of nanocellulose and semiconducting polymers towards next generation bio-based electronics. **B. Risteen, E. Reichmanis**
- 2:00** **258.** Bio-derived molecular materials: Ability to adapt, clean, energy storage and therapeutic. **G. John**
- 2:30** **259.** Graft-modification of chitosan biopolymer with phosphonated polymer via nitroxide-mediated polymerization. **X. Solimando, P. Champagne, M. Cunningham**
- 3:00** **260.** Customization of chemical structure and reactivity of agro-based materials for applications in coatings. **V.M. Mannari**
- 3:30** Intermission.
- 3:45** **261.** Characterization of carbohydrate polymers using molecular rotor as a structural probe. **Y. Yao**
- 4:15** **262.** Preparation and characterization of hemicellulose-derived materials. **H.N. Cheng, A. Biswas**
- 4:45** **263.** Cosmeceutical ingredients from commodity crop oils. **D.L. Compton, K.O. Evans, M. Appell, J.R. Goodell**

SECTION B

San Diego Convention Center
Room 33A

AGFD Award Symposium Honoring Dr. Fidel Toldra

Cosponsored by PROF
X. Fan, *Organizer*
F. Shahidi, *Organizer, Presiding*

- 2:00** Introductory Remarks.
- 2:10** **264.** Protein hydrolysates and biopeptides from seafood and processing by-products thereof. **F. Shahidi**
- 2:30** **265.** Pea protein-derived peptides as inhibitory agents against carbohydrate and lipid-digesting enzymes. **T. Awosika, R. Aluko**
- 2:50** **266.** Computational approach to mimic gastrointestinal digestion and predict novel peptides with angiotensin converting enzyme-I (ACE-I) inhibitory activity. **S. Hazra, K. Majumder**
- 3:10** **267.** Chemistry and biological significance of food-derived pyroglutamyl peptides. **C. Udenigwe**
- 3:30** **268.** Investigation of the concept of refreshing perception, related flavor components, and its application in sugar-reduced beverage by flavor instrumental analysis and sensory evaluation. **X. Du**
- 3:50** **269.** Considerations in the hydrolysis of insect proteins to improve their bioactivity and decrease allergenicity. **A. Liceaga**

- 4:10 **270.** Recent progress in enzymatic release of food-derived peptides and assessment of bioactivity. **F. Toldra**

SECTION C

San Diego Convention Center

Room 32B

Nutrition, Diet, Functional Foods in Health

W. Chen, T. Hofmann, Y. Ito, M. Kobori, L. Liu, D. Ren,
Organizers, Presiding

- 1:20 Introductory Remarks.
- 1:30 **271.** Microbial metabolization of glycosylated amino acids. **M. Hellwig, T. Henle**
- 2:10 Intermission.
- 2:30 **272.** Combined proteomics and transcriptomics analysis of *Lactococcus lactis* under different culture conditions. **L. Li, X. Yang, R. Hong**
- 2:50 **273.** Comparative kinetics of soy protein gel digestion: Role of mechanical structure and spatial organization. **Y. Guo, P. Takhistov**
- 3:10 **274.** Consequences of superfine grinding treatment on structure, physicochemical, and rheological properties of transglutaminase-crosslinked whey protein isolate. **C. Wang, T. Li, L. Ma, T. Li, J. Hou, Z. Jiang**
- 3:30 **275.** Phenolic composition of blue honeysuckle and its protective effect against oxidative damage following gastrointestinal digestion and gut microbiota fermentation. **T. Bao, L. Xie, J. Xie, W. Chen**
- 3:50 **276.** Evaluation of *trans*-resveratrol levels in grape wine using laser-induced graphene-based electrochemical sensors. **C. Zhang, J. Ping, Y. Ying**

SECTION D

San Diego Convention Center

Room 32A

Proposition 65 on Food Safety

Cosponsored by AGRO

M. Granvogl, *Organizer*

S. MacMahon, *Organizer, Presiding*

M. Granvogl, *Presiding*

- 1:30 Introductory Remarks.
- 1:35 **277.** Food-borne toxicants in Proposition 65: Formation and analysis. **M. Granvogl**
- 2:05 **278.** Risk assessment of inherent chemical contaminants. **P. Hanlon**
- 2:35 **279.** Analysis and occurrence of bound 3-MCPD and glycidol in refined vegetable oils, infant formulas, and other processed foods. **J. Beekman, M. Granvogl, S. MacMahon**

- 3:05 Intermission.
- 3:20 **280.** Free 2- & 3-MCPD as urinary biomarker of exposure for 2- & 3-MCPD fatty acid esters: Controlled exposure study in humans. **J. Kuhlmann, B. Monien, A. Lampen, K. Abraham**
- 3:50 **281.** Toxicokinetics and metabolism of 3-monochloropropane 1,2-diol dipalmitate in Sprague-Dawley rats. **G. Huang, B. Gao, Y. Zhang, L. Yu**
- 4:20 **282.** Styrene, the undesired and toxicologically relevant brother of the desired key aroma compounds of wheat beer. **V. Kalb, T. Hofmann, M. Granvogl**

SECTION E

San Diego Convention Center

Room 31C

Functional Foods: The Chemistry, Bioactivity, Bioavailability, & Biomarkers of Dietary Phytochemicals

Y. Zhu, *Organizer*

J. Daily, S. Sang, *Organizers, Presiding*

- 1:30 Introductory Remarks.
- 1:35 **283.** Polymethoxyflavones from citrus: Chemistry, metabolism and selected bioactivity. **C. Ho, S. Li**
- 2:00 **284.** Variability of bioactive compounds and antioxidant capacity of three morphotypes of *Mauritia flexuosa* L. f. from the Amazon region of Peru. **I. Best, S. Casimiro, A. Portugal, J. Gomez-Mendoza, L. Olivera, R. Nakandakare, F. Ramos-Escudero, A. Muñoz**
- 2:25 **285.** Microbiota facilitates tea polyphenols to trap deleterious reactive endogenous metabolites. **S. Zhang, Y. Zhao, C. Ohland, C. Jobin, S. Sang**
- 2:50 Intermission.
- 3:00 **286.** Protective effects of flaxseed oil and fish oil on TMAO-exacerbated atherogenesis. **Z. He, Z. Chen**
- 3:25 **287.** Inhibition of colonic inflammation and colon tumorigenesis by strawberry and cranberry. **Y. Han, X. Wu, H. Xiao**
- 3:50 **288.** Renal function improvement of diabetic nephropathy mice with ethanol extract of *Pueraria lobata* (Willd.) Ohwi. **F. Chen**
- 4:15 **289.** *In vivo* acrolein-trapping capacities of tea EGCG and soy genistein were mainly mediated by individual bioavailability and biotransformation. **Y. Zhu, Q. Huang, L. Lv, S. Sang**
- 4:40 **290.** Honey of *Apis cerana* Fabricius from China: Structures, biological functions and emerging health benefits. **w. cao, H. Zhao**

SECTION A

San Diego Convention Center

Room 33B

Innovative Approaches to Enhancing Food Safety & Reducing Food Waste

Cosponsored by AGRO

M. Guo, *Organizer*T. Z. Jin, *Organizer, Presiding*X. Fan, *Presiding*

- 8:30 Introductory Remarks.
- 8:35 **291.** Food safety: Critical consideration in reducing food losses and waste. **R. Rolle**
- 9:00 **292.** Advanced oxidation process to enhance microbial safety of fresh produce. **X. Fan**
- 9:25 **293.** High pressure processing (HPP) as an innovative approach in value-added product development of superfruits with aronia berry as the main model. **C. Xu**
- 9:50 Intermission.
- 10:00 **294.** Waterless gaseous antimicrobial intervention for produce safety. **V. Wu**
- 10:30 **295.** Nature inspired synergistic antimicrobial approaches for enhanced microbial inactivation. **N. Nitin**, X. Yang, E. Oliveria, C. Nguyen Huu
- 11:00 **296.** DBD and GlidArcs in plasma agriculture and food safety. **G. Fridman**

SECTION B

San Diego Convention Center

Room 33A

Teaching & Learning Food Chemistry & Analysis

E. Choe, M. H. Tunick, *Organizers, Presiding*

- 8:30 Introductory Remarks.
- 8:40 **297.** Best practices in teaching food chemistry. **M.H. Tunick**
- 8:50 **298.** Teaching analytical chemistry to food science students. **A.E. Mitchell**
- 9:00 **299.** Learning outcome of food analysis for undergraduate students in food science and technology. **M.C. Qian**
- 9:10 **300.** Learning food chemistry as a graduate student and a teaching assistant. **K. Luo**
- 9:20 **301.** My path from chemist to food scientist. **Z. Wang**
- 9:30 **302.** Learning industry standard methods of food analysis as a student, and learning to emphasize critical material for making confident, knowledgeable, industry-bound food science graduates as a teaching assistant. **Q. Ferraris**
- 9:40 Discussion.

Nutrition, Diet, Functional Foods in Health

L. Liu, *Organizer*W. Chen, Y. Ito, M. Kobori, D. Ren, *Organizers, Presiding*

- 8:00 **303.** Enhancement, characterization of phenolic compounds by *Agaricus bisporus* (Qué.) Sacc. ZJUCDMA12 and its anti-proliferation activity. **H. Kuang**, D. Gu, Y. Jiao, Q. Chen
- 8:40 **304.** Nutrient utilization of a gut microbial community: Metabolic analysis of the distinct regional communities *in vitro*. **J. Firrman**
- 9:05 **305.** Impact of Stevia leaf extract on the human gut microbial community *in vitro*. **K.K. Mahalak**, J. Firrman, A. Thomas-Gahring, J. Lee, L. Liu
- 9:30 **306.** Modulation of the luminal and mucosal gut microbiome of cats and dogs by a novel short-term colonic fermentation model. **P. van den Abbeele**
- 9:55 Intermission.
- 10:10 **307.** Stabilization of liposomes by incorporation of block copolyptide. **Y. Ito**
- 10:35 **308.** Transcriptomics of *L. monocytogenes* treated with olive leaf extract. **Y. Liu**, G. Baranzoni, Y. Suo, L. McKeever
- 11:00 **309.** *In vitro* and *in vivo* studies on anti-inflammatory effects of traditional Okinawan vegetable methanol extracts. **J. Nagata**, H. Yokodera, G. Maeda
- 11:25 **310.** Different sources of glucomannans protects against immunosuppression in cyclophosphamide-induced mice. **M. Li**, X. Huang, J. Hu, S. Nie, M. Xie

SECTION D

San Diego Convention Center

Room 32A

Proposition 65 on Food Safety

Cosponsored by AGRO

M. Granvogl, *Organizer*S. MacMahon, *Organizer, Presiding*M. Granvogl, *Presiding*

- 8:30 **311.** Strategy for acrylamide reduction in different bakery products: Breads, cookies, and muffins. **M. Starowicz**, Z. Ciesarova, H. Zielinski
- 9:00 **312.** Testing the next generation of handheld devices for screening acrylamide in high-risk products. **L.E. Rodriguez-Saona**
- 9:30 **313.** Acrylamide levels in commercially available baby biscuits. **S. Elmore**, L. Das, S. Arafa, M. Oruna-Concha
- 10:00 Intermission.

- 10:15 314.** Influence of matrix and coatings in the analysis of acrylamide in nuts and nut products. **A.E. Mitchell**, K. Luo, E. Nojima
- 10:45 315.** Reducing the acrylamide-forming potential of wheat, rye, and potato: From crop management to variety selection and genome editing. **N. Halford**
- 11:15 316.** Pyrrolizidine alkaloids: Occurrence, properties, and analysis. **J. Kuhlmann**
- 11:45 317.** Withdrawn

SECTION E

San Diego Convention Center
Room 31C

Functional Foods: The Chemistry, Bioactivity, Bioavailability, & Biomarkers of Dietary Phytochemicals

S. Sang, *Organizer*

J. Daily, Y. Zhu, *Organizers, Presiding*

- 8:00** Introductory Remarks.
- 8:05 318.** Chungkookjang, a fermented soybean food, fermented with *Bacillus amyloliquefaciens* SRCM100730 and SRCM100731 protected against ischemic stroke and post-hyperglycemia by improving blood flow in gerbils. **J. Daily**, S. Park
- 8:30 319.** Modulation of energy sensing targets by natural products: Effects on health span. **M.B. Zemel**
- 8:55 320.** Oxidative fragmentation of aspalathin leads to the formation of dihydrocaffeic acid and the related lysine amide adduct. **M.A. Glomb**, N. Mertens
- 9:20 321.** Mechanistic investigation of methylglyoxal adducts of 5-hydroxytryptamine in mice. **T. Yao**, C. Hu, S. Sang
- 9:45** Intermission.
- 9:55 322.** Quantitative analysis, bioactive evaluation, and biotransformation of oat avenanthramides with two double bonds. **C. Hu**, Y. Tang, S. Sang
- 10:20 323.** Isolation and purification of 5-n-alkylresorcinols from 21 different wheat varieties and its inflammation inhibitory potential under LPS induced RAW264.7 macrophages. **J. Liu**, Y. Hao, Z. Wang, **J. Wang**
- 10:45 324.** Phytochemical investigation, biological assessment, and quantitative analysis of *Ziziphus jujuba* resources from China. **N. Bai**, S. Guo, L. Bai, T. Wang, S. Zhang
- 11:10 325.** Physicochemical characterization and antioxidant capacity of four native populations of fine or flavour cocoa (*Theobroma cacao* L.) from Peru. **I. Best**, K. Grabiell, C. Plasencia, L. Mendoza, F. Pérez-Cano, M. Castell, S. Pastor-Soplín

- 11:35 326.** Glabrous canary seed: Novel and functional food ingredient. **E.M. Abdelaal**

Agrochemical Residue & Metabolism Chemistry

Sponsored by AGRO, Cosponsored by AGFD

Biological Considerations for Agrochemical Control

Sponsored by AGRO, Cosponsored by AGFD

WEDNESDAY AFTERNOON – AGFD

SECTION A

San Diego Convention Center
Room 33B

Innovative Approaches to Enhancing Food Safety & Reducing Food Waste

Cosponsored by AGRO

M. Guo, *Organizer*

T. Z. Jin, *Organizer, Presiding*

X. Fan, *Presiding*

- 1:30** Introductory Remarks.
- 1:35 327.** Introduction of food waste reduction & recovery program in San Diego. **G. Grootenhuis**
- 2:00 328.** Systems approach to reducing postharvest losses of fresh fruits due to rot-causing pathogens. **C. Xiao**
- 2:30 329.** Withdrawn
- 2:55 330.** Edible coating to keep fresh-cut fruits fresh and safe. **T.Z. Jin**
- 3:20** Intermission.
- 3:30 331.** Novel biocidal materials for prevention of foodborne disease contaminations. **G. Sun**, N. Nitin, Y. Ma, Z. Zhang, L. Wang
- 3:55 332.** Light-activated antimicrobial plastic material with chitosan: Characterization and reusability. **L.J. Bastarrachea**, A. Gagon
- 4:20 333.** Targeted inactivation of antibiotic-resistant *Escherichia coli* and *Pseudomonas aeruginosa* in a soil-lettuce system by combined polyvalent bacteriophage and biochar treatment. **Y. Mao**, S. Mingming

SECTION B
San Diego Convention Center
Room 33A

Edible Functional Food Packaging from Agricultural Biomacromolecules

Cosponsored by AGRO

L. Chen, X. Liu, *Organizers, Presiding*

- 1:30** Introductory Remarks.
- 1:35** **334.** Chain conformation and biological activities of fungal polysaccharides. **L. Zhang**, X. Xu
- 2:25** **335.** Silver nanoclusters embedded zein films as antimicrobial coating materials for food packaging. **L. Mei**, Q. Wang
- 2:45** **336.** Development of functional packaging for food application. **M. Lacroix**
- 3:05** Intermission.
- 3:20** **337.** Molecular structure, physicochemical characterization, and *in vitro* degradation of cereal protein films for edible food packaging application. **L. Chen**, Z. Tian, A. Xia
- 3:40** **338.** Characteristic evaluation of natural plant-derived dyes in food freshness indicator system: Color sensitivity, stability, and security. S. Huang, H. Lin, X. Liu, **H. Li**
- 4:00** **339.** Anti-glycation effect and advanced glycation end-products protein cross-links breaking ability of *Psidium guajava* leaf extracts. **O.I. Adeniran**, M.A. Mogale
- 4:20** Concluding Remarks.

SECTION C
San Diego Convention Center
Room 32B

Nutrition, Diet, Functional Foods in Health

L. Liu, *Organizer*

W. Chen, Y. Ito, M. Kobori, D. Ren, *Organizers, Presiding*

K. Deibler, *Presiding*

- 1:30** **340.** Natural anthocyanin ameliorates type 2 diabetes through targeted inhibition of α -glucosidase activity and coordinately regulating autophagy pathway and gut microbiota composition. **W. Chen**, H. Su
- 2:10** **341.** Functional foods: Advancement of definition and evaluation of scientific investigations. **D.M. Martirosyan**
- 2:50** **342.** Probiotic characteristics of *Lactobacillus plantarum* E680 and its effect on hypercholesterolemic mice. Z. Zheng, W. Wang, J. Liu, J. Firman, J. Renye, **D. Ren**

- 3:15** Intermission.
- 3:30** **343.** *Lactobacillus rhamnosus* GG components exert protective effects on mouse macrophages upon lipopolysaccharide challenge. **H. Wang**, **S. Qi**, X. Luo
- 3:55** **344.** Rumen-protected methionine improve lactation performance of late lactation goats fed with amino acids-deficient diet. **Y. Sun**, Z. Wang, P. Hou, C. Wang, J. Liu, **H. Liu**
- 4:20** **345.** Effects of dietary supplementation of rumen-protected betaine on lactation performance and serum metabolites of dairy cows. **C. Wang**, H. Liu, C. Wang, J. Liu, **H. Liu**
- 4:45** **346.** ASCT2 and SARS are involved in Met-stimulated β -casein synthesis in bovine mammary epithelial cells. **W. Dai**, F. Zhao, J. Liu, H. Liu

SECTION D
San Diego Convention Center
Room 32A

Proposition 65 on Food Safety

Cosponsored by AGRO

M. Granvogl, *Organizer*

S. MacMahon, *Organizer, Presiding*

M. Granvogl, *Presiding*

- 1:30** **347.** Reliable analysis of bisphenol A in beverage, food, infant formula, feed and dietary supplement matrices. **K. Mastovska**, S. Li, J. Shippar
- 2:00** **348.** Plasticiser residues in edible oils and fats: Occurrence & analysis. **J. Kuhlmann**
- 2:30** **349.** Non-targeted screening of nuts and nut products for Proposition 65 compounds. **J. Zweigenbaum**, A.E. Mitchell
- 3:00** Intermission.
- 3:15** **350.** Distinguishing between natural and industrial lead in consumer products and other environmental matrices. **A. Flegal**, K. Odigie
- 3:45** **351.** Toxic elements in food in the United States. **J. Fong Sam**
- 4:15** **352.** Prop 65: Analysis of As, Se, Cd, Hg, & Pb in traditional foods and “new foods” using inductively coupled mass spectrometry (ICPMS). **J. Nelson**, C. Jones

Plant-Insect-Microbe Communications in Agriculture: General Session

Sponsored by AGRO, Cosponsored by AGFD

SECTION A

San Diego Convention Center
Room 33B

Innovative Approaches to Enhancing Food Safety & Reducing Food Waste

Cosponsored by AGRO

M. Guo, *Organizer*

T. Z. Jin, *Organizer, Presiding*

X. Fan, *Presiding*

- 8:30 Introductory Remarks.
- 8:35 353. Antioxidant activities of potato peel extractives. **C. Wu**, K. Yang, J. Li, E. Ebikade, D.G. Vlachos
- 9:00 354. Microbial volatile biomarkers for MP charcoal rot and Rhizopus soft tissues in sweet potatoes. **C. Gamlath Mohottige**, T. Mlsna, R. Baird
- 9:25 355. Microencapsulation of antibiotic alternatives to modulate microflora at target intestinal location. **Y. Wu**
- 9:50 356. Efforts to improve the long-term precision of fumonisin quantitation by LC/MS using a ¹³C labeled internal standard and a well characterized trending sample. **B. Strong**, R. Sarver, E. Bergeron
- 10:15 Intermission.
- 10:25 357. Detection of beef quality by using impedance characteristics. **Z. Sun**, L. Liang, T. Wang, X. Zou, X. Yan, J. Li, X. Liu
- 10:50 358. The discrimination of production process and age of Zhenjiang aromatic vinegar based on SPME-MS. **Z. Sun**, X. Yan, T. Wang, X. Zou, L. Liang, X. Liu, J. Li
- 11:15 359. Withdrawn

SECTION B

San Diego Convention Center
Room 33A

Edible Functional Food Packaging from Agricultural Biomacromolecules

Cosponsored by AGRO

L. Chen, X. Liu, *Organizers, Presiding*

- 8:30 360. Visible colorimetric oxygen indicator for quick response and real-time monitoring of the integrity of modified atmosphere packaging. **X. Liu**
- 8:50 361. Fabrication of chitin nanofiber/calcium alginate sponges and their application as wound healing. **Y. Du**, Z. Pang
- 9:30 362. Protein unfolding and aggregation of PSE-like chicken meat protein at an extreme alkaline pH: Influence on edible film-forming properties. **X. Zhao**, T. Xing, X. Xu

- 9:50 Intermission.
- 10:05 363. RFID-enabled wireless humidity sensor for food packaging. **S. Ye**
- 10:25 364. Improved thermal stability of W₁/O/W₂ double emulsions with bioactive peptide/polysaccharide complexes prepared by self-assembled electrostatic interaction. **Y. Jo**, U. van der Schaaf, S. Min

SECTION C

San Diego Convention Center
Room 32B

The Role of the Microbiome in Mediating Health Effects of Dietary Components

Role of the Microbiome in Mediating Health Effects of Dietary Components

H. Xiao, G. Zhang, *Organizers, Presiding*

- 8:00 Introductory Remarks.
- 8:05 365. Impact of gut microbiota on the metabolism and bioactivity of [6]-shogaol in ginger. **S. Sang**
- 8:30 366. Dietary flavonoid and gut microbiota interaction: Critical in anti-inflammation and anti-cancer in the colon. **H. Xiao**
- 8:55 367. Vitamin E forms: Protective effects on gut health and modulation of gut microbiome. **Q. Jiang**
- 9:20 Intermission.
- 9:35 368. Mildly oxidized vegetable oil exaggerates colitis and colitis-associated colon tumorigenesis. **G. Zhang**
- 10:00 369. An *in vitro* small intestine model with simulated resident microbiome. **L.A. Doherty**, J. Whitman, S. Arcidiacono, K. Conca, J.W. Soares
- 10:25 370. Targeted metabolomics identifies linoleic acid-derived epoxyoctadecenoic acids (EpOMEs) as critical regulators of colon tumorigenesis. **G. Zhang**
- 10:50 371. Impact of different starter cultures on the quality of salami sausages. **Y. Liu**, J. Wei, J. Wang

SECTION D

San Diego Convention Center
Room 32A

General Papers

L. Yu, *Organizer*

B. Gao, E. Kreger, C. Shao, *Presiding*

- 8:30 Introductory remarks.
- 8:35 372. Studies on the effect of processing method on the loss of nutrients in some grains and legumes. **M.C. Azih**

- 8:55 373.** Elucidating composition and structure of purified condensed tannins: Corroboration of thiolysis and spectroscopic data. **W. Zeller**, L.A. Reinhardt, E.E. Hardcastle, J.T. Robe, I. Mueller-Harvey, A. Ramsay, H.M. Ropiak, C. Fryganas, R.H. Brown, C. Drake, R. Sepela, A.E. Hagerman
- 9:15 374.** Water for coffee: Impact of solvated minerals on coffee flavor. **C.H. Hendon**
- 9:35 375.** Pru du 8: First member of a new food allergen family. **Y. Zhang**, H. Che, S. Jiang, T. Jin, S. Lyu, K. Nadeau, T. McHugh
- 9:55 376.** Defining typicity of Pennsylvania-grown Grüner Veltliner wines using instrumental and human sensory methods. **S. Keller**, M. Centinari, H. Hopfer, R. Elias
- 10:15** Intermission.
- 10:25 377.** Effect of post-harvest moisture exposure on stored roasted almonds. **K. Luo**, D.M. Chapman, A.E. Mitchell

- 10:45 378.** 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
- 11:05 379.** Dietary intake of estrogen-mimicking endocrine disruptors and breast cancer. **D.A. Bowes**, R.U. Halden

Plant-Insect-Microbe Communications in Agriculture: General Session

Sponsored by AGRO, Cosponsored by AGFD

AGRO

DIVISION OF AGROCHEMICALS

C.B. Cleveland, *Program Chair*

SUNDAY MORNING – AGRO

SECTION A

San Diego Convention Center
Ballroom 20B-D Theater 1

New Herbicides & Their Modes of Action

Financially supported by Corteva Agriscience and FMC Corporation

F. Dayan, *Organizer*

S. O. Duke, T. M. Stevenson, *Organizers, Presiding*

- 8:40** Introductory Remarks.
- 8:45** 1. Explorations into the development of new herbicides and modes of action. **K. Stubbs**
- 9:10** 2. Tetflupyrolimet: New mode-of-action herbicide that interferes with pyrimidine biosynthesis. **K.A. Hughes**, T.P. Selby, A.D. Satterfield, A. Puri, D.A. Travis, M.J. Campbell, A.E. Taggi
- 9:35** 3. Inhibition of a step in plant *de novo* pyrimidine biosynthesis by a new class of herbicide causes selective phytotoxicity with commercial levels of activity. **I. Kang**, J.L. Andreassi, S. Gutteridge
- 10:00** Intermission.
- 10:20** 4. Novel herbicidal agents based on a substituted pyrazole core with an unknown mode of action. **T. Mueller**, S. Lehr, H. Helmke, J. Tiebes, U. Doeller, C. Kallus, B. Kuhn
- 10:45** 5. Discovery of cyclopyrimorate, new mode of action herbicide in paddy rice fields. **T. Hamada**, M. Shino, Y. Shigematsu, K. Hirase, S. Banba, Y. Tsukamoto, J. Kadotani
- 11:10** 6. Benzoxaboroles as starting points for new herbicides. **J. Roth**, J. Gruber, D. Riar, K. Bravo-Altamirano
- 11:35** Concluding Remarks.

SECTION B

San Diego Convention Center
Ballroom 20B-D Theater 2

Breaking Chemistry Barriers to Feed the World

L. Rossi, *Organizer*

H. B. Irrig, C. Tiu, *Organizers, Presiding*

- 8:15** Introductory Remarks.
- 8:20** 7. EPA's role in ensuring a safe food supply. **R. Keigwin**, M. Goodis
- 8:45** 8. Global challenges in trade policy: Pesticide MRLs. **L. LaPointe**, R. Vanderberg
- 9:10** 9. Chemical registrant perspective on challenges to breaking barriers to feed the world. **C. Smith**
- 9:35** 10. Import pesticide tolerance pilot project. **L. Rossi**
- 10:00** Intermission.
- 10:20** 11. Importance and consequences of MRL disharmony in the trade of almonds. **G. Ludwig**, J. Adam, J. Roseman, G. Bogart
- 10:45** 12. U.S. potato challenges regarding MRL's of different countries. **D. Robinson**
- 11:10** 13. Navigating World Trade Organization activities to promote science-based trade. **A. Markitanova**
- 11:35** Panel Discussion.
- 11:55** Concluding Remarks.

SECTION C

San Diego Convention Center
Ballroom 20B-D Theater 3

CRISPR/Gene Editing & RNAi: Utilization for Enhanced Crop Production

Cosponsored by AGFD and BIOL

P. Reibach, M. C. Ruebelt, *Organizers, Presiding*

- 8:40** Introductory Remarks.
- 8:45** 14. Development of Cibus' Trait Machine™ to efficiently apply gene editing. **D. Songstad**
- 9:10** 15. Transient expression of CRISPR-Cas systems to mature plant tissues with nanoparticle-mediated delivery. **F. Cunningham**, G.S. Demirer, S. Jeong, J. Wang, N. Goh, A.J. Aditham, M. Landry
- 9:35** 16. Rise of new CRISPR technologies and their potential to reverse the loss of nutritional and health benefits in the modern food system, caused by decades of intensive breeding. **M. Oufattole**
- 10:00** Intermission.
- 10:20** 17. Antiviral siRNA nanoparticles protect shrimp against white spot disease. **A. Schroeder**
- 10:45** 18. DNA nanostructures coordinate gene silencing in mature plants. **H. Zhang**, G.S. Demirer, H. Zhang, N. Goh, A.J. Aditham, F. Cunningham, M. Landry

- 11:10** 19. Journey of effectively and efficiently developing a formulated dsRNA product. **L. Aulisa**
- 11:35** 20. EPA registration of dsRNAi plant incorporated protectants: Implications for genome edited products. **K. Matthews**
- 12:00** Concluding Remarks.

SECTION D

San Diego Convention Center
Ballroom 20B-D Theater 4

Creative Thinking in Designing E fate Studies & Data Analysis to Meet Agrochemical Regulatory Challenges

Cosponsored by ENVR

C. Fang, A. K. Sharma, M. Zhang, *Organizers, Presiding*

- 8:40** Introductory Remarks.
- 8:45** 21. Comparing hot versus cold metabolism studies. **C. Seigneur**
- 9:10** 22. Derivation of soil aged sorption parameters of pesticides from field dissipation studies: Theoretical considerations. **X. Huang**
- 9:35** 23. Separation of highly polar photolytic degradation products of benzophenone pesticide. **D. Safarpour**
- 10:00** Intermission.
- 10:20** 24. Development of plant uptake factor study for regulatory environmental fate modeling. **X. Zhou**, C. Schriever, M. Lamshoeft, H. Reseler, R. Sur, P. Volz
- 10:45** 25. Test design modifications to assess the transformation of chemical compounds in aquatic sediment (OECD 308) and soil (OECD 307) test systems: Simulated natural sunlight, algae, pesticide mixtures. **C. Wijntjes**, Y. Weber, D. Adam, W. Völkel, A. Schäffer
- 11:10** 26. Modifications to laboratory based surface water mineralisation tests to investigate persistence. **C. Lowrie**
- 11:35** 27. Biphasic sorption and transformation are key factors in the environmental fate of the herbicide monosodium methylarsenate. **S.Z. Cohen**, M. Williams, M. Eldan, Y. Masue-Slowey, P. Miner, J. Cheplick, C. Hoogeweg
- 12:00** Concluding Remarks.

SECTION E

San Diego Convention Center
Ballroom 20B-D Theater 5

Plant-Insect-Microbe Communications in Agriculture: Early Career Scientist Symposium

P. Kendra, J. Niogret, N. Tabanca, *Organizers, Presiding*

- 8:15** Introductory Remarks.
- 8:20** 28. Withdrawn
- 8:45** 29. Development of a push-pull system for the redbay ambrosia beetle *Xyleborus glabratus*, vector of the laurel wilt pathogen. **X. Martini**, L. Stelinski
- 9:10** 30. Semiochemicals in context: How status of target interactions for behavioral manipulation influences application. **M.J. Rivera**
- 9:35** 31. Chemical ecology of host and vector manipulation by plant viruses. **K.E. Mauck**, Q. Chesnais, J. Kenney
- 10:00** Intermission.
- 10:20** 32. Microbial metabolites mediate bumble bee attraction and feeding. **R. Schaeffer**, C.C. Rering, I. Maalouf, J.J. Beck, R.L. Vannette
- 10:45** 33. Belowground semiochemicals mediating multi-trophic cascades. **D. Willett**, H.T. Alborn, L. Stelinski
- 11:10** 34. Plant chemical responses to herbivory by the imported cabbageworm and two parasitic wasps. **R. Paul**, F.E. Dayan, D. Vyas, P. Ode
- 11:35** 35. Characterisation of the volatile chemical signalling from the beneficial soil fungus *Trichoderma hamatum*. **G. Thomas**, M. Birkett, J. Pickett, M. Grant, D. Withall, J. Sidda, J. Vuts, C. Thornton
- 12:00** Concluding Remarks.

Chemistry & Utilization of Agro-Based Materials Water in Chemistry & Agriculture

Sponsored by AGFD, Cosponsored by AGRO

Metals & Trace Elements in Food Safety, Health & Food Quality

Toxicology

Sponsored by AGFD, Cosponsored by AGRO

Chemistry of Water Reuse Processes Toward Water Sustainability

Sponsored by ENVR, Cosponsored by AGRO and PRES

SUNDAY AFTERNOON – AGRO

SECTION A

San Diego Convention Center
Ballroom 20B-D Theater 1

New Herbicides & Their Modes of Action

Financially supported by Corteva Agriscience and FMC Corporation

F. Dayan, S. O. Duke, T. M. Stevenson, *Organizers, Presiding*

- 1:00** Introductory Remarks.
- 1:05** **36.** Discovery of new herbicide modes of action by quantification of plant primary metabolite and enzyme pools. **S.O. Duke**, F.E. Dayan
- 1:30** **37.** Reactive oxygen species trigger the fast action of glufosinate. H. Takano, R.S. Beffa, C. Preston, P. Westra, **F.E. Dayan**
- 1:55** **38.** Competitors, non-competitors, and un-competitors in herbicide sites of action. **R. Sammons**
- 2:20** **39.** Resistance-gene directed discovery of a natural product herbicide with a new mode of action. **Y. Tang**, S. Jacobsen
- 2:45** Intermission.
- 3:05** **40.** Splicing inhibition is responsible for spliceostatin C phytotoxicity. **J.N. Bajsa-Hirschel**, L. Boddy, M. Sabat, Z. Pan, S.O. Duke
- 3:30** **41.** Unusual sugar from cyanobacteria acts as natural inhibitor of the shikimate pathway. **K. Brilisauer**, J. Rapp, P. Rath, S. Grond, K. Forchhammer
- 3:55** Discussion.
- 4:15** Concluding Remarks.

SECTION B

San Diego Convention Center
Ballroom 20B-D Theater 2

Breaking Chemistry Barriers to Feed the World

C. Tiu, *Organizer*

H. B. Irrig, L. Rossi, *Organizers, Presiding*

- 1:00** Introductory Remarks.
- 1:05** **42.** Crop grouping and other tools to enable trade of specialty crops. **J.j. Baron**, D. Kunkel, M.P. Braverman, W. Barney
- 1:30** **43.** Update on international industry MRL coalition work. **G. Kurbis**, E. Bergeron
- 1:55** **44.** Risk, hazard, human health, and international standards setting for pesticide and veterinary drug maximum residue levels. **B. Bryant**
- 2:20** **45.** Withdrawn
- 2:45** Intermission.
- 3:05** **46.** Global harmonization of MRLs: New threads, old threads, lost threads. **M. Sharpe**
- 3:30** **47.** Urea cocrystal design for improved agrochemical nitrogen management. **J. Baltrusaitis**, M. Silva, D. Kiani
- 3:55** **48.** ONE MRL concept. **C. Tiu**
- 4:20** **49.** Communicating science to an audience that no longer understands what we are trying to say. **G. O'Sullivan**
- 4:45** Concluding Remarks.

SECTION C

San Diego Convention Center
Ballroom 20B-D Theater 3

Agrochemical Residue & Metabolism Chemistry

Cosponsored by AGFD

J. J. Johnston, K. Mastovska, D. J. Smith, X. Zhou,
Organizers, Presiding

- 1:00** Introductory Remarks.
- 1:05** **50.** Chromatographic separations of several functional analogs. H. Kandala, **T. Chowdhury**
- 1:30** **51.** Evolution of the multi-residue method: Epic quest to perfect the pesticide residue analytical method. **S. Perez**, J. Adams
- 1:55** **52.** Withdrawn
- 2:20** **53.** Trials and tribulations of glyphosate analysis in raw agricultural commodities, foods, and dietary supplements. **J.P. Zulkoski**, S. Avula, L. Vaclavik, K. Mastovska
- 2:45** Intermission.
- 3:05** **54.** Fate and distribution of ³⁶Cl-chlorine dioxide gas on animal and plant-based foods. **D.J. Smith**, A. Scapanski
- 3:30** **55.** Investigation into the detection of semicarbazide, a nitrofurazone indicator, in chicken. R. Duverna, **J.J. Johnston**, R. Kishore, J. Jarosh, C. Yee
- 3:55** Discussion.
- 4:10** Concluding Remarks.

SECTION D

San Diego Convention Center
Ballroom 20B-D Theater 4

Pest Management Economics: Present & Future Considerations

Cosponsored by BMGT

C. Hawkins, J. Roseman, *Organizers*

M. Dobbs, L. Duzy, *Organizers, Presiding*

- 1:00** Introductory Remarks.
- 1:05** **56.** Benefit and impact analyses under FIFRA. **T. Wyatt**
- 1:30** **57.** Economic and pest management analysis of proposed pesticide regulations. J. Steggall, R. Goodhue, **K. Mace**, S. Blecker, R. Van Steenwyk
- 1:55** **58.** Agricultural consolidation and digitization: Future development landscape. **A. Duehl**, B. Brauer, W. Poulson
- 2:20** **59.** How ecosystem services credit exchanges allow private companies and public agencies an opportunity to comply with environmental laws, regulations, policies and guidelines with a cost-effective, environmentally superior outcome. **B. Monaghan**, J. Bickel

- 2:45 Intermission.
- 3:05 60. Precision agriculture adoption and farm chemical use: Regions, soil variability, and farm size. **D. Schimmelpfennig**
- 3:30 61. Economics of pest eradication programs: Lessons for resistance management. **G. Frisvold**
- 3:55 62. Analysis of agrochemical use in California almonds during bloom. J. Durant, **B. Goodrich**
- 4:20 63. Role of IPM in farm sustainability. **D. McCallister**, M. Parajulee
- 4:45 Concluding Remarks.

SECTION E

San Diego Convention Center
Ballroom 20B-D Theater 5

Plant-Insect-Microbe Communications in Agriculture: Early Career Scientist Symposium

P. Kendra, J. Niogret, N. Tabanca, *Organizers, Presiding*

- 1:00 Introductory Remarks.
- 1:05 64. Interactions between spotted-wing *Drosophila* and fruit rot fungi in fall red raspberries. **M. Lewis**, K. Hamby
- 1:30 65. Microbiome in host plant colonization and foraging of an invasive fruit fly. **C. Wong**, J. Hernandez, J.J. Beck, O. Liburd
- 1:55 66. Additive microbe studies to elucidate semiochemicals responsible for attractive and/or repellent effects on *Drosophila suzukii*. **J.T. Brown**, C. Wong, J.J. Beck
- 2:20 Intermission.
- 2:40 67. New ion chromatography method for the quantification of ammonia, putrescine, and trimethylamine salts from cones used to trap female Mediterranean fruit flies, *Ceratitis capitata* (Diptera: Tephritidae). **A. Vazquez**, H. Pierre, R.A. King, L.K. Mosser, P. Kendra
- 3:05 68. Stilbenes and fatty acids as mosquitocides for control of the malaria vector, *Anopheles gambiae*. **F. Démares**, Q. Coquerel, G. Richoux, K. Linthicum, J.R. Bloomquist
- 3:30 69. Natural and synthetic compounds display multiple mechanisms of synergism and resistance-breaking properties. **E.J. Norris**, J.R. Bloomquist
- 3:55 70. Spatial repellency and antennal responses of *Aedes aegypti* to plant-derived chemicals. **L. Yang**, S. Jiang, K. Linthicum, J.R. Bloomquist
- 4:20 Concluding Remarks.

Chemistry & Utilization of Agro-Based Materials Value-Added Products from Agricultural Raw Materials

Sponsored by AGFD, Cosponsored by AGRO

Food Bioactives: Chemistry & Health Effects

Sponsored by AGFD, Cosponsored by AGRO

Metals & Trace Elements in Food Safety, Health & Food Quality

Food Quality and Safety

Sponsored by AGFD, Cosponsored by AGRO

Chemistry of Water Reuse Processes Toward Water Sustainability

Sponsored by ENVR, Cosponsored by AGRO and PRES

Agnes Rimando Memorial International Student Symposium

Biomedical & Biochemical Research

Sponsored by AGFD, Cosponsored by AGRO

MONDAY MORNING – AGRO

SECTION A

San Diego Convention Center
Ballroom 20B-D Theater 1

Analytical Methodologies for Process Chemistry & Formulation Research

Cosponsored by ENVR

M. Evenson, D. Knueppel, Y. Shi, *Organizers, Presiding*

- 9:00 Introductory Remarks.
- 9:05 71. Global food analysis. **P.C. Dorrestein**
- 9:30 72. Agrochemical forced degradation studies and their role in analytical method and formulation development. **D.S. Malkin**, R. Samame, M. Bishop, D. Knueppel
- 9:55 Intermission.
- 10:15 73. Determination of anionic polar pesticides as residual impurities in pesticide formulations by LC-MS/MS. **C. Love-Nkansah**
- 10:40 74. Isolation of trace level impurities from agricultural technical grade active ingredients using semi-preparatory scale LC/MS. **M.D. Evenson**, D. Knueppel, P. Graupner, B. Moscato, C. Zu, R. Samame
- 11:05 75. Optimizing separation for complex samples using two-dimensional liquid chromatography. **L. Zang**, **R. Giuffre**
- 11:30 76. Application of SFC to achiral agricultural active ingredients. **J. Richards**, J. Houchins
- 11:55 Concluding Remarks.

SECTION B

San Diego Convention Center
Ballroom 20B-D Theater 2

Agrochemicals & Water: Advances in Prevention, Monitoring, & Treatment

Cosponsored by ENVR

H. B. Irrig, S. Mathys, *Organizers, Presiding*

- 9:00 Introductory Remarks.
- 9:05 77. Passive samplers for surface water pesticide occurrence in remote areas of Northern California. **M.L. Hladik**, M. De Parsia, C. Sanders, J. Orlando
- 9:30 78. Agrochemicals and water: Postharvest applications toward insect pest control. **S.S. Walse**
- 9:55 Intermission.
- 10:15 79. Implications of tertiary recycled water use for watering nondairy livestock on animal health and safety of food animal products. **D.J. Smith**, R.H. Poppenga
- 10:40 80. Seasonal changes in glyphosate concentrations in the Lake Erie tributaries using high throughput monitoring with IC-ICP-MS. **S. Biswas**, L. Johnson, D.D. Snow
- 11:05 81. Extrapolation of US prospective groundwater monitoring study to Colombia using GIS techniques for consideration of coffee uses. **M. Kim**, M. Robert
- 11:30 82. Residues of synthetic pyrethroids in water bodies of different cropping system. **T. Jindal**, S. Thakur, K. Gulati
- 11:55 Concluding Remarks.

SECTION C

San Diego Convention Center
Ballroom 20B-D Theater 3

Agrochemical Residue & Metabolism Chemistry

Cosponsored by AGFD

K. Mastovska, X. Zhou, *Organizers*

J. J. Johnston, D. J. Smith, *Organizers, Presiding*

- 9:00 Introductory Remarks.
- 9:05 83. Avian exposure to current-use pesticides: Method development and environmental application. **M. Gross**, A. Elgin, C. Morrissey, M.L. Hladik, K. Kuivila
- 9:30 84. Antemortem fluids as indicator of agrochemical exposure in food animals. **W.L. Shelver**, D.J. Smith
- 9:55 Intermission.
- 10:15 85. Establishing baseline sensitivity data using LCMS/MS to investigate dermal *in-vitro* absorption toxicological application. **A. Patel**, P. Trivedi

- 11:05 86. Metabolism studies of dicamba in dicamba-tolerant crops. **A. Adio**
- 11:30 87. Using metabolomics to provide evidence of a reactive metabolite of an avicide. **D.A. Goldade**
- 11:55 Concluding Remarks.

SECTION D

San Diego Convention Center
Ballroom 20B-D Theater 4

Advances in Exposure Modeling for Human Health Assessments

Cosponsored by TOXI

Financially supported by Syngenta

C. B. Cleveland, *Organizer*

A. Z. Szarka, *Organizer, Presiding*

K. Tatum-Gibbs, *Presiding*

- 9:00 Introductory Remarks.
- 9:05 88. Application of an integrated approach for chemical evaluation of human cancer risk. **D.C. Wolf**
- 9:55 Intermission.
- 10:15 89. RISK21: Overview of a transparent, exposure-driven, and fit-for-purpose risk assessment framework. **S. Deglin**, M. Embry
- 10:40 90. Determination of the kinetics of metabolism of dimethoate in rat and human liver microsomes. **G.C. Nallani**, K. Kassahun, L. Shen, A. Chandrasekaran
- 11:05 91. High-throughput exposure assessment: Overview and integration on non-target dust analysis. **D.H. Bennett**
- 11:30 92. Guidance for assessing human dietary exposure to newly expressed proteins in genetically modified crops. C. Mathesius, A. Sauve-Ciencewicki, J.A. Anderson, **C.B. Cleveland**, C. Fleming, G. Frierdich, L. Goodwin, M.C. Grunenwald, F. Laporte, E.A. Lipscomb, R. Oberdoerfer, J. Petrick, P.A. Bauman
- 11:55 Concluding Remarks.

SECTION E

San Diego Convention Center
Ballroom 20B-D Theater 5

Off-Target Transport of Field Applied Agricultural Chemicals: Study Designs, Monitoring, Modelling, & Risk Assessment

Cosponsored by ENVR

R. Lerch, M. A. Locke, L. L. McConnell, P. J. Rice, N. Thurman, C. Truman, Q. Yao, *Organizers*

S. Grant, A. M. Ritter, *Organizers, Presiding*

- 9:00 Introductory Remarks.
- 9:05 **93.** Review of fumigant field emission studies for human exposure assessment. **W. Jiang**, E. Kwok, S. DuTeaux
- 9:30 **94.** Development of the soil fumigant exposure assessment (SOFEA) model. **J. Buonagurio**, S. Cryer, I. van Wesenbeeck, R. Reiss
- 9:55 Intermission.
- 10:15 **95.** Comparison of three flux models across five field studies. **N. Pai**, E. Sall, J. Stryker, J. Popovic, R. Reiss, J. Cabbage
- 10:40 **96.** Transport and deposition of pesticide residues in fog. **J.N. Seiber**
- 11:05 **97.** Landscape-scale field studies to evaluate fate and transport of an agricultural fungicide to farm ponds. **A.M. Moore**, T. Wiepke, C. Truman, M. Cox, J.P. Hanzas
- 11:30 **98.** Wetland water monitoring within intensive agricultural areas of Western Canada. **C.R. Harrington**, S.M. Chen, W. Chen, R. Underwood
- 11:55 Concluding Remarks.

SECTION F

San Diego Convention Center
Room 33C

2019 ACS International Award for Research in Agrochemicals: Advances in the Physiology & Biochemistry of Insect Control

Cosponsored by AGFD, BIOL, MEDI, POLY and PROF
M. D. David, K. D. Wing, *Organizers, Presiding*

- 8:05 Introductory Remarks with Presentation of International Award.
- 8:15 **99.** Many faces of nicotinic receptors as insecticide targets. **V.L. Salgado**
- 9:05 **100.** Genetic analysis of nicotinic acetylcholine receptors and their interactions with insecticides. **T. Perry**, W. Chen, R. Ghazali, D. Christesen, T.C. Sparks, P. Batterham
- 9:30 **101.** Spider toxins as novel allosteric modulators of insect nicotinic receptors. **F. Earley**, C. Chambers, P. Cutler, Y. Huang, D.J. Craik
- 9:55 Intermission.
- 10:15 **102.** Toward understanding the mechanism of selectivity of neonicotinoids: Interactions with loop C and loop DEG triangle of *Drosophila* Dα1 subunit with imidacloprid and thiacloprid. **K. Matsuda**
- 10:40 **103.** Photochromic insecticidal molecules for insect behavior regulation. **X. Shao**
- 11:05 **104.** Functional genomics of cys-loop ligand-gated ion channels, a superfamily of insecticide targets. **A.K. Jones**
- 11:30 Concluding Remarks.

Chemistry & Utilization of Agro-Based Materials Agro-Based Fibers & Textiles

Sponsored by AGFD, Cosponsored by AGRO

Current Advances in Water Analysis: From Citizen Scientists to Laboratory Breakthroughs

Sponsored by ENVR, Cosponsored by AGRO and CEI

Food Bioactives: Chemistry & Health Effects

Sponsored by AGFD, Cosponsored by AGRO

Metals & Trace Elements in Food Safety, Health & Food Quality

Health & Nutrition

Sponsored by AGFD, Cosponsored by AGRO

Chemistry of Water Reuse Processes Toward Water Sustainability

Sponsored by ENVR, Cosponsored by AGRO and PRES

Agnes Rimando Memorial Symposium in honor of the Scientist & International Ambassador of Agricultural & Food Chemistry

Sponsored by AGFD, Cosponsored by AGRO

MONDAY AFTERNOON – AGRO

SECTION A

San Diego Convention Center
Ballroom 20B-D Theater 1

2019 ACS International Award for Research in Agrochemicals: Advances in the Physiology & Biochemistry of Insect Control

Cosponsored by AGFD, BIOL, MEDI and PROF
M. D. David, K. D. Wing, *Organizers, Presiding*

- 1:50 Introductory Remarks.
- 1:55 **105.** Discovery and mode of action of a novel insecticide, broflanilide. **T. Nakao**, H. Katsuta, M. Nomura, T. Wakita, H. Daido, Y. Kobayashi, A. Kawahara, S. Banba
- 2:20 **106.** Effects of amino acid substitutions at the intersubunit cavity on the sensitivity of the GABA receptor to fluralaner. **Y. Ozoe**, K. Yamato, F. Ozoe, M. Asahi, M. Kobayashi
- 2:45 Intermission.
- 3:05 **107.** Crop protection industry and the new age of insecticide discovery. **T.C. Sparks**, B.A. Lorsbach, F. Wessels

- 3:30 **108.** Conservation of the voltage-sensitive sodium channel protein within the *Insecta*. J. Silva, **J.G. Scott**
- 3:55 **109.** Insecticides that inhibit sodium channels. **D.M. Soderlund**
- 4:20 **110.** Molecular basis of pyrethrum repellency in mosquitoes. **K. Dong**
- 4:45 Concluding Remarks.

SECTION B

San Diego Convention Center
Ballroom 20B-D Theater 2

Challenges & Opportunities Facing Early Career Scientists: Early Career Scientist Symposium

Cosponsored by AGFD and BIOL

X. Zhou, *Organizer*

S. Whiting, *Organizer, Presiding*

X. Zhou, *Presiding*

- 1:00 Introductory Remarks.
- 1:05 **111.** Lessons learned from starting career at a contract research organization. **S. Whiting**
- 1:30 **112.** Starting a career in academia: Navigating the first couple of years of a tenure-track position. **A.D. Gross**
- 1:55 **113.** Challenges of transitioning from a small college to a large world. **K. Maurey**
- 2:20 **114.** What is work/life balance? Reconciling parenthood with an academic career in STEM. **S. O'Neal**
- 2:45 Intermission.
- 3:05 **115.** Stop signs and alternative routes: Navigating the road to a successful career. **K. Tatum-Gibbs**
- 3:30 **116.** More than a box of rocks: Experiences of a U.S. Geological Survey research chemist. **M. Gross**
- 3:55 **117.** Withdrawn
- 4:20 **118.** Excel in your career: Tips and advice. **M. Ma**
- 4:45 Concluding Remarks.

SECTION C

San Diego Convention Center
Ballroom 20B-D Theater 3

Water Scarcity: Challenges for Agriculture

Cosponsored by ENVR and PRES

Financially supported by Golden Pacific Labs

T. F. Moate, M. D. PazCarpio-Obeso, J. N. Seiber, *Organizers*

J. Carvalho, *Organizer, Presiding*

- 1:00 Introductory Remarks.
- 1:05 **119.** Aftermath of California's most recent drought: 2012–2016. **S. Sandoval**

- 1:30 **120.** Salt mitigation in irrigated crops: Reducing negative impacts past, present and possibilities for the future. **S. West**
- 1:55 **121.** Biogeosystem technique for healthy soil, water, and environment. **V.P. Kalinitchenko**, A. Glinushkin, M. Sokolov, A. Batukaev, T. Minkina, V. Zinchenko, V. Chernenko, V. Startsev, S. Mandzhieva, S. Sushkova, D. Makarenkov, L. Il'ina, A. Rykhlik, G. Larin
- 2:20 **122.** Saltwater greenhouse: Combining engineering and plant science to deliver a new concept in food and water security. **M. Tester**
- 2:45 Intermission.
- 3:05 **123.** Impact of the application of natural biostimulants on water use in crop production under adequate and reduced water availability. **G. Povero**, A. Biasone, A. Santaniello, N. Briglia, A. Petrozza, A. Piaggese
- 3:30 **124.** Skincare meets agriculture: Cross-over idea creates a novel, water-saving biostimulant with field results presented. **C. Jordan**
- 3:55 **125.** Chemists Without Borders' model for saving water and capturing carbon through biochar production and use. **A.W. Cooper**, B. Vaccaro, R. Kronquist
- 4:20 **126.** Best management practices to keep pesticides out of water. **S. Sandoval**
- 4:45 Panel Discussion.

SECTION D

San Diego Convention Center
Ballroom 20B-D Theater 4

Advances in Exposure Modeling for Human Health Assessments

Cosponsored by TOXI

Financially supported by Syngenta

C. B. Cleveland, *Organizer*

A. Z. Szarka, *Organizer, Presiding*

K. Tatum-Gibbs, *Presiding*

- 1:00 Introductory Remarks.
- 1:05 **127.** Benchmark dose modeling and 21st century application in predictive safety assessment. **V. Bhat**
- 1:55 **128.** Tiered approach for exposure and risk assessment of inert ingredients in pesticide product formulations. **M.C. Grunenwald**, A.Z. Szarka, T.S. Ramanarayanan
- 2:20 **129.** Reevaluation as a starting point to implement the risk assessment of pesticides for operators, workers, residents, and bystanders in Brazil. **J. Braz**, F. Neves
- 2:45 Intermission.

- 3:05 **130.** Survey of the Brazilian agricultural scenarios to support the development of the database of occupational exposure in Brazil. **F.C. Cremaschi Palma, D. Laustenchalaeger, K. Cazarin, M. Grigoli**
- 3:30 **131.** Development of metrics for screening for chemical storage near drinking water sources. **C.N. Lowe, K. Isaacs**
- 3:55 Discussion.
- 4:15 Concluding Remarks.

SECTION E

San Diego Convention Center
Ballroom 20B-D Theater 5

Off-Target Transport of Field Applied Agricultural Chemicals: Study Designs, Monitoring, Modelling, & Risk Assessment

Cosponsored by ENVR

S. Grant, R. Lerch, A. M. Ritter, N. Thurman, C. Truman, Q. Yao, *Organizers*

M. A. Locke, L. L. McConnell, P. J. Rice, *Organizers, Presiding*

- 1:00 Introductory Remarks.
- 1:05 **132.** Optimization of farm agronomic practices to meet environmental quality requirements. **M. Winchell, B. Patterson**
- 1:30 **133.** Field methods for assessing vegetative filter strip (VFS) impacts on benzovindiflupyr runoff transport in the Southeastern United States. T. Wiekpe, C. Truman, J.P. Hanzas, **M. Arpino, C. Harris**
- 1:55 **134.** Multi-year field studies evaluating the benefits of vegetative filter strips. **A.M. Ritter, D.A. Desmarteau, G. Goodwin, J. Trask, L. Carver, M. Cox, A.M. Moore, C. Truman**
- 2:20 **135.** Modelling experiments with vegetated filter strips with a new version of VFSSMOD: Calibration, uncertainty analysis and recommendations for regulatory use. **R. Sur, S. Reichenberger, C. Kley, S. Sittig, S. Multsch**
- 2:45 Intermission.
- 3:05 **136.** Effect of the VFSSMOD pesticide trapping equation on environmental exposure assessments. R. Munoz-Carpena, G. Fox, **A.M. Ritter**
- 3:30 **137.** Regulatory perspective: Opportunities and challenges in considering vegetative filter strips in pesticide risk assessments. **N. Thurman, M. Appleyard, K. Costello**
- 3:55 Concluding Remarks.

SECTION F

San Diego Convention Center
Room 33C

Metabolomics & Metabolite Identification in Agricultural Research

J. Balcer, A. Chen, J. Ferguson, P. Wei, *Organizers, Presiding*

- 12:55 Introductory Remarks with JAFC Award Presentation.
- 1:05 **138.** Antifungal metabolite profiling of high value compounds in fruit peel waste. **A. Munkacsi, M. Mokhtari, M. Jackson, M. Hooker, J. Harvey, A. Brown, D. Ackerley, N. Ritson, R. Keyzers**
- 1:30 **139.** Novel mass spectrometry tools to speed the identification of metabolites and impurities. **J.R. Gilbert, J. Balcer, Y. Adelfinskaya, D. McCaskill, N. Wang, J.A. Godbey, M. Madary, M.P. Mawn, C. Zu**
- 1:55 **140.** *In vitro* metabolism of semi natural product TL-909 and identification of its complex metabolic products by HPLCMSTOF, UPLCMSTOF and CECMSTOF. **D. Safarpour, L. O'Brien**
- 2:20 **141.** Metabolism prediction and metabolite identification using biotransformer: Applications in crop protection discovery. **Y. Djoumbou Feunang, J. Balcer, D. Tomandl**
- 2:45 Intermission.
- 3:05 **142.** Discovery of plant-derived metabolite markers for pest management strategies. J.H. Kim, G.P. Head, **P. Wei**
- 3:30 **143.** Establishing a spatial metabolomics workflow that integrates MALDI imaging with new trapped ion mobility metabolomics for more comprehensive identification and validation. **D.S. Cornett, A. Barsch, C. Henkel, M. Witt, M. Szesny**
- 3:55 Concluding Remarks.

Chemistry & Utilization of Agro-Based Materials

Improved Utilization of Agricultural Raw Materials

Sponsored by AGFD, Cosponsored by AGRO

Sensors & Biosensors for Widespread Environmental Monitoring

Sponsored by ENVR, Cosponsored by AGRO

Nanotechnology Applications for Food & Agriculture

Sponsored by AGFD, Cosponsored by AGRO

Food Bioactives: Chemistry & Health Effects

Sponsored by AGFD, Cosponsored by AGRO

Chemistry of Water Reuse Processes Toward Water Sustainability

Sponsored by ENVR, Cosponsored by AGRO and PRES

Metals & Trace Elements in Food Safety, Health & Food Quality

Analytical Methods of Metals & Trace Elements

Sponsored by AGFD, Cosponsored by AGRO

Agnes Rimando Memorial International Student Symposium

Sponsored by AGFD, Cosponsored by AGRO

MONDAY EVENING – AGRO

SECTION A

San Diego Convention Center
TBD

Sci-Mix

C. B. Cleveland, *Organizer*

8:00 - 10:00

255, 256, 257, 269, 271, 272, 273, 274, 275, 276, 277, 278, 279, 280, 281, 286, 288, 289, 307. See Subsequent Listings.

TUESDAY MORNING – AGRO

SECTION A

San Diego Convention Center
Ballroom 20B-D Theater 1

Advances in Analytical Technologies Supporting Environmental Fate, Metabolism, & Residue Analysis

Cosponsored by ENVR

Y. Yuan, *Organizer*

K. Kuppannan, M. Ma, *Organizers, Presiding*

8:05 Introductory Remarks.

8:10 **144.** Determination of nitrite residues in feral swine tissues. **B.G. Abbo**

8:35 **145.** Use of PolyCYPs[®] enzymes for accessing mammalian metabolites of agrochemicals and pharmaceutical drugs. S. Lai, A. de Riso, **L. Evans**, W. Hodds, E. Hopkins, A. Khan, K. Nytko, R. Phipps, V. Poon, F. Scheffler, J. Shanu-Wilson, J.C. Steele, S. Wrigley

- 9:00 **146.** Temporal and spatial study of neuropeptidomic changes in response to hypoxia via a multi-faceted mass spectrometry platform. **L. Li**, A. Buchberger, C. Sauer, K. DeLaney, N. Vu, Y. Liu
- 9:25 **147.** Determination of drugs and pesticides in catfish feed for contaminant traceback. **D.L. Sparks**, J.S. Boone, C.V. Childers, A. Meredith, G. Hagood, A.E. Brown
- 9:50 Intermission.
- 10:10 **148.** In-house suspect screening database as a tool to increase detection coverage for analysis of contaminants in environmental samples. **M.E. Guardian**, P. He, D.S. Aga
- 10:35 **149.** US EPA CompTox Chemicals Dashboard to support mass spectrometry targeted and non-targeted analysis. **A.J. Williams**, A. Chao, T. Cathey, T. Transue, E.M. Ulrich, J. Sobus
- 11:00 **150.** Innovative method for simultaneous determination of pesticides, veterinary drugs, and environmental contaminants residues in beef. **S. Monteiro**, E. Ninga, S.J. Lehotay, Y. Sapozhnikova
- 11:25 Concluding Remarks.

SECTION B

San Diego Convention Center
Ballroom 20B-D Theater 2

2019 ACS International Award for Research in Agrochemicals: Advances in the Physiology & Biochemistry of Insect Control

Cosponsored by AGFD, BIOL, MEDI and PROF M. D. David, K. D. Wing, *Organizers, Presiding*

8:05 Introductory Remarks.

8:10 **151.** Nicotinamide is an endogenous modulator of insect chordotonal organs. V.L. Salgado, **K. Lelito**

8:35 **152.** Genetics of resistance to Cry1 proteins in *Spodoptera frugiperda*. **G. Head**, R. Nauen, L. Flagel, D. Boaventura, S. Martinelli, P. Dourado

9:00 **153.** Insect glia as a cellular target for insecticide development. **D. Swale**

9:25 **154.** Proinsecticides as potential resistance management tools. **M.D. David**

9:50 Intermission.

10:10 **155.** Novel biomedical technologies which may apply to insecticide discovery. **K.D. Wing**

10:35 **156.** Unusual modes of action of pyrethroid-derived spatial repellents. **J.R. Bloomquist**

11:00 Discussion.

11:15 Concluding Remarks.

SECTION C
San Diego Convention Center
Ballroom 20B-D Theater 3

Metabolomics & Metabolite Identification in Agricultural Research

J. Balcer, A. Chen, J. Ferguson, P. Wei, *Organizers, Presiding*

- 8:30** Introductory Remarks.
- 8:35** **157.** Novel approach for the non-targeted profiling of oligomeric nutraceuticals in fruits using reporter-ion triggered tandem mass spectrometry. **N. Tharayil**, E. Leonard
- 9:00** **158.** New methods for the automated structural classification of natural products. **W.H. Gerwick**, C. Zhang, R. Reher, S. Zhu, N. Roberts, G. Cottrell
- 9:25** **159.** Advanced software tools for metabolite identification and metabolomics analysis in agrochemical research. **C. Ding**, M.P. Mawn, J. Balcer
- 9:50** Intermission.
- 10:10** **160.** Insect repellents and insecticides from plants and microbes. **K.M. Meepagala**
- 10:35** **161.** Determining characteristics of cannabis plants to distinguish cultivars and growing conditions using high resolution QTOF mass spectrometry. **P. Winkler**, C. Butt, D. Hughes, S. Churchill, M. Aiello
- 11:00** **162.** Putative gene mode of action discovery by GC/MS and LC/MS metabolomics. **J. Hazebroek**, B. Ruddy, T. Harp, C. Vlahakis, L. Perugini, L. Peddicord
- 11:25** Concluding Remarks.

SECTION D
San Diego Convention Center
Ballroom 20B-D Theater 4

Surfactant & Colloid Science Applied to Formulations

Cosponsored by COLL

R. Acosta Amado, B. Rauzan, S. Sumulong, *Organizers, Presiding*

- 8:30** Introductory Remarks.
- 8:35** **163.** Designing tools for improving the performance of automotive clear coat system. **B. Cao**, C. Harris
- 9:00** **164.** Removing the guesswork from stability analysis: Quantifying and prediction of the physical stability of dispersions. **M. Vanden Eynden**, C. Tisserand, Y. Lefeuvre, P. Bru, G. Meunier
- 9:25** **165.** Using design of experiments to optimize complex formulations. **B. Rauzan**, R. Acosta Amado, H. Jeon, M. Evenson, T. Minnicks, N. Skaggs
- 9:50** Intermission.
- 10:10** **166.** Structured surfactant technology: Novel suspensive system by surfactant self-assembly,

allowing for complex agrochemical formulations not achievable through conventional methods. **E. Weber**

- 10:35** **167.** Formulations based on self-assembled polymer systems. **R. Nagarajan**
- 11:00** **168.** Structuring of fertilizer compatible suspension concentrates. **J. Wall**
- 11:25** Concluding Remarks.

SECTION E
San Diego Convention Center
Ballroom 20B-D Theater 5

Biostimulants in Agriculture: Chemistry & Regulatory Aspects

Cosponsored by BIOL, MEDI and TOXI

P. Halarnkar, K. D. Wing, *Organizers*

M. E. Koivunen, *Organizer, Presiding*

P. Halarnkar, *Presiding*

- 8:20** Introductory Remarks.
- 8:25** **169.** Biostimulants: Their function and effective use in modern agriculture. **P.H. Brown**, D. Amaral, M. Park
- 9:00** **170.** Mining phytomicrobiomes for microbial compounds to replace synthetic fertilizers and fungicides for sustainable agriculture. **A.M. Hirsch**, N. Khan, P. Martínez-Hidalgo, T. Ice, M. Maymon, E.A. Humm, K.F. Faull
- 9:25** **171.** Commercial *Ascophyllum nodosum* extracts (Acadian Plant Health) reduce plant stress resulting in improved plant growth and productivity. **H. Little**
- 9:50** Intermission.
- 10:10** **172.** M-trophs for sustainable agriculture. **J. Kerovuo**
- 10:35** **173.** Analysis of *Ascophyllum nodosum* extracts and other biostimulant products using NMR metabolomics and other analytical methods to evaluate final product composition and consistency. **D. Hiltz**, E. Kerrin, L. Hamilton, A. Banskota
- 11:25** Concluding Remarks.

SECTION F
San Diego Convention Center
Room 33C

Kenneth A. Spencer Award & Related Presentations

S. J. Leibowitz, *Organizer, Presiding*

B. A. Lorsche, *Presiding*

- 8:05** Introductory Remarks with Presentation of Spencer Award.

- 8:15** **174.** Science at the interface: Natural products and computational approaches to understanding and exploiting their chemistry. **T.C. Sparks**
- 9:00** **175.** Synthesis of GABA_AR antagonists and related chemical space. **R.A. Shenvi**
- 9:25** **176.** Innovative approaches to deliver natural product and natural-derived solutions for crop protection. **B.A. Lorsbach**, R. Cicchillo, N. Garizi, D. Hahn, K.G. Meyer, T.C. Sparks
- 9:50** Intermission.
- 10:10** **177.** Discovery and use of natural products as mosquito repellents. **C.L. Cantrell**, A. Ali
- 10:35** **178.** NCI program for natural product discovery: Creating natural product libraries for high-throughput screening. **C. Thornburg**, J. Britt, J. Evans, R. Akee, J. Whitt, S. Trinh, M. Harris, J. Thompson, T. Ewing, S. Shipley, P. Grothaus, D. Newman, J. Schneider, T. Grkovic, B. O’Keefe
- 11:00** Concluding Remarks.

Chemistry & Utilization of Agro-Based Materials Nanoscience & Related Materials

Sponsored by AGFD, Cosponsored by AGRO

Chemistry & Applications of Free Radical-based Technologies for Water Treatment & Purification

UV-Based Free Radicals-Based Technologies & Application

Sponsored by ENVR, Cosponsored by AGRO

Nanotechnology Applications for Food & Agriculture

Sponsored by AGFD, Cosponsored by AGRO

Chemistry of Water Reuse Processes Toward Water Sustainability

Sponsored by ENVR, Cosponsored by AGRO and PRES

Non-targeted Analysis to Understand Fate & Effects of Pharmaceuticals & Emerging Contaminants in Agriculture & Natural Environments

Sponsored by ENVR, Cosponsored by AGRO

USDA-ARS Sterling B. Hendricks Memorial Lectureship Symposium

Sponsored by AGFD, Cosponsored by AGRO

Sensors for Water Quality Assessment in Resource Limited Environments

Sponsored by ENVR, Cosponsored by AGRO

SECTION A

**San Diego Convention Center
Ballroom 20B-D Theater 1**

Kenneth A. Spencer Award & Related Presentations

S. J. Leibowitz, *Organizer, Presiding*
B. A. Lorsbach, *Presiding*

- 2:15** Introductory Remarks.
- 2:20** **179.** Two scalable platforms for large scale discovery of microbial natural products. **N.L. Kelleher**
- 2:45** **180.** Development of novel carbohydrate-based macrocyclic picolinamide fungicides. **K. Bravo-Altamirano**, F. Li, R. Heemstra, K.G. Meyer, P. Graupner, C. Yao
- 3:10** Intermission.
- 3:30** **181.** AI and natural agricultural active agent discovery. **N. Magarvey**
- 3:55** **182.** Discovery of florylpicoxamid, a new picolinamide for disease control. **K.G. Meyer**, C. Yao, Y. Lu, K. Bravo, Z. Buchan, J. Daeuble, K. DeKorver, J. Herrick, D.M. Jones, B.A. Loy, J. Rigoli, N. Wang, J. Wilmot, D. Young
- 4:20** Concluding Remarks.

SECTION B

**San Diego Convention Center
Ballroom 20B-D Theater 2**

Simulating Fumigant Transport & Emissions: The Evolving Role of Modeling in California Regulations

Cosponsored by ENVR
S. Krepich, *Organizer*
E. Vidrio, *Organizer, Presiding*

- 1:00** Introductory Remarks.
- 1:05** **183.** Comparison between field-estimated and HYDRUS-simulated emission of 1,3-Dichloropropene from agricultural fields. **M. Kandelous**, C. Brown
- 1:30** **184.** Estimation of bystander exposure of sulfuryl fluoride during structural fumigations of California detached single family houses. **J. Tao**
- 1:55** **185.** Environmental effects on fumigant emission from soil surface: Modeling perspective. **M. Kandelous**, C. Brown
- 2:20** **186.** Procedure to select meteorological data for air dispersion modeling of pesticide applications in California. **J. Tao**

- 2:45 **187.** Refining dispersion modeling to meet evolving regulatory requirements. **R. Sullivan, D.A. Sullivan**
- 3:10 Intermission.
- 3:30 **188.** Using HYDRUS to estimate 1,3-D emissions under California conditions. **C. Brown, M. Kandelous, F. Sartori, C. Collins, F. Spurlock**
- 3:55 **189.** AERFUM: Integrated air dispersion modeling system for soil fumigants. **Y. Luo**
- 4:20 Concluding Remarks.

SECTION C

San Diego Convention Center
Ballroom 20B-D Theater 3

What does Nanotechnology Have to do with Agriculture?

Cosponsored by COLL

J. Hughes, S. Kweskin, *Organizers, Presiding*

- 1:00 Introductory Remarks.
- 1:05 **190.** Effects of nanotechnology fertilizers on soybean plant runoff water. **J. Taylor**
- 1:30 **191.** Nanoscale agrochemicals for precision agriculture and sustainable environment. **R. Raliya**
- 1:55 **192.** Nanoparticles of Cu and Si for the suppression of plant diseases. **W. Elmer, C. Ma, L. Pagano, N. Zuverza-Mena, R. De La Torre-Roche, C. Perez, J. Borgata, J.T. Buchman, C.L. Haynes, R.J. Hamers, J.C. White**
- 2:20 **193.** Molecular and physiological responses of alfalfa (*Medicago sativa*) plants exposed to nano, bulk, and ionic copper compounds. **K. Cota-Ruiz, Y. Yuqing, C. Valdes, E. Eguiarte, J.I. García-López, J.A. Hernández-Viezcas, J. Peralta-Videa, J.L. Gardea-Torresdey**
- 2:45 **194.** High aspect ratio nanomaterials enable biomolecule delivery and transgene expression or silencing in intact plants. **G.S. Demirer, H. Zhang, J. De Lima Matos, N. Goh, F. Cunningham, Y. Sung, B. Staskawicz, M. Landry**
- 3:10 Intermission.
- 3:30 **195.** Evaluating the potential of a suite of metal colloids for the treatment of pathogenic diseases: Case study for citrus greening disease. **T. Ameh, C. Sayes, E. Braswell**
- 3:55 **196.** Bioinspired development of crop foliage-adhesive nanopesticides to enhance folia retention. **Z. Zeng, M. Yu, H. Chen, H. Cui**
- 4:20 **197.** Utilization of cellulose nanomaterials in agriculture: Current status and future prospects. **G. Kandhola, J. Batta-Mpouma, M. Lisunova, J. Kim**
- 4:45 Concluding Remarks.

SECTION D

San Diego Convention Center
Ballroom 20B-D Theater 4

Surfactant & Colloid Science Applied to Formulations

Cosponsored by COLL

R. Acosta Amado, B. Rauzan, S. Sumulong, *Organizers, Presiding*

- 1:25 Introductory Remarks.
- 1:30 **198.** Enhanced microbial pesticides via rainfastness and UV resistance improvement. **C. Woelfle-Gupta, S. Arumugam, D. Saucy, M. Carter, Y. Tan, S.L. Jordan, A. Izmitli, B. Ajayi**
- 1:55 **199.** Approaches in waterborne basecoat formulation practice to minimize volatile organic compounds (VOCs). **M. MacDonald, L. Humbert**
- 2:20 **200.** Influence of solvent chemistry on the viscosity of high-load emulsifiable concentrate agrochemical formulations. **R. Acosta Amado, N. de Castro, H. Jeon**
- 2:45 **201.** Emulsifiable concentrate (EC) development and beyond. **F. Tu**
- 3:10 Intermission.
- 3:30 **202.** Colloidal nanocrystal approach to fighting counterfeit products. **A.F. Smith, S.E. Skrabalak, J.D. Smith**
- 3:55 **203.** Natural wax nanoparticles induce changes in morphology and physical properties of polysaccharides after spray drying: Applications for development of controlled-release formulations. **C. Espinoza-González, N. Navarro-Guajardo, C. Villanueva-González, C. Martínez-Lara, L. Arizmendi-Galaviz, A. Ledezma-Pérez, J. Romero-García**
- 4:20 Concluding Remarks.

SECTION E

San Diego Convention Center
Ballroom 20B-D Theater 5

Next Generation Watershed Modeling of Agrochemicals

Cosponsored by ENVR

N. Peranginangin, N. Thurman, M. Winchell, *Organizers, Presiding*

- 1:25 Introductory Remarks.
- 1:30 **204.** Overview and application of the SWAT+ model for watershed scale simulation of agrochemicals. **H. Rathjens, M. Winchell, P.L. Havens**
- 1:55 **205.** Modeling the co-occurrence of pesticides and degradation products in surface water at the landscape scale. **P.K. Janney, J.J. Jenkins**

- 2:20** **206.** Methods for representing watersheds in a tiered approach for pesticide risk assessments. **N. Thurman**, J. Hook
- 2:45** **207.** Towards the derivation of realistic dilution factors for drinking water abstraction combining GIS analysis and landscape level modelling. **S. Gebler**, T. Schröder, **E. Henry**
- 3:10** Intermission.
- 3:30** **208.** Comparison of pesticide concentrations observed in community water systems to predictions from US regulatory aquatic exposure models. **J. Dunne**, N. Peranginangin, L. Padilla, M. Winchell
- 3:55** Panel Discussion.
- 4:20** Concluding Remarks.

SECTION F
San Diego Convention Center
Room 33C

Biostimulants in Agriculture: Chemistry & Regulatory Aspects

Cosponsored by BIOL, MEDI and TOXI
 P. Halarnkar, *Organizer*
 M. E. Koivunen, K. D. Wing, *Organizers, Presiding*
 P. Halarnkar, *Presiding*

- 1:20** Innovation Award Ceremony and Introductory Remarks.
- 1:30** **209.** History, status, and future potential of natural products for pest management and plant health. **P.G. Marrone**
- 2:20** **210.** Managing the challenges associated with continued growth of biostimulant technologies. **S. Semones**
- 2:45** **211.** Guidance for plant regulator label claims, including plant biostimulants. **R.S. Jones**
- 3:10** Intermission.
- 3:30** **212.** U.S. regulation and legislation impacting the plant biostimulant industry. **D.G. Beaudreau**
- 3:55** **213.** Update on regulatory developments related to biostimulants. **K. Matthews**
- 4:20** Discussion.
- 4:35** Concluding Remarks.

Chemistry & Applications of Free Radical-based Technologies for Water Treatment & Purification
Various Free Radicals-Based Technologies

Sponsored by ENVR, Cosponsored by AGRO

Chemistry & Utilization of Agro-Based Materials
Advanced Materials from Agricultural Sources

Sponsored by AGFD, Cosponsored by AGRO

Biochar & Hydrochar for Energy, Environmental & Agricultural Applications

Sponsored by ENVR, Cosponsored by AGRO

Proposition 65 on Food Safety

Sponsored by AGFD, Cosponsored by AGRO

TUESDAY EVENING – AGRO

Biochar & Hydrochar for Energy, Environmental & Agricultural Applications

Sponsored by ENVR, Cosponsored by AGRO

Chemistry & Applications of Free Radical-based Technologies for Water Treatment & Purification

Sponsored by ENVR, Cosponsored by AGRO

Chemistry of Water Reuse Processes Toward Water Sustainability

Sponsored by ENVR, Cosponsored by AGRO and PRES

Non-targeted Analysis to Understand Fate & Effects of Pharmaceuticals & Emerging Contaminants in Agriculture & Natural Environments

Sponsored by ENVR, Cosponsored by AGRO

Sensors & Biosensors for Widespread Environmental Monitoring

Sponsored by ENVR, Cosponsored by AGRO

Sensors for Water Quality Assessment in Resource Limited Environments

Sponsored by ENVR, Cosponsored by AGRO

SECTION A

San Diego Convention Center
Ballroom 20B-D Theater 1

Process Research & Development in Crop Protection

W. Su, Q. Yang, *Organizers*
K. Gray, *Organizer, Presiding*

- 8:05 Introductory Remarks.
- 8:10 **214.** Evaluation of [3 + 2] cyclization strategies to 3-(3-Chloro-1 *H*-pyrazol-1-yl)pyridine, a key intermediate for the insecticidal active tyclopyrazoflor. **Q. Yang**, X. Li, B.A. Lorsbach, G. Roth, D. Pordhorez, R. Ross, N. Niyaz, A. Buysse, D. Knueppel, J. Nissen
- 8:35 **215.** Fit-for-purpose optimization of the route to tyclopyrazoflor featuring [3 + 2] cyclization of 3-hydrazinopyridine dihydrochloride and methyl acrylate. **X. Li**, Q. Yang, B.A. Lorsbach, J. Muhuhi, **G. Roth**, K. Gray, D.E. Podhorez
- 9:00 **216.** Streamlining the chemical development process through continuous flow and task automation. **C. Breen**, T.F. Jamison
- 9:25 Intermission.
- 9:45 **217.** Scalable synthesis of methyl 3-((3,3,3-trifluoropropyl)thio)propanoate via thiol-ene chemistry. **K. Gray**, P. Heider, P. McGough, M. Ondari, J. Devaraj, Q. Yang, G. Frycek, B. Graham, J. Neuman, B.A. Lorsbach, Y. Zhang
- 10:10 **218.** Withdrawn
- 10:35 **219.** Development of a scalable synthesis of chiral allyl ether 6, a key intermediate *en route* to an experimental picolinamide fungicide. **S.N. Good**, F. Li, G.T. Whiteker
- 11:00 Concluding Remarks.

SECTION B

San Diego Convention Center
Ballroom 20B-D Theater 2

Pollinators in Agroecosystems: Current Science Issues & Risk Assessment Approaches

Cosponsored by ENVR
Financially supported by Intrinsic
V. Kramer, J. R. Purdy, T. Steeger, *Organizers*
C. Douglass, A. Krueger, *Organizers, Presiding*
J. Purdy, *Presiding*

- 8:05 Introductory Remarks.
- 8:10 **220.** Protecting pollinators in agricultural land: Toolbox of risk mitigation measures associated to pesticide use. **A. Alix**

- 8:35 **221.** Pollinators as keystones of agriculture and natural ecosystems: Impact of organosilicone spray adjuvants on their health and reproduction. **D.L. Cox-Foster**, E. Klinger, W.J. Doucette
- 9:00 **222.** Pesticides in honey bee colonies: Real world exposure and associated morbidity over seven years (2011–2017) in the USA. **D. van Engelsdorp**, K. Traynor, R. Rose, K. Rennich
- 9:25 **223.** Quantification of neonicotinoid residues in a pollinator attractive habitat. **M.J. Hall**, V. Dang, G. Zhang, M.E. O’Neal, S.P. Bradbury, J.R. Coats
- 9:50 Intermission.
- 10:10 **224.** Toxicity of some ready-to use and common garden pesticides to non-*Apis* bees. **N. Joshi**, O. Kline, J. Belsky
- 10:35 **225.** Semi-field testing to address the risk of the insecticide chlorantraniliprole on the brood of the honey bee (*Apis mellifera*, *Hymenoptera*, *Apidae*). **A. Dinter**, A. Samel, K. Brugger
- 11:00 **226.** Movement of Varroa mites and the spread of viruses they transmit among colonies: Challenges to quantification of pesticide effects. **G. De Grandi-Hoffman**, V. Corby Harris, J. Chen, M. Chambers, H. Graham, E. Watkins DeJong, N. Ziolkowski
- 11:25 Concluding Remarks.

SECTION C

San Diego Convention Center
Ballroom 20B-D Theater 3

Transfer of Analytical Methods: The Good, the Bad, & the Ugly

R. M. Bennett, K. Clark, J. E. Foster, L. Riter, *Organizers, Presiding*

- 8:05 Introductory Remarks.
- 8:10 **227.** Method development and validation for determination of mancozeb and its metabolite ETU via LC-MS/MS in soil, water, plant, and animal matrices. **A. Li**, A.D. Budgeon Jr, C.M. Bianca
- 8:35 **228.** Two perspectives on transfer of residue analytical methods. **L. Riter**, K. Clark
- 9:00 **229.** Key elements of successful method transfers. **K. McInerney**
- 9:25 **230.** Method development and optimization for extracting a pesticide from bee and corn pollen. **S. Whiting**, W. Fain, E. Vogl, K. Clark
- 9:50 Intermission.
- 10:10 **231.** Contract laboratory perspective on the transfer of LC-MS/MS methods. **S. Sharp**, S. Perez
- 10:35 **232.** Stay tuned! Strategically-developed GLP EPA residue analytical methods to meet the regulatory requirements of different global regions. **J.E. Foster**
- 11:00 Discussion.
- 11:25 Concluding Remarks.

SECTION D
San Diego Convention Center
Ballroom 20B-D Theater 4

Environmental fate, transport, & modeling of agriculturally-related chemicals

Financially supported by Stone Environmental
S. Jackson, R. L. Warren, *Organizers, Presiding*

- 8:30** Introductory Remarks.
- 8:35** **233.** Challenges, approaches and achievements on surface water mineralization with amended solids: Case study for insoluble compounds and high volatility. **R. Lomax**, M. Ponte
- 9:25** **234.** Hydrolysis of dichloroacetamide herbicide safeners: Rates and transformation products. **M.E. McFadden**, J.D. Sivey, G.H. LeFevre, D.M. Cwiertny
- 9:50** Intermission.
- 10:10** **235.** Sorption-desorption hysteresis linked to formation of metastable states: How much does it cost (in terms of free energy). **M. Borisover**
- 10:35** **236.** Summary of ‘Scientific opinion about the guidance of the Chemical Regulation Directorate (UK) on how aged sorption studies for pesticides should be conducted, analysed and used in regulatory assessments’: Released in August 2018 by EFSA. **P. Sharma**
- 11:00** **237.** Inverse modeling approaches for derivation of aged sorption parameters from terrestrial field dissipation studies. **P. Sharma**
- 11:25** Concluding Remarks.

SECTION E
San Diego Convention Center
Ballroom 20B-D Theater 5

Development of Novel Vector Control Technologies

Cosponsored by MEDI
A. D. Gross, E. J. Norris, D. Swale, *Organizers, Presiding*

- 8:05** Introductory Remarks.
- 8:10** **238.** Convergence of the octopaminergic and muscarinic signal transduction pathways in *Drosophila melanogaster*. **A.D. Gross**, N. Xie
- 8:35** **239.** Will resistance render pyrethroids ineffective for house fly control in the near future?. J.C. Freeman, **J.G. Scott**
- 9:00** **240.** How many sodium channel mutations confer pyrethroid resistance in *Aedes aegypti*?. **K. Dong**
- 9:25** **241.** Towards new modes of action for reducing arthropod-borne disease in honey bee colonies. **T.D. Anderson**
- 9:50** Intermission.

- 10:10** **242.** Developing novel mechanism insecticides to inhibit feeding and vectorial capacity of the cotton aphid, *Aphis gossypii*. **D. Swale**
- 10:35** **243.** Do ABC transporters contribute to pyrethroid resistance in the Puerto Rico strain of *Aedes aegypti*?. **L. Rault**, E. Johnson, S. O’Neal, T.D. Anderson
- 11:00** **244.** Vapor delivery of plant essential oils alters pyrethroid efficacy and detoxification enzyme activity in mosquitoes. **S. O’Neal**, E.J. Johnson, L. Rault, T.D. Anderson
- 11:25** Concluding Remarks.

SECTION G
San Diego Convention Center
TBD

Advances in Analytical Technologies Supporting Environmental Fate, Metabolism, & Residue Analysis

Cosponsored by ENVR
K. Kuppanan, M. Ma, Y. Yuan, *Organizers*

- 11:30 - 2:00**
- 245.** Development of analytical method of cyantraniliprole residue in Wilford swallow-wort (*Cynanchum wilfordii* (Maxim.) Hemsl.). **J. Choi**, S. Leem, H. Ham, J. Kim, H. Choi, **J. Hur**
- 246.** SFC-MS based analytical strategy for stereoisomer analysis in environmental fate and metabolism studies. **X. Zhou**, J.A. Godbey, T.K. Trullinger
- 247.** Method development for analysis of herbicide glyphosate and its metabolite aminomethylphosphonic acid in human urine samples using GC-MS/MS. **J. Tang**, T. Baker, K. LeVanseler, N. Cole
- 248.** Degradation of tetracycline antibiotics in livestock and poultry manure during anaerobic digestion. **J. Kasumba**, K. Appala, G. Agga, J.H. Loughrin, E.D. Conte
- 249.** Application of multiple mass defect filters to improve the quality of total ion chromatograph in high resolution MS analysis. **M. Zhang**, D. Nabb
- 250.** Development of the analytical method for carbendazim in a traditional herbal medicine, *Astragalus membranaceus*, using HPLC. **B. Ju**, J. Lee, E. Park, X. Yuan, R. Go, M. Rehan, E. Jung, H. Han, J. Kim
- 251.** Withdrawn
- 252.** Efficiency evaluation of extraction and clean-up for multi pesticides by LC-MS/MS in agricultural commodities. **S. Lee**, S. Kwak, H. Kim, H. Jeong, A. Nam, J. Kim

SECTION G
San Diego Convention Center
TBD

Agrochemical Residue & Metabolism Chemistry

Cosponsored by AGFD

J. J. Johnston, K. Mastovska, D. J. Smith, X. Zhou, *Organizers*

11:30 - 2:00

253. Hydrolysis of amisulbrom in various pH buffer solutions: Kinetic and products identification. **J. Hu**, K. Pang, H. Lin

254. Withdrawn

255. Application of kinetic models for degradation rate of triazole pesticides in perilla leaves. **H. Kim**, S. Lee, S. Kwak, A. Sarker, H. Jeong, A. Nam, T. Kim, J. Kim

256. Structure determination of DNA adducts from chlorobenzonitrile pesticides. **M. Byron**, D.W. Boerth

257. Development of multi-residue analysis method of pesticides in organic agro-materials. **H. Jeong**, S. Kwak, S. Lee, A. Sarker, H. Kim, A. Nam, J. Kim

258. Dissipation of fomesafen in fumigated and organic-amended soil in Florida tomato systems.

Z. Li, F. Di Gioia, J. Hwang, J. Hong, M. Ozores-Hampton, X. Zhao, C. Pisani, E. Roskopf, P. Wilson

259. Method optimization for the trace analysis of planar pesticides in pigmented plant matrices. **E. Leonard**, C. Palmer, N. Tharayil

SECTION G
San Diego Convention Center
TBD

Biological Considerations for Agrochemical Control

Cosponsored by AGFD

C. B. Cleveland, *Organizer*

11:30 - 2:00

260. Alternative water source contaminant concerns for greenhouse agriculture. **J.C. Czarnecki**, T.M. Vadas, D. Kelemen, C. Kirchhoff, A. Tashev, R. Raudales

261. Semiochemicals for attraction of *Euwallacea* nr. *forficatus*, a pest ambrosia beetle in southern Florida. **N. Tabanca**, P. Kendra, D. Owens, T. Narvaez, W. Montgomery, E. Schnell, D. Carrillo

262. Evaluation of repellents for *Euwallacea* nr. *forficatus*, a pest ambrosia beetle in Florida avocado groves. P. Kendra, **N. Tabanca**, W. Montgomery, T. Narvaez, E. Schnell, A. Vazquez, D. Carrillo

263. Toxicity changes during photolysis of Triton X-100 in water. **E. Jho**, D.G. Yoo

264. Elucidating the influence of nanoparticle chemical and physical properties on their translocation and distribution in crop leaves. **P. Hu**, J. An, M. Faulkner, H. Wu, Z. Li, X. Tian, J. Giraldo

265. Acephate risk characterization. **W. Zhao**

266. Effect of polyethylene microplastics on strawberry plant growth, soil enzyme activity, and microbial community composition. **S. Chahal**, P. Wang, V. Bueno, H. Anand, S. Bayen, S. Ghoshal, V. Gravel, N. Tufenkji

SECTION G
San Diego Convention Center
TBD

Biostimulants in Agriculture: Chemistry & Regulatory Aspects

Cosponsored by BIOL, MEDI and TOXI

P. Halarnkar, M. E. Koivunen, K. D. Wing, *Organizers*

11:30 - 2:00

267. Foliar application of inositol-based biostimulant boosts zinc uptake and accumulation in wheat (*Triticum aestivum* L.). **D. Amaral**, P.H. Brown

268. Field methods for evaluating nutrient enhancement effects of biostimulants. **R.E. Ross**

269. Field screening approaches for monitoring whole-plant response modulated by biostimulants. **M. Park**, D. Amaral, P.H. Brown

SECTION G
San Diego Convention Center
TBD

Development of Novel Vector Control Technologies

Cosponsored by MEDI

A. D. Gross, E. J. Norris, D. Swale, *Organizers*

11:30 - 2:00

270. Phenalenones-based photosensitizers for mosquito control. **X. Shao**

271. Larvicide activity of biorational compounds to pyrethroid-resistance *Aedes aegypti* mosquitoes. **E. Johnson**, S. O'Neal, L. Rault, T.D. Anderson

272. Plant terpenoids as a source of novel nematicides. **C. Wong**, J.R. Coats

273. Combatting plant-parasitic nematodes with biorational pesticides. **J.S. Klimavicz**, J.O. Barizon, G.L. Tylka, J.R. Coats

274. Giving ticks 'dry mouth' through chemical modulation of inward rectifier potassium channels as a mechanism to prevent blood feeding. **Z. Li**, D. Swale

- 275.** Inducing neural failure through chemical inhibition of insect inward rectifier potassium channels. **R. Chen**, D. Swale
- 276.** Identification of novel target sites to reduce salivary gland function and feeding of *Aedes aegypti*. **A. Soohoo-Hui**, D. Swale
- 277.** Toxicological relevance of potassium ion channels to honey bee immune health. **C.J. Fellows**, T.D. Anderson, D. Swale
- 278.** Toxicological and neurophysiological characterization of natural product based chromene analogs to insect pests. **S. McComic**, D. Swale, K.M. Meepagala
- 279.** Repurposing isoxazoline and diamide insecticides to control the sand fly, *Phlebotomus papatasi*. **M. Nguyen**, Z. Li, L. Foil, D. Swale
- 280.** Developing an alternative method for deploying toxic sugar bait technologies. **C.L. Corona**, J.S. Klimavicz, J.R. Coats
- 281.** Synergistic effects of potassium channel blockers and pyrethroids: Mosquitocidal activity and neuronal mode of action. **S. Jiang**, J.R. Bloomquist
- 282.** Transcriptome analysis of the chicken mite *Dermanyssus gallinae* for the characterization of major acaricide target genes. K. Kim, S. Kim, J. Kim, S. Lee

SECTION G

San Diego Convention Center

TBD

Ecological Considerations of Crop Protection

Cosponsored by ENVR

C. B. Cleveland, *Organizer*

11:30 - 2:00

- 283.** Growing good neighbors using technology to improve outreach and communication. **S. Regagnon**
- 284.** Toxicology of a pyrethroid insecticide in the monarch butterfly and interactions with host plant defense chemicals. **A. Krueger**, T.D. Anderson
- 285.** Some challenges of analytical method transfer for ecotoxicology study in CRO. **J. Wang**
- 286.** Evaluation of DDT bioaccumulation in earthworms from a historically-contaminated orchard using Bayesian hierarchical modelling. **Z. Yang**, M.O. Anderson, T. LaChance, R.E. Plummer, D. Jackson, L.L. McConnell, C.J. Hapeman, A. Torrents

Environmental Fate, Transport, & DRIFT Modeling of Agrichemicals

Financially supported by Stone Environmental

S. Jackson, R. L. Warren, *Organizers*

11:30 - 2:00

- 287.** Quantum yields and product studies for photolysis of neonicotinoids solid films. **W. Wang**, K.Z. Aregahegn, S.T. Andersen, A.Z. Ni, A. Rohrbacher, O. Nielsen, B.J. Finlayson Pitts
- 288.** Atmospheric fate of neonicotinoids as pure compounds and in formulations. **A. Rohrbacher**, B.J. Finlayson Pitts
- 289.** Ion-specific influences on the photodegradation of benzobicyclon hydrolysate in seawater. M. Knight, E.N. Vebrosky, **L. Basirico**, **K.L. Armbrust**
- 290.** Common Issues in agrochemical risk communication. **D. Barrett**, M. Williams
- 291.** Uptake, translocation, and metabolism of trace organic contaminants in water-plant. **J. Hwang**, P. Wilson
- 292.** Evaluation of end points derived from soil rate of degradation studies dosed with cold and radio-labeled test substances and their impact on exposure assessment. **C. Fang**
- 293.** Spray drift characterization using an ambient breeze tunnel. **T. Lane**, C. Mohler, F. Salzman, J. Arnold
- 294.** Assessing lateral hydraulic connectivity of edge-of-field groundwater monitoring wells using a tiered modeling approach. **N. Kehrein**, W. He, F. Hegler, R. Sur
- 295.** Higher tier refinement on the tier 1 AgDRIFT buffer distance using REGDISP model for environmental risk assessment in New Zealand. **M. Kim**, M. Robert

SECTION G

San Diego Convention Center

TBD

New Herbicides & Their Modes of Action & Design

F. Dayan, S. O. Duke, T. M. Stevenson, *Organizers*

11:30 - 2:00

- 296.** Highly functionalized herbicidal natural product: Synthesis, SAR and stereochemistry. **B. Kuhn**,

H. Dietrich, D. Barber, U. Doeller, M. Hoffmann, D. Schmutzler, S. Schnatterer, M.E. Maier, T. Kocakaya, M. Morkunas

297. Computational modeling of inhibition of acetyl CoA carboxylase by cyclohexanedione and aryloxypropionic acid herbicides. **V. Sammeta**, D.W. Boerth

298. Complex nanoparticles for delivering crop protection agents. **J. Zhang**

SECTION G

San Diego Convention Center
TBD

Off-Target Transport of Field Applied Agricultural Chemicals: Study Designs, Monitoring, Modelling, & Risk Assessment

Cosponsored by ENVR

S. Grant, A. M. Ritter, Q. Yao, *Organizers*

11:30 - 2:00

299. Establishment of soil management guideline for spinach cultivation in soils contaminated with endosulfan. **S. Kwak**, S. Lee, A. Sarker, H. Kim, H. Jeong, A. Nam, J. Kim

300. Results of a multi-stakeholder workshop on incorporating the benefits of vegetative filter strips into aquatic risk assessment and risk management of pesticides. D. Carley, Z. Tang, R. Munoz-Carpena, G. Fox, P.J. Rice, C. Truman, K.L. Armbrust, **L.L. McConnell**

301. Edge-of-field management to mitigate potential off-site pesticide movement. **M.A. Locke**, M. Moore, L. Yasarer, R. Bingner

302. Effectiveness of vegetated filter strips based on modeling with VFSSMOD or fixed reduction percentages from the European regulatory framework. **R. Sur**, S. Reichenberger, H. Meyer, C. Kley

303. Regulatory implementation of VFS as a mitigation for transport of pesticides via runoff and erosion: European approach. **E. Henry**, B. Erzgräber, Z. Tang, R. Sur

304. Phytoremediation of atrazine using switchgrass (*Panicum virgatum*). **K. Hatch**, R. Lerch, K.W. Goyne, C. Willett, K.J. Robert, R. Craig

SECTION G

San Diego Convention Center
TBD

Pollinators in Agroecosystems: Current Science Issues & Risk Assessment Approaches

Cosponsored by ENVR

Financially supported by Intrinsic

C. Douglass, V. Kramer, A. Krueger, J. R. Purdy, T. Steeger, *Organizers*

11:30 - 2:00

305. Pollinator research task force: Overview of accomplishments and upcoming projects. **V.J. Kramer**

306. Residue analysis of cyantraniliprole and its metabolites in bee products in support of ecotoxicology studies. **M.Y. Cabusas**

307. Sublethal effects of chlorantraniliprole exposure to a beneficial insect species. **J. Williams**, D. Swale, T.D. Anderson

308. Addressing multiple factors impacting honey bee colonies in large colony feeding studies with a mechanistic honey bee colony model. A. Schmolke, F. Abi-Akar, **D. Perkins**, N. Galic, S. Hinarejos

309. Contamination of bee-collected pollen in multiple landscapes. **J. Zawislak**, G. Lorenz, J. Adamczyk, N. Joshi

310. Toxicity of premixed insecticide chemistries to blue orchard bees. **J. Belsky**, N. Joshi

SECTION G

San Diego Convention Center
TBD

Surfactant & Colloid Science Applied to Formulations

Cosponsored by COLL

R. Acosta Amado, B. Rauzan, S. Sumulong, *Organizers*

11:30 - 2:00

311. Optimization of manufacturing process to improve the physical stability of oil-in-water emulsion agricultural formulation. **J. Xu**, R. Acosta Amado

312. Use of polar co-solvents to improve dilution properties at low temperature of high-load emulsifiable concentrate (EC) agrochemical formulations. **N. de Castro**, R. Acosta Amado

313. Overview of the application of surface chemistry in pesticide formulations. **V. Shing**

Innovative Approaches to Enhancing Food Safety & Reducing Food Waste

Sponsored by AGFD, Cosponsored by AGRO

Chemistry & Applications of Free Radical-based Technologies for Water Treatment & Purification

Sulfate Radicals- & Electrochemical Production of Radicals-Based Technologies

Sponsored by ENVR, Cosponsored by AGRO

Biochar & Hydrochar for Energy, Environmental & Agricultural Applications

Sponsored by ENVR, Cosponsored by AGRO

Proposition 65 on Food Safety

Sponsored by AGFD, Cosponsored by AGRO

WEDNESDAY AFTERNOON – AGRO

SECTION A

San Diego Convention Center
Ballroom 20B-D Theater 1

Innovative Approaches to Managing the Interface Between Pesticide Use & Non-Target Species Habitat Protection

Cosponsored by ENVR

A. Beehler, A. Frank, L. Moreno, *Organizers, Presiding*
K. Bissell, *Presiding*

- 2:00 Introductory Remarks.
- 2:05 **314.** Ontogeny of a pesticide application with respect to FIFRA/ESA endangered species risk interpretation. **B. McGaughey**
- 2:30 **315.** Conservation measures and their role in the endangered species act consultation process. **K. Bissell, L. Laniawe**
- 2:55 **316.** Tools developed to inform landowners about sensitive habitats and conservation options. **J. Peters, M. Crowder, A. Rivers**
- 3:20 **317.** Ensuring safety of sensitive listed plants to new crop protection products. **D.E. Edwards, P.J. Rice, S.R. Mortensen**
- 3:45 Intermission.
- 4:05 **318.** What do we actually do? Review of modern integrated mosquito control programs in the United States. **G. White**
- 4:30 **319.** Best management practices: Using species specific technology to control *Aedes aegypti* mosquitoes at Anastasia Mosquito Control District. **R. Xue**
- 4:55 **320.** Quantitative analysis of traditional and non-traditional techniques to minimize spray drift. **J. Bonds**

- 5:20 **321.** Endangered Species Act considerations in planning and implementing pesticide use. **C.A. Roberts**
- 5:45 Concluding Remarks.

SECTION B

San Diego Convention Center
Ballroom 20B-D Theater 2

Plant-Insect-Microbe Communications in Agriculture: General Session

Cosponsored by AGFD

P. Kendra, J. Niogret, N. Tabanca, *Organizers, Presiding*

- 2:00 Introductory Remarks.
- 2:05 **322.** Role of semiochemicals in plant-insect-entomopathogenic nematode interactions. **H.T. Alborn**
- 2:30 **323.** Constitutive, herbivore- and microbe-induced *Citrus jambhiri* (lemon) volatiles differentially influence African citrus trioqid *Trioza erytreae* behavior. **B. Torto, A.K. Antwi-Agyakwa, S.A. Mohamed**
- 2:55 **324.** Exploring the role of phenolic and terpenoid compounds in grapevine defense against pathogens and insects. **C.M. Wallis**
- 3:20 **325.** Interaction of ants and microbes with special emphasis on the fire ant, *Solenopsis invicta*. **R.K. Vander Meer**
- 3:45 Intermission.
- 4:05 **326.** Developing microbial odor based repellents to manage spotted wing drosophila, *Drosophila suzukii*. **D. Cha, G. Loeb**
- 4:30 **327.** Development of infestation detection and population monitoring tool for invasive species, spotted wing *Drosophila*. **A. Zhang, Y. Feng, N. Larson**
- 4:55 **328.** Agricultural screening of volatile organic compounds as indicators of infestation by portable gas chromatography. **L.D. Mosser**
- 5:20 **329.** Nectar microbe mixtures differ from single species in volatile emission and pollinator acceptance. **C.C. Rering, R.L. Vannette, R. Schaeffer, J.J. Beck**
- 5:45 Concluding Remarks.

SECTION C
San Diego Convention Center
Ballroom 20B-D Theater 3

Transfer of Analytical Methods: The Good, the Bad, & the Ugly

R. M. Bennett, K. Clark, J. E. Foster, L. Riter, *Organizers, Presiding*

- 2:00** Introductory Remarks.
- 2:05** **330.** Transferring a verified method for the analysis of pesticides in cannabis to contract laboratories: Lessons learned. **P.C. Winkler**, D. Tran, R. DiLorenzo, S. Roberts, C. Butt, K. Oetjen, K. Hyland, C. Borton
- 2:30** **331.** Transfer of a trace level dicamba method between industry and a state agency to enable assessment of off-target transport. **A. Meredith**, M. Green, J. Toler, P. Jensen, L. Riter, A. Chen, D.L. Sparks, A.E. Brown
- 2:55** **332.** Methods of miscommunication: Series of unfortunate events. **E.A. Schoenau**, **T.F. Moate**
- 3:20** **333.** Challenges for developing a method, validation and method transfer. **R.M. Bennett**
- 3:45** Intermission.
- 4:05** **334.** LC-MS/MS analysis of neonicotinoids and their metabolites in different environmental matrices by modified QuEChERS. **M.J. Hall**, V. Dang, D.J. Borts, S.P. Bradbury, J.R. Coats
- 4:30** **335.** Obstacle course of running SANCO compliant method validations to support ecotoxicology studies. **L. Zhang**, K. Martin
- 4:55** Discussion.
- 5:10** Concluding Remarks.

SECTION D
San Diego Convention Center
Ballroom 20B-D Theater 4

Environmental fate, transport, & modeling of agriculturally-related chemicals

Financially supported by Stone Environmental
S. Jackson, R. L. Warren, *Organizers, Presiding*

- 2:25** Introductory Remarks.
- 2:30** **336.** Pesticide quantitative structure-biodegradability relationship models. **D. Tomandl**, D. Cirovic, M. Hastings, K. Lynn, S. Gehen, R. Rasoulpour
- 2:55** **337.** US EPA CompTox Chemicals Dashboard providing access to experimental and predicted environmental fate and transport data. **A.J. Williams**, C. Grulke, K. Mansouri, T. Martin
- 3:20** **338.** Improved lipophilicity (clogD) QSAR models for agrochemicals. **Y. Djoumbou Feunang**, D. Tomandl

- 3:45** Intermission.
- 4:05** **339.** Refinement of consumer use pesticides application practices and resulting improvements to exposure predictions in ecological risk assessments. **S. Castro-Tanzi**, L. Padilla, W. Hillwalker, M. Winchell
- 4:30** **340.** Screening for regions vulnerable to runoff in Brazil: Case study using the exposure model PRZM. **N. Kehrein**, H. Lißner
- 4:55** **341.** Spatially explicit modeling of static, flowing, and intermittent water bodies in probabilistic pesticide exposure assessments. **M. Winchell**, H. Rathjens, P. Whatling
- 5:20** Discussion.
- 5:45** Concluding Remarks.

SECTION E
San Diego Convention Center
Ballroom 20B-D Theater 5

Development of Novel Vector Control Technologies

Cosponsored by MEDI

A. D. Gross, E. J. Norris, D. Swale, *Organizers, Presiding*

- 2:00** Introductory Remarks.
- 2:05** **342.** Potential of spatial repellents for the control of mosquito-borne disease. **N.L. Achee**
- 2:30** **343.** Challenges in developing new vector control tools. **R. Koganemaru**, K. Ohashi, N. Sakamoto
- 2:55** **344.** Avoiding silent spring: Revolutionizing vector control by redesigning insecticide discovery and delivery. S. Shruti, M. Murgia, J. Kaur, J. Scott, W. Austin, S. Nakatake, D. Flaherty, M. Scharf, L. Raymond, L. Pfeiffer, V. Watts, **C.A. Hill**
- 3:20** **345.** Using semiochemicals to control disease vectors. **A. Mafrá Neto**
- 3:45** Intermission.
- 4:05** **346.** Investigations for reducing fitness in peridomestic mosquitoes using spatial repellents. **C.S. Bibbs**, J.R. Bloomquist, D.A. Hahn, P.E. Kaufman, R. Xue
- 4:30** **347.** Solid-state form dependent lethality of fast-acting fluoro analogs of the contact insecticide DDT. **X. Zhu**, M.D. Ward, B.E. Kahr
- 4:55** **348.** Structure-activity relationship analysis of potential new insecticides and repellents. **G. Richoux**, Q. Coquerel, F. Démarets, L. Yang, K. Linthicum, J.R. Bloomquist
- 5:20** Concluding Remarks.

Innovative Approaches to Enhancing Food Safety & Reducing Food Waste

Sponsored by AGFD, Cosponsored by AGRO

Chemistry & Applications of Free Radical-based Technologies for Water Treatment & Purification

Novel Materials Application for Free Radicals-Based Technologies

Sponsored by ENVR, Cosponsored by AGRO

Edible Functional Food Packaging from Agricultural Biomacromolecules

Sponsored by AGFD, Cosponsored by AGRO

Proposition 65 on Food Safety

Sponsored by AGFD, Cosponsored by AGRO

Biochar & Hydrochar for Energy, Environmental & Agricultural Applications

Sponsored by ENVR, Cosponsored by AGRO

THURSDAY MORNING – AGRO

SECTION A

San Diego Convention Center
Ballroom 20B-D Theater 1

Advances in Spray Drift Deposition Characterization & Measurement

Cosponsored by ENVR

G. Goodwin, G. Kruger, J. W. Perine, D. Perkins, *Organizers, Presiding*

- 8:15** Introductory remarks.
- 8:20** **349.** Standardizing methods of spray drift measurement. **J. Bonds**, A.C. Chappel, N. Mackay
- 8:45** **350.** Withdrawn
- 9:10** **351.** Assessment of spray drift and resulting plant effects in a non-target plant field study. **D. Moore**, C. Banman, B. Brayden, A.C. Chappel, T. Hall, J.P. Hanzas, R. Isemer, L. Ortego, I.M. Rodea Palomares, S. Rodney, Z. Tang, K. Watson, T. Xu, Y. Yang
- 9:35** **352.** Remote-sensing based assessment of long-term riparian vegetation health in proximity to agricultural lands with herbicide use history. **L. Ghebremichael**, F. Yousef, J.W. Perine, M. Gebremichael
- 10:00** Intermission.
- 10:20** **353.** Drift potential from glyphosate and 2,4-D applications as influenced by nozzle type and adjuvants. **G. Sousa Alves**, B.C. Vieira, T.R. Butts, S.M. Silva, J. Cunha, G. Kruger
- 10:45** **354.** Effect of adjuvants on dicamba droplet size and physicochemical properties of the solution. **G. de Castro Macedo**, G. Obear, F. Sexton, J.A. Golus, J. Gizotti-de-Moraes, G. Kruger

- 11:10** **355.** Characterizing worker exposure to pesticides without personal monitors: Developing challenge for all pesticides. R.D. Sullivan, **D.A. Sullivan**
- 11:35** **356.** Application of FTIR spectroscopy and chemometrics for the classification of auxin herbicides in damaged cotton and soybean tissue. **A.E. Brown**, J. Buol, C.X. Reid, D. Reynolds, B. Blackburn, D.L. Sparks, K. Greg
- 12:00** Concluding Remarks.

SECTION B

San Diego Convention Center
Ballroom 20B-D Theater 2

Plant-Insect-Microbe Communications in Agriculture: General Session

Cosponsored by AGFD

P. Kendra, J. Niogret, N. Tabanca, *Organizers, Presiding*

- 8:15** Introductory Remarks.
- 8:20** **357.** Phytochemicals are key drivers of host and range expanding insect herbivores. **N. Erbilgin**
- 8:45** **358.** Controlling fusarium dieback: Shot hole borers throughout avocado groves in California. S.C. Lynch, R. Stouthamer, G.S. Gilbert, **A. Eskalen**
- 9:10** **359.** Stink bug pheromones of bisabolane structural motif: Identification, synthesis, and use in pest management. **A. Khrimian**, M. Blassioli Moraes, M. Borges, R. Laumann, E. Hickel, D.C. Weber
- 9:35** **360.** Pheromonal regulation of reproduction in a plant bug. **C.S. Brent**
- 10:00** Intermission.
- 10:20** **361.** Tracking female moths (*Lepidoptera: Tortricidae*) in orchards with new kairomonal blends. **A.L. Knight**
- 10:45** **362.** Traps and attractants for monitoring for *Amyelois transitella* in the presence of mating disruption. **C.S. Burks**, J.J. Beck, B. Higbee
- 11:10** **363.** Identification of novel host plant volatiles for use as navel orangeworm attractants. N. Mahoney, W. Gee, B. Reynolds, **L.W. Cheng**
- 11:35** **364.** Advances in the synthesis, design, and formulation of semiochemicals used to control tephritid fruit flies (*Diptera: Tephritidae*). **D. Kuzmich**, S.S. Walse
- 12:00** Concluding Remarks.

SECTION C
San Diego Convention Center
Ballroom 20B-D Theater 3

Interpreting, Communicating & Managing Risk in the FIFRA/ESA Regulatory Setting

J. Rodgers, G. Watson, *Organizers*
B. McGaughey, *Organizer, Presiding*
G. Bahr, N. Golden, *Presiding*

- 8:15** Introductory Remarks.
- 8:20** **365.** Informing national-level assessments with FESTF's "gopher" data integration tool. **A. Frank**, T. Hall, D.D. Campbell
- 8:45** **366.** Mitigating risk with technology communication tools. **S. Regagnon**
- 9:10** **367.** Pesticide use in the Pacific Northwest: Enabling compliance with the Endangered Species Act. **J.J. Jenkins**, P.K. Janney
- 9:35** **368.** Making the intersection of FIFRA and ESA work!. **M. Dobbs**, T. Hall
- 10:00** Intermission.
- 10:20** **369.** Participating in the registration review and Endangered Species Act processes for the protection of endangered species. **L.A. Moreno-Matiella**, C. Bilheimer
- 10:45** **370.** Lesson for agriculture: when the Endangered Species Act interferes with management of an invasive species. **G. Watson**
- 11:10** **371.** Leveraging national compensatory mitigation conservation offset strategies to proactively address endangered species section 7 authorized take of residual, unavoidable impacts permitted within national scale pesticide biological opinions. **W. White**, J. Bickel, N.J. Snyder
- 11:35** **372.** Investigating the adoption of conservation activities by agricultural stakeholders. **L. Duzy**
- 12:00** Concluding Remarks.

SECTION D
San Diego Convention Center
Ballroom 20B-D Theater 4

To GLP or Not? How-To's for the AGRO Professional

Financially supported by SQA
C. Lee, J. Mazlo, *Organizers*
K. Watson, *Organizer, Presiding*
V. Erickson, *Presiding*

- 8:15** Introductory Remarks.
- 8:20** **373.** To GLP or not to GLP: That is the question. **K. Watson**
- 8:45** **374.** Good documentation practices, data quality, and data integrity. **J. Franchetti**

- 9:10** **375.** Digital data documentation: Good documentation practices for electronic data for EPA GLP studies when electronic laboratory notebook is used to record study data. **L. Hayes**
- 9:35** **376.** Management of multisite studies: Challenges and solutions. **L.U. Sanghani**
- 10:00** Intermission.
- 10:20** **377.** Interactions between the study director and quality assurance experts on GLP agricultural field studies: Challenges and bright spots. **A.M. Moore**, J. Mazlo
- 10:45** **378.** Failure to comply: How does this happen?. **V. Erickson**
- 11:10** **379.** EPA good laboratory practice compliance. **F. Liem**, D. Myers, M. Lehr
- 11:35** Concluding Remarks.

SECTION E
San Diego Convention Center
Ballroom 20B-D Theater 5

Development of Novel Vector Control Technologies

Cosponsored by MEDI
A. D. Gross, E. J. Norris, D. Swale, *Organizers, Presiding*

- 8:40** Introductory Remarks.
- 8:45** **380.** Natural and biorational repellents to protect against disease vectors. **J.R. Coats**, J.S. Klimavicz, C.L. Corona, C. Wong, E.J. Norris
- 9:10** **381.** Improvements to biorational mosquito repellents: Beyond simple monoterpenoid esters. **J.S. Klimavicz**, C.L. Corona, J.R. Coats
- 9:35** **382.** Plant essential oils enhance public health insecticides through diverse modes of action. **E.J. Norris**, J.R. Bloomquist
- 10:00** Intermission.
- 10:20** **383.** Use of volcanic rock to kill mosquitoes and other vector important arthropods. **R.M. Roe**, J. Deguenon, R. Mitchell, A. Dhammi, C. Apperson, J. Strider, J. Zhu, G. Cave, M. McCord, D. Stewart, F. Agossa, R. Azondekon, J. Ahoga, B. N'dombidje, R. Anagonou, G. Padonou, M. Akogbeto, K. Chen
- 10:45** **384.** Liriodenine, a natural plant alkaloid, as a tool to explore new targets for mosquitocidal activity. **Q.R. Coquerel**, F. Démares, A. Le Ray, C. Legros, J.R. Bloomquist
- 11:10** **385.** Withdrawn
- 11:35** **386.** Insecticidal activity of essential oil-derived compounds and their possible synergy mechanisms in the yellow fever mosquito, *Aedes aegypti*. **J. Tak**, J.R. Bloomquist
- 12:00** Concluding Remarks.

Innovative Approaches to Enhancing Food Safety & Reducing Food Waste

Sponsored by AGFD, Cosponsored by AGRO

Edible Functional Food Packaging from Agricultural Biomacromolecules

Sponsored by AGFD, Cosponsored by AGRO

THURSDAY AFTERNOON – AGRO

SECTION A

San Diego Convention Center
Ballroom 20B-D Theater 1

Unmanned Aerial Vehicles (aka Drones): Pesticide Spraying & other Agricultural Applications

Cosponsored by ENVR

A. Jacobson, *Organizer*

J. W. Perine, *Organizer, Presiding*

- 1:15 Introductory Remarks.
- 1:20 **387.** Implementation of sUAVs into public health vector control programs. **E.S. Horvath, D.M. Smith**
- 1:45 **388.** Spray drift from drone application. **T. Lane, C. Scott, F. Salzman, J. Arnold**
- 2:10 **389.** Precision pesticide applications with remotely-piloted aerial spray systems (RASS) in a steep vineyard setting. **J. Bonds, A. Herbst, C. Wang, X. He**
- 2:35 **390.** Best management practices (BMP) for unmanned aerial vehicle (UAV) applications to improve rice pest control in China with FMC's Rynaxypyr® products. **X. Li, J. Andaloro, E.B. Lang**
- 3:00 **391.** Unmanned aerial spraying of pesticides in Brazil: Regulation and expectations. **L. Souza, M. Ceccon**
- 3:25 Panel discussion.
- 3:45 Concluding Remarks.

SECTION B

San Diego Convention Center
Ballroom 20B-D Theater 2

Formulating Complex Agrochemical Mixtures

R. Acosta Amado, B. Rauzan, J. Whitteck, *Organizers*

J. Whitteck, *Presiding*

- 1:15 Introductory Remarks.
- 1:20 **392.** Metribuzin crystal growth inhibition in a premixture formulation: Fierce® MTZ herbicide. **J. Tanuwidjaja, S. Cheung**

- 1:45 **393.** Layered formulating to improve stability of seed treatment blends. **R.F. Colletti, M. Migliazzo, S. Selness, D.J. Seyer**
- 2:10 **394.** Finally: An application designed to meet the research needs of formulators. **M.A. Strausbaugh, M.A. Pozenel**
- 2:35 **395.** Addressing physical stability of complex suspension formulations. **J. Zhang, G.J. Klopff**
- 3:00 **396.** *Escherichia coli* inactivation during biosolarization using tomato and grape pomaces as soil amendments. **J. toniato, E. Shea, C.W. Simmons**
- 3:25 Discussion.
- 3:35 Concluding Remarks.

SECTION C

San Diego Convention Center
Ballroom 20B-D Theater 3

High Throughput Approaches to Support Pesticide Discovery & Development

K. Lynn, M. Zhang, *Organizers*

L. Riter, *Organizer, Presiding*

M. Ma, *Presiding*

- 1:15 Introductory Remarks.
- 1:20 **397.** Finding novel lead compounds in pesticide discovery inspired by pharmaceutical research. **F. van den Broek, M. Shkrob, A. Yuryev**
- 1:45 **398.** High throughput environmental fate and metabolism assays to support pesticide discovery & development. **M. Ma, V. Badwaik, K. Lynn, P. Yu, M. Huang, Y. Adelfinskaya, M. Hastings, A. Eatherall, S. Gehen, G. Shan**
- 2:10 **399.** High-throughput experimental and computational technologies at the National Center for Computational Toxicology. **A.J. Williams, J. Wambaugh, K. Houck, R. Judson, K. Paul-Friedman**
- 2:35 **400.** Sorption of pesticides in soil: Screen data, QSAR, and prediction. **X. Huang, M. Ma, P. Yu, A. Eatherall**
- 3:00 **401.** Development of optimized extraction and pass-through SPE cleanup protocols for LC-MS and GC-MS multiresidue pesticide and veterinary drug analysis. **M.S. Young, M. Blaze, K. Tran**
- 3:25 Concluding Remarks.

SECTION D
San Diego Convention Center
Ballroom 20B-D Theater 4

Novel Applications of Mathematics, Statistics, & Modeling to Agrochemical Problems

J. R. Purdy, K. Schnelle, *Organizers*
W. Al-Akhdar, W. Chen, *Organizers, Presiding*
J. Purdy, *Presiding*

- 1:15** Introductory Remarks.
- 1:20** **402.** In silicon investigation on agrochemical toxicities against aquatic organism: QSTR models on *Daphnia Magna*. **J. Cheng**, L. He, **Z. Xu**, **Z. Li**
- 1:45** **403.** Relating environmental parameters to dicamba emissions under humidome conditions. **T.C. Mueller**, L.E. Steckel
- 2:10** **404.** Mechanistic modeling the breakup of liquid sheets of agricultural spray. **N. Rajan**, S. Cryer
- 2:35** **405.** Pooled data approach for percentile estimates of pesticide surface water monitoring data. **P. Mosquin**, J. Aldworth, W. Chen
- 3:00** **406.** Exposition of the SEAWAVE-QEX model and other developments for the modeling of surface-water concentration monitoring data. **J. Aldworth**, P. Mosquin, W. Chen
- 3:25** **407.** Mathematics chemistry and toxicology in the design of pesticide monitoring programs for surface water. **J.R. Purdy**, S. Purdy
- 3:50** Concluding Remarks.

SECTION E
San Diego Convention Center
Ballroom 20B-D Theater 5

Legal Challenges & Landmark Lawsuits in Agrochemicals

Cosponsored by CHAL
J. Van Emon, *Organizer*
R. M. Bennett, A. Coates, *Organizers, Presiding*
J. M. Van Emon, *Presiding*

- 1:00** Introductory Remarks.
- 1:05** **408.** What next for the chemist? Regulation in a changing legal environment. **R.M. Bennett**
- 1:30** **409.** Taste of water. **A. Ehrlich**
- 1:55** **410.** NAICC advocating for crop and research consultants. **D. Hattermann**
- 2:20** **411.** How the US Constitution impacts agriculture. **A. Coates**
- 2:45** **412.** New agrochemical products: Clearing a path for commercialization. **J.L. Krieger**
- 3:10** **413.** Appealing from patent examiner's rejections to USPTO's patent, trial and appeal board (PTAB) can improve the chances of obtaining patents on agricultural products. **X. Pillai**
- 3:35** Panel Discussion.

DIVISION OF ANALYTICAL CHEMISTRY

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

SUNDAY MORNING – ANYL

SECTION A

Marriott Marquis San Diego Marina
San Diego Ballroom Salon C

Nanotechnology & Single Cell Analysis in Biology & Medicine

Nanoscience, Biology & Medicine

Cosponsored by BIOL, COLL, MPPG and PHYS

X. Xu, *Organizer, Presiding*

- 8:00 1. Cellular adaptability to nanoparticle stress. **C.J. Murphy**
- 8:30 2. Study of cytotoxic and therapeutic effects of silver nanoparticles against colon tumor cells. **R.M. Richardson**, K. Raut, T. Zvonare, P. Songkiatisak, P. Cherukuri, X. Xu
- 8:45 3. Biophysical and bio-nano-mechanical insights from tracking single gold nanoparticles in live cells. **N. Fang**
- 9:15 4. Profiling cells inside and out using magnetic nanoparticles. **S.O. Kelley**
- 9:45 5. Endocytosis and exocytosis of nanoparticles by cells. **Y. Xia**
- 10:15 Intermission.
- 10:25 6. Nanoscale structures modulates protein signaling at the cell membrane. **B. Cui**
- 10:55 7. Photonic modification of cell-culture landscapes. **J. Shear**, K. Michelson, J. Connell, D. Hernandez, E. Ritschdorff
- 11:25 8. Metallic nanoislands on graphene as multimodal biomechanical sensors. **D.J. Lipomi**
- 11:55 9. Subcellular control over focal adhesion anisotropy, independent of cell morphology, dictates stem cell fate. **C.A. Mirkin**

SECTION B

Marriott Marquis San Diego Marina
Torrey Pines 3

Zarefest: Symposium in honor of Richard Zare's Love for Science

Cosponsored by PHYS

M. Dulay, A. Orr-Ewing, H. Park, *Organizers, Presiding*

- 8:00 Introductory Remarks.
- 8:05 10. Applying analytical tools to ovarian cancer detection: Proteomics and aptamers. **R.J. Whelan**
- 8:35 11. Adventures with plasmons: Molecular sensing, chemical reactions, and energy transfer processes. **J.P. Camden**
- 9:05 12. Nanoscale chemical analysis and imaging using tip-enhanced Raman spectroscopy. **R. Zenobi**
- 9:35 Intermission.
- 10:00 13. New eyes for nanocatalysis: Molecular-scale investigations of nanocatalyst chemistry. **M.A. Hines**
- 10:30 14. Ultrabright probes for highly multiplexed cellular analysis. **D.T. Chiu**
- 11:00 15. From chiral cavity polarimetry, to ultrahigh-density spin-polarized hydrogen. **T. Rakitzis**

SECTION C

Marriott Marquis San Diego Marina
Presidio 1

Origins & Future of Metabolite & Small Molecule Identification

Cosponsored by BIOL, BIOT and MEDI

Financially supported by Waters

R. S. Plumb, *Organizer*

G. Siuzdak, *Organizer, Presiding*

- 8:00 16. Metabolism's future and its inextricable link to identifying new metabolites. **G. Siuzdak**
- 8:30 17. *In-silico* characterization of metabolites using artificial intelligence. **L. Pirhaji**
- 9:00 18. Identifying metabolites using mass spectrometry and stable isotopes. **C. Guijas**, J. Montenegro-Burke, A. Palermo, G. Siuzdak

- 9:30** 19. Using stable isotope labeling to facilitate unknown metabolite identification. **W. Lu**, L. Wang, X. Xing, Y. Xu, J. Rabinowitz
- 10:00** 20. Molecular composition of alcoholic beverages: The good, the bad, and the unnecessary. **L. Silva**, T. Shulman, M. Chua, A. Lee, J. Jastrzembski
- 10:30** 21. The alkynes we eat: Where do they come from and how do we identify them?. **C. Fischer**, J. Jeon, K. Smith, E. Sattely
- 11:00** 22. Identifying metabolites from scratch. **J. Montenegro-Burke**, C. Guijas, A. Palermo, G. Siuzdak

SECTION D

Marriott Marquis San Diego Marina
Presidio 2

Measuring Protein Conformations & Folding Inside the Cell

Cosponsored by BIOL, BIOT and MEDI
J. Genereux, *Organizer, Presiding*

- 8:00** Introductory Remarks.
- 8:05** 23. Global analysis of methionine oxidation provides a census of folding stabilities for the human proteome. **S. Ghaemmaghami**
- 8:30** 24. In-cell footprinting coupled with mass spectrometry to study protein folding. **L.M. Jones**
- 8:55** 25. Covalent protein painting reveals aberrant protein folding in cells *in vivo*. **C.C. Bamberger**, S. Pankow, S. Martínez-Bartolomé, J.R. Yates
- 9:20** 26. Measuring cellular protein stability through Hsp40 affinity purification coupled with mass spectrometry. **J. Genereux**
- 9:45** 27. Molecular code for intracellular collagen assembly. **M. Shoulders**
- 10:10** Intermission.
- 10:20** 28. Quantifying a protein-protein interaction in living cells. S.L. Speer, A.J. Guseman, **G.J. Pielak**
- 10:45** 29. Structural biology in cellular environments using sensitivity enhanced NMR. **K.K. Frederick**
- 11:10** 30. Probing thiol-reactivity to monitor proteome foldedness and conformational change under proteostasis stress. **D. Hatters**
- 11:35** 31. Detecting the multi-step protein aggregation process in live cells using the AggTag method. **X. Zhang**

SECTION E

Marriott Marquis San Diego Marina
Torrey Pines 2

Chemical Forensics

C. Fraga, *Organizer*
C. Timperley, *Presiding*

- 8:00** Introductory Remarks.
- 8:05** 32. The changing nature of analytical and investigate chemistry for chemical disarmament and non-proliferation. **J.E. Forman**
- 8:20** 33. Chemical forensics capability expansion. **R. Bull**
- 8:40** 34. Standardization of impurity profiling for chemical forensics international collaborative research. **C. Fraga**, A.S. Breton-Vega, K. Höjer Holmgren, L. de Reuver, H. Lignell
- 9:05** 35. Score based likelihood ratio approaches to chemical profiling of methylphosphonic dichloride (DC) and derived products. **M.E. Sigman**, D. Ramos, K. Jarman, **C. Fraga**
- 9:30** Intermission.
- 9:50** 36. Source attribution of sulfur mustard in complex matrices. **K. Höjer Holmgren**, L. Mören, L. Ahlinder, D. Wiktelius, R. Norlin, C. Åstot
- 10:15** 37. Reaction pathways in the synthesis of Levinstein mustard. **G.n. Hondrogiannis**
- 10:40** 38. Chemical attribution of ricin by profiling of fatty acids using gas chromatography mass spectrometry. **R. Webster**, S. Ovenden
- 11:05** 39. Highly accurate classification of biological spores by culture medium for forensic attribution using multiple chemical signature types and machine learning. **P. Ippoliti**, M.D. Crenshaw, F. Nargi, T. Boettcher, M. Walsh, A. Casale, J. Han, J. Dettman

SECTION F

Marriott Marquis San Diego Marina
Leucadia

Advances in Wearable & Implantable Sensors

M. A. Daniele, L. Deravi, M. Yokus, *Organizers, Presiding*

- 8:00** Introductory Remarks.
- 8:05** 40. Ultra-flexible and stretchable electronic systems for monitoring brain activities. **T. Sekitani**
- 8:35** 41. Mechanically-softening intracortical implants for sensing and drug delivery. **A. Dunning**, G. Maguire, E. Szabo, S.J. Rowan, D. Tyler, J. Capadona
- 9:05** 42. Eavesdropping on neurochemical signaling *in vivo*. **A.M. Andrews**
- 9:35** 43. Micro-invasive biochemical sampling of brain interstitial fluid for investigating neural pathology. **R. Raman**, E. Rousseau, M. Wade, R. Langer, M. Cima

- 10:05** Intermission.
- 10:20** **44.** Wearable biomarker analysis for health and wellness monitoring at the point of person. **S. Emaminejad**
- 10:50** **45.** Implantable optoelectronic devices based on CMOS LSI technology. **T. Tokuda**, M. Haruta, K. Sasagawa, J. Ohta
- 11:20** **46.** Lysozyme sensing in tear using a contact lens. **Z. Ballard**, S. Bazargan, D. Jung, S. Sathianathan, A. Clemens, D. Shir, S. Al-Hashimi, A. Ozcan

Characterization of Plastics in Aquatic Environments

Sponsored by POLY, Cosponsored by ANYL, BIOL, CEI, ENVR, I&EC, PMSE and PRES

Getting to the Bottom: Optical & Electron Imaging of Reactive Chemical Systems

High-Resolution Optical Imaging of Chemical Processes

Sponsored by PHYS, Cosponsored by ANYL

SUNDAY AFTERNOON – ANYL

SECTION A

Marriott Marquis San Diego Marina
San Diego Ballroom Salon C

Nanotechnology & Single Cell Analysis in Biology & Medicine

Nanoscience

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

- 1:00** **47.** Electrochemical zero-mode waveguide nanovials for capture and bimodal interrogation of single entities. J. Kim, S. Baek, S. Kwon, G. Crouch, H. Do, **P.W. Bohn**
- 1:30** **48.** Nanopore induced phase-shift sequencing (NIPSS) for universal biomolecule sequencing. **S. Huang**
- 2:00** **49.** Imaging membrane viscosity of single cells through second harmonic light scattering. **H. Dai**
- 2:30** **50.** Endogenous second harmonic and two photon coherence imaging of substructures in neurons in 3D. **S. Roke**
- 3:00** Intermission.
- 3:10** **51.** Sensing the biological membranes. **W. Cho**
- 3:40** **52.** Photoluminescent cellular probes based on mesoporous silicon nanoparticles. **M.J. Sailor**

- 4:10** **53.** Nanoscale-manipulation of the force field fluctuation and energy landscape entanglement in protein non-covalent recognition dynamics. **H. Lu**
- 4:40** **54.** Nanoplasmonics for characterizing EGFR heterogeneity. **S. Zhang**, B.M. Reinhard
- 4:55** **55.** Generation of a compact quantum dot conjugate for imaging dopamine transporter membrane dynamics in acute brain slices. **L.B. Thal**, V.R. Mann, I.D. Tomlinson, D. Sprinzen, J.R. McBride, K.R. Reid, D.G. McMahon, B.E. Cohen, S.J. Rosenthal

SECTION B

Marriott Marquis San Diego Marina
Torrey Pines 3

Zarefest: Symposium in honor of Richard Zare's Love for Science

Cosponsored by PHYS

M. Dulay, A. Orr-Ewing, H. Park, *Organizers, Presiding*

- 1:00** **56.** Microdroplet chemistry for catalysis, material synthesis, and biology. **J. Lee**
- 1:30** **57.** Reaction dynamics is really interesting, but is it useful?. **K.G. McKendrick**
- 2:00** **58.** Ambient ionization mass spectrometry and machine learning to guide clinical decisions and improve patient outcome. **L. Schiavinato Eberlin**
- 2:30** Intermission.
- 2:55** **59.** Finding the smoking gun: Solving the mystery of soot formation. **H.A. Michelsen**, K.O. Johansson, J. Hendrix, D. Hait, M.P. Head-Gordon, P.E. Schrader, K.R. Wilson
- 3:25** **60.** To see a world in a grain of sand: CAESAR comet sample return mission. **S.J. Clemett**
- 3:55** **61.** From Halley's comet to metabolomics: How the Zarelab conquered the spectroscopy of the masses. **M.A. Johnson**
- 4:25** Concluding Remarks.

SECTION C

Marriott Marquis San Diego Marina
Presidio 1

Origins & Future of Metabolite & Small Molecule Identification

Cosponsored by BIOL, BIOT and MEDI
Financially supported by Waters
G. Siuzdak, *Organizer*
R. S. Plumb, *Organizer, Presiding*

- 1:00** **62.** Identification of putative bio markers of breast, liver, and bladder cancer with IOn mobility enabled LC/MS based metabolomics. **R.S. Plumb**

- 1:30** **63.** Metabolite identification and unknown characterization for metabolomics activity screening. **A. Palermo**, J. Montenegro-Burke, C. Guijas, G. Siuzdak
- 2:00** **64.** Development of a shark health matrix using metabolomics coupled with metagenomics. **E.M. Forsberg**, A.Z. Goodman, Z. Walters, R.A. Edwards, E. Dinsdale
- 2:30** **65.** Advanced metabolomics and chemical biology approaches for selective analysis of microbiota and human co-host metabolism. **M. Pova Correira**, C. Ballet, L. Conway, N. Garg, D. Globisch
- 3:00** **66.** Applying a comprehensive reference tandem mass spectral library to accurate identification of human metabolites. **X. Yang**, P. Neta, S.E. Stein
- 3:30** **67.** Investigation of host-microbiota co-metabolism as a new strategy for biomarker discovery: New chemical biology tools for metabolomics analysis. **M. Pova Correira**, L. Conway, W. Lin, C. Ballet, N. Garg, **D. Globisch**
- 4:00** **68.** Withdrawn

SECTION D

Marriott Marquis San Diego Marina
Presidio 2

Advances in Fluorescence & Bioluminescence Imaging Probes

Cosponsored by PHYS
H. Ai, *Organizer, Presiding*
X. Zhang, *Presiding*

- 1:00** Introductory Remarks.
- 1:05** **69.** Optical biosensors for illuminating the biochemical activity architecture of the cell. **J. Zhang**
- 1:25** **70.** Coordinated histone modifications and chromatin reorganization in a single cell revealed by FRET biosensors. **Y. Wang**, Q. Peng
- 1:45** **71.** Role of local electric field in controlling fluorescence quantum yield of red fluorescent proteins. **M. Drobizhev**, J. Scott, P.R. Callis, R. Molina, G. Lambert, N.C. Shaner, A. Salih, T.E. Hughes
- 2:05** **72.** AgHalo: HaloTag-based multi-color fluorogenic sensor that visualizes and quantifies proteome stress in live cells using solvatochromic and molecular rotor-based fluorophores. **X. Zhang**
- 2:25** **73.** Fluorescence imaging of Fe(II) flux in ischemic stroke. **Y. Wei**, L. Wan, R. Pan, K. Liu, **W. Wang**
- 2:45** Intermission.
- 3:00** **74.** Genetically encoded fluorescent indicators for 2-photon imaging. **A. Aggarwal**, K. Podgorski
- 3:20** **75.** Development of a genetically encoded intensimetric lactate indicator iLACCO1. **Y. Nasu**, Y. Wen, J. Lemieux, S. Zhang, R.E. Campbell

- 3:40** **76.** Development of mNG-GECO1. **L.C. Zarowny**
- 4:00** **77.** Fluorescent protein based biosensors for metabolism and neurotransmission. **S. Zhang**
- 4:20** **78.** *In situ* two-photon fluorescence imaging of depression related active molecules. **P. Li**, B. Tang
- 4:40** **79.** Mycophenolic acid core intermediates as a new chemosensing fluorophore class: Selenium-based ROS biological probes. **J. Choi**, D.G. Churchill

SECTION E

Marriott Marquis San Diego Marina
Torrey Pines 2

Chemical Forensics

C. Fraga, *Organizer, Presiding*

- 1:00** Introductory Remarks.
- 1:05** **80.** Tool box for forensic investigations in the environment. **S.M. Mudge**
- 1:30** **81.** Tracing Soman precursors through site specific isotope ratio NMR spectroscopy. **S. Lindberg**, M. Engqvist, K. Höjer Holmgren, C. Åstot, R. Norlin
- 1:55** **82.** Analysis of chlorohydrins of phospholipids as chlorine biomarkers in biomedical samples of exposed animal models. **P. Lindén**, P. Hemstrom, L. Elfsmark, S. Jonasson, A. Larsson, **C. Astot**
- 2:20** **83.** Investigation of the use of deuterium and oxygen in illicit fentanyl analysis. **J. Casale**, M. Lott, **J. Mallette**
- 2:45** Intermission.
- 3:05** **84.** Source attribution of calcium ammonium nitrate (CAN) by handheld Raman spectroscopy. **O.M. Primera**, C. Fraga, A.S. Breton-Vega, M. Philip, N.S. Mirjankar
- 3:30** **85.** Chemometric analysis of spectroscopic and spectrometric data from energetic materials. **R. Lehmann**, S. Walker, D. Armitt
- 3:55** **86.** THz/Far-Infrared spectroscopy at the Australian Synchrotron for the detection and identification of energetic materials and discrimination between energetic materials and precursors. **G.S. Walker**, R. Lehmann, B.M. Fischer, D. Appadoo

SECTION F

Marriott Marquis San Diego Marina
Leucadia

Advances in Wearable & Implantable Sensors

M. A. Daniele, L. Deravi, M. Yokus, *Organizers, Presiding*

- 1:00** **87.** Soft, skin-interfaced, wireless, battery-free, microfluidic devices for chronometric sweat capture and analysis. **A.J. Bandodkar**
- 1:30** **88.** Flexible lab on the skin for personalized molecular monitoring. **W. Gao**

- 2:00 89. Wearable sweat sensors: Towards big data for human health. **A. Javey**
- 2:30 Intermission.
- 2:45 90. Materials challenges and opportunities for carbon nanotubes-based flexible electronics and wearable sensors. **Y. Wang**
- 3:15 91. *In vivo* biosensing of steroid hormones using corona phase molecular recognition (CoPhMoRe) and nIR fluorescent single walled carbon nanotubes for health monitoring and biologgging. **M. Strano**
- 3:45 92. Wearable multimodal patches: Concurrent monitoring of human physiology and biochemistry. **M. Yokus**, T. Songkakul, V. Pozdin, A. Bozkurt, M.A. Daniele

Characterization of Plastics in Aquatic Environments

Sponsored by POLY, Cosponsored by ANYL, BIOL, CEI, ENVR, I&EC, PMSE and PRES

Getting to the Bottom: Optical & Electron Imaging of Reactive Chemical Systems

Visualizing Biology in Living Cells and In Vitro

Sponsored by PHYS, Cosponsored by ANYL

SUNDAY EVENING – ANYL

SECTION G

San Diego Convention Center
TBD

Analytical Division Poster Session

K. Agnew-Heard, *Organizer*

8:00 - 10:00

93. Rapid vertical flow assay on AuNP plasmonic paper for SERS-based point of need diagnostics. **R. Frimpong**, W. Jang, J. Kim, J.D. Driskell
94. Quantification of hydrophilic layer on bioresolve SCX mAb particles. **B. Niu**, M. Xu, X. Song, Y. Xu
95. Effect of cultivation elevation of tea leaves on the formation and size control of silver nanoparticles for mercury ion sensing. **B. Giri**, A. Bhattarai, A. Chandra, J. Adhikari, N. Sharma, A. Yadav, M. Singh
96. Quantitative analysis of organic nitrogen in the atmosphere. **X. Huang**
97. Design hub for early phase drug discovery. **A. Stracz**

98. Simulation of fluid catalytic riser and regenerator used for monitoring catalyst retention: Case study of Kaduna refining and petrochemical company FCC reactor. **J. Olujinmi**
99. Diurnal cycle effects on ocean biochemistry during a mesocosmic algal bloom. **M.M. Rogers**, S. Baumler, H.C. Allen
100. Mesoporous CaCO₃-based alkaline stable reversed-phase HPLC packing material. **M. Mochida**, Y. Nagai, H. Kumagai, H. Imai, D. Citterio, Y. Hiruta
101. Tuning carbon nanodots and antioxidant studies. **Z. Ji**
102. Use of ATR FT-IR spectroscopy in identification of immature fiber (*im*) mutant and Texas Marker-1 (TM-1) cotton fibers. **Y. Liu**, H. Kim
103. Attaining quantitative speciation by leveraging varying strengths of amalgamation by mercury species in gold-bead traps. **A.J. Boggess**, B. Looney, M. Jones, T. White
104. *In situ* characterization of protein corona formation within ordered porous nanostructures. **W. Qian**, Q. Su
105. Electric field assisted electrode modification. **H. Wang**, C. Ma
106. Potential role of halogen bonding in the gas phase: Ambient ionization mass spectrometry utilizing iodine. **J. Ganske**, L.M. Wingen, V. Perraud, B.J. Finlayson Pitts
107. Microfluidic thread-based electrode system to detect glucose and acetylthiocholine. **K. Uchida**, L. Duenas, M. Gaines, M. Gonzalez-Guerrero, **F.A. Gomez**
108. 3D microfluidic paper-based analytical devices for colorimetric bioassays. **N. Neris**, A. Wong, A. Fernandez, **F.A. Gomez**
109. Effects of short chain fatty acids on fatty acid and glycogen synthesis in Hep G2 cells. **L. Ma**, **J.K. Yee**, S. Lim, W. Lee
110. Colorimetric detection of carcinogenic alkylating fumigants on nylon 6 nanofibrous membrane with self-catalytic function. **P. Tang**, G. Sun
111. Detection of steroids and human growth hormone using color-changing cyclodextrin systems. **A. Haynes**, J. Racicot, D. Jones, M. Levine, A. Yonchak, B. Point
112. Sensitive analysis of breast cancer biomarkers using laser wave-mixing detector interfaced to microfluidics. **J. Liang**
113. Evaluation of statistical techniques to normalize mass spectrometry-based urinary metabolomics data. **S. Gamagedara**, T. Cook

- 114.** Colorimetric detection of aliphatic alcohols in β -cyclodextrin solutions. **A. Haynes**, M. Levine, P. Halpert
- 115.** Withdrawn
- 116.** Deep ultraviolet resonance Raman spectroscopy of hydrogen bonding along transmembrane α -helices. **X. Wei**, R.D. Jiji, C. Greenlief
- 117.** Enzyme-specific imaging achieved by labeling with enzyme activatable probes. **A. Owen**, R.L. McCarley
- 118.** Analysis of commercially available mineral supplements: Microwave plasma atomic emission spectroscopy (MP-AES) and X-ray fluorescence (XRF) spectroscopy study. **K.J. Kolonko**, J. Pulvidente
- 119.** Gradient chromatofocusing of proteins: Comparison of weak/strong anion/cation exchange HPLC columns. **S. Rayaprolu**, D.J. Anderson
- 120.** Isorhamnetin-cyclodextrin inclusion: Sensitive fluorescent probe for copper (II). S. Yang, **L. Xu**, X. Sun, H. Xue, J. Chen
- 121.** Preliminary study on impurities and by-products formed in the synthesis of CWC-related chemicals. **H. Kiljunen**, **H. Lignell**, **T. Kauppila**, **P. Vanninen**
- 122.** Comparison study of the phytochemicals and antioxidant activity of fully matured and averagely natured *Crinum jagus* bulbs. **D.L. Abiona**, O.O. Onawumi, S.O. Oladoye
- 123.** Microfluidic device for oxygen quantitation in anoxic environments. **M. Clayson**, **M.J. Evans**, L. Miller, S. Mckay, **C.F. Monson**
- 124.** Rapid detection of bisphenol A in a microfluidic device through the use of hydrogels and aptamers. **B. Phelps**, N. Perera, M. Piyasena
- 125.** Development of an analytical method to detect microplastics in the wastewater treatment plant. **M. Kim**, K. Zoh
- 126.** Molecular insights into ultras-small nanoparticle-protein interactions through measurement of binding kinetics. **R.S. Ferreira**, A.L. Lira, R.J. Torquato, **S. Hassan**, A.A. Sousa
- 127.** Rapid screening and semi-quantification of zilpaterol in incurred sheep tissue samples using ambient and semi-ambient mass spectrometry. **S. Chakrabarty**, W.L. Shelver, D.J. Smith
- 128.** Probing the rheology of model sea spray aerosol particles using a dual-balance linear quadrupole trap as a micro-analytical tool. **D.S. Richards**, K. Trobaugh, R.D. Davis
- 129.** Automated low density solvent based demulsification dispersive liquid-liquid microextraction followed by gas chromatography-mass spectrometry for the determination of pharmaceutically active compounds in water. **L. Guo**, H. Lee
- 130.** Comparative quantitative analysis of cetirizine dihydrochloride by HPLC (high performance liquid chromatography) and q-NMR (quantitative nuclear magnetic resonance) techniques. **S. Kumar**, M. Villanueva
- 131.** Development of a simple extraction method for tetracycline analogues from milk with UV detection. **O. Cordova**, T. Le, K. Ng
- 132.** Mass spectrometry analysis and theoretical study of the enrichment of phosphopeptides by different crystal forms of TiO_2 . **Y. Qi**, **X. Yang**, **W. Zhang**, **R. Jiang**, **J. Zhang**, **H. Zhong**
- 133.** Efficiency study of pH sensitive drug release of carbon dots-doxorubicin conjugation in glioblastoma brain tumor cells. **S.D. Hettiarachchi**, R.M. Graham, S. Paudyal, E. Seven, R.M. Leblanc
- 134.** Rapid and accurate determination of the pH of environmental water samples using smartphone colorimetry. **Z. Naing**, H. Liang, D. Sarmiento, J. Brannon, Y. Liu
- 135.** Evaluation of human serum albumin nanoparticles for drug delivery and biomedical imaging. D. Bwambok, **L.A. Arrijoja**, **A. Bituin**
- 136.** Indium phosphide quantum dots as benign fluorescent probes for enzymatic assays. **D. Bwambok**, A. Acoba, S. Uriosttigue
- 137.** Screening for fungal infections using LC/MS. **C. Allison**, M.M. Reynolds
- 138.** Early diagnosis of colon cancer with rapid hybridization of DNA biomarkers. **S. Lee**
- 139.** Super-resolution stimulated Raman scattering microscopy. **D. Kim**, Y. Lee, D. Choi, J. Kwon, H. Lee, M. Cho, S. Shim
- 140.** Preparation of magnetic molecularly imprinted polymer for the electrochemical analysis of melamine. W. Ho, M. Tse, **S. Cheng**
- 141.** Improvement of a sensor for urine creatinine using a copper electrodeposited gold electrode. **N. Sato**, K. Takeda, H. Ohno, N. Nakamura
- 142.** Withdrawn
- 143.** Silicone membrane modified with chitooligosaccharide *in situ* purification and detection of *Salmonella*. C. Yan, **C. Ma**
- 144.** New isothermal amplification technique for POCT of foodborne pathogenic bacterium *Listeria monocytogenes*. **J. Chen**, **Y. Shi**
- 145.** Loop-mediated isothermal amplification based on naked visualization dye for *Salmonella* POCT testing. J. Chen, **Y. Shi**
- 146.** Evidence of direct reaction between ozone and oleanolic acid in plant cuticular waxes under

- laboratory and ambient conditions. **T.L. Longin**, V. Huerta Navarro, B. Romero, C. Smith, T. Rogoff, T. Kochar, D.P. Soulsby
- 147.** Forensic analysis of disposable nitrile gloves utilizing FTIR, XRF, TGA/DSC/Pyrolysis-MS. **J. Angst**, D.J. Lecaptain
- 148.** Rapid colorimetric detection of *Salmonella typhimurium* based on polyamide film and strand exchange amplification. **S. Liu**, S. Kuang
- 149.** Practical derivatization protocol for phosphonic acid markers of G-agents at low levels in various soils. **C.A. Valdez**, R.N. Leif, S. Hok, E.P. Salazar, A.K. Vu, A. Alcaraz
- 150.** Internal calibration potentiometric aptasensors for simultaneous detection of Hg²⁺, Cd²⁺, and As³⁺ based on a screen-printed carbon electrodes array. **W. Tang**, P. He
- 151.** Multiorganelle concurrent imaging in single cells by 3D superlocalization of dual-code enhanced dark-field microscopy. **S. Lee**, S.H. Kang
- 152.** Colorimetric breath analyzer using photonic gel in hydrophobic ionic liquid. **H. Choi**, W. Lee
- 153.** Fabrication of inverse opal hydrogel sensors on flexible substrate by transfer process. **S. Yoon**, W. Lee, H. Lee
- 154.** Development of *N,N,N*-Trimethyl-2-oxo-2-(2-((7-sulfinobenzo [c][1,2,5]oxadiazol 4-yl) sulfonyl)hydrazinyl)ethan-1-aminiium (TOSBA) as a thiol specific fluorogenic agent for cell surface thiol imaging in live cells. **S. Wang**, Y. Huang, Y. Alqahtani, A. Najmi, T.M. Seefeldt, X. Guan
- 155.** 2D HPLC coupled with MS to examine cold medicines using compendial methods as the first dimension. **W. Long**, K.W. Whitaker
- 156.** Sensitive detection of heart failure biomarkers using multiphoton laser wave-mixing spectroscopy. **J. Suprpto**, I. Chavez, M. Mohamed, W.G. Tong
- 157.** Analysis of chemicals generated from plastic decomposition in the ocean. H. Kimukai, **K. Koizumi**, B. Kwon, K. Kim, K. Metori, M. Okada, T. Hiaki, T. Kusui, K. Takatama, **K. Saïdo**
- 158.** Accelerated charge separation and stabilization in a fused bis zinc porphyrin-quinone conjugate via cation-quinone interactions. **M. Thomas**, Y. Hu, H. Wang, F. D'Souza
- 159.** Development of substitutable interface on dandelion-like SiO₂ / Au thin film and application to sensitive and selective VOCs gas detection. J. Kim, H. Son, Y. Choi, **S. Hong**
- 160.** Forensic applications of analytical chemistry: Funding programs at the National Institute of Justice. **G.J. Dutton**
- 161.** State-of-the-art technologies for relative response normalization of metabolites in mass spectrometry. **S. Dell'Aiera**, **E. Isin**, **C. Delatour**
- 162.** Analysis of total mercury in radioactive waste using a direct mercury analyzer instrument. **T.L. White**, B. Looney, L. Brown
- 163.** Improved method for the measurement of tobacco-specific carcinogen biomarker urinary 4-(Methylnitrosamino)-1-(3-pyridyl)-1-butanol (NNAL) in tobacco users. **J. Brown**, B. Xia, J. Lee, B. Blount, L. Wang
- 164.** Polycyclic aromatic hydrocarbons and polyacenes: Analyzing the band structure and elemental composition of organic, heterocyclic crystals. **K. Erlitz**, S. Brady, B. Schatschneider
- 165.** Effect of gold nanoparticles on MCP-1 guided monocytic cell line (THP-1) chemotaxis in 3D μ -slide. **X. Zhang**, P. Falagan Lotsch, C.J. Murphy
- 166.** Determination of cholesterol concentrations in aqueous solutions using screen-printed carbon electrodes and cyclic voltammetry. **D.E. Martyn**, S.K. Buehler
- 167.** HPLC-UV method development for baseline resolution of 17 cannabinoids. **M.J. Wilcox**, E. Franklin
- 168.** Development of efficient extraction and detection method for the active components in commercial kratom products. **F. Ceja**, P. Tuitt, K. Ng
- 169.** Development of a peptide mapping protocol to minimize oxidation and deamidation for biotherapeutic characterization. **K. Chanthamontri**, P. Jalili, K. Ray
- 170.** Separating chiral steroid compounds by isocratic C18 reversed phase HPLC: Optimization of the acetonitrile/methanol ratio to maximize separation. **E. Kipruto**
- 171.** Ultrasensitive fluorescent DNA detection through signal amplification and target regeneration via dual-cycling reactions. **I.A. Iwe**
- 172.** Microfluidic trapping and observation of size-sorted liposomes prepared by water-in-oil emulsion transfer method. **H. Sugiyama**, T. Osaki, S. Takeuchi, T. Toyota
- 173.** Chemometric analysis of multidimensional fluorescence data recorded from benzo[a]pyrene metabolites in frozen matrixes. **M. Chehelamirani**
- 174.** Thermal desorption coupled gas chromatography-mass spectrometry analysis of low emission polyurethane foam for automobile applications. **Y. Tan**, A.L. Grzesiak, Y. Zhang, E. Pearce, G. Marr, K. Kiszka
- 175.** Ultrasensitive, colorimetric, paper-based devices for the detection of ppb levels of nitrate and nitrite. **T. Mako**, A. Levenson, M. Levine

176. Silver-chlorosilver(I) reference electrodes of the first and second kind for alkylimidazolium bis(trifluoromethylsulfonyl)imide room temperature ionic liquids from solubility and complexation studies. **A. García-Mendoza, J.C. Aguilar**

177. Fungal degradation of defense materials and assets. **T.T. Brown, J.S. Lee**

178. Aptamer-modified microelectrodes for the measurement of neuropeptide Y using electrochemical impedance spectroscopy. **L.F. Lopez, N.G. Hernandez, K. Flores, J. Cruz, L. Cunci**

179. Electrochemical detection of viable bacterial cells using a tetrazolium salt. **K. Ishiki, D. Nguyen, H. Shiigi**

180. Real-time monitoring of α -synuclein-induced cell membrane disruption in Parkinson's disease by scanning ion conductance microscopy. **J. Parres-Gold, S. Wong Su, A. Chieng, M. Chang, Y. Wang**

181. Cancer DNA detection using gold nanoparticle colorimetry and three ways target switching catalytic hairpin assembly. **C. Park, S. Na**

182. Determination of a quantitative indicator of the lytic strength of cell lysing reagents. **A. Zhao, M. Brody, X. Zhao**

183. Development of a glycan reference material for therapeutic proteins. **M. Lowenthal, G. Boons, B. Lang, K. Phinney**

184. 2D IR spectroscopy for the characterization of protein side-chain dynamics. **S. Ramos, R. Horness, A. Le Sueur, M.C. Thielges**

185. Investigation of 2-amino-thiazole and 2-amino-benzothiazole salicylidene as sensitive probes for detection of anions and cations. **R.O. Alzu'bi, Y. Hijji**

186. Co-release of dopamine and serotonin upon optogenetic stimulation of dopaminergic neurons. **K. Perrotta, H. Yang, A. Hachisuka, M. Dagher, S. Erwin, S. Masmanidis, A.M. Andrews**

187. Resorufin derived fluorescent probes for the selective detection of ONOO⁻. **M. Weber, T. James, A. Mackenzie, S. Bull**

188. Hierarchical surfaces with biomimetic polydopamine coatings for efficient capture of circulating tumor cells. **X. Zhou**

189. Protein profiling and pseudo-parallel reaction monitoring to monitor the fusion-associated conformational switch in hemagglutinin. **K.K. Nguyen**

190. Separation and detection of fentanyl from complex mixtures using gradient elution moving boundary electrophoresis. **S. Krauss, T. Forbes, D. Ross**

191. Enhancing the disposal wells permeability monitoring by applying ASTM D7678 for the measurement of oil in water in GOSPs disposal lines. **A.M. AlSubaie**

192. Electrochemical biosensor using *p*-AP oxidation reaction on the mixed SAM Au electrode. **Y. Song**

193. Study on mechanism of single silver nanoparticle collided upon copper ultramicroelectrode in alkaline solution. **K. Kim**

194. Multifunctional, aramid-wrapped, multiwalled carbon nanotubes as an analytical microextraction sorbent. **A. Alhendal, S. Sharaif, R. AbdulMoan, Z. Ahmad**

195. Conductometric titration as a method for measurement of elevated sulfate levels in groundwater. **R. Srinivasan, M.B. Mudd, H.C. Stephen, B.R. Rothrock, L.D. Schultz**

196. Organosilica-based adsorbents for treatment PFAS impacted groundwater. **H.A. Hartmann, P. Edmiston**

197. A single molecule examination of salting out in protein-polymer membrane interactions. **N. Moringo, L.D. Bishop, N.C. Carrejo, H. Shen, W. Wang, A. Misiura, R. Baiyasi, F. Ye, J.T. Robinson, C.F. Landes**

SECTION H

San Diego Convention Center
TBD

Biosensing: New Strategies & Latest Development

Cosponsored by BIOL, BIOT and MEDI
Q. J. Cheng, *Organizer, Presiding*

8:00 - 10:00

198. Bacteria identification using a DNA-nGO based sensing array. **L. Wang, Y. Wen, X. Yang, L. Li, Y. Li, L. Xu, W. Liang, F. Gong, G. Liu**

199. Far- and deep-ultraviolet surface plasmon resonance sensors. **I. Tanabe, K. Fukui**

200. Competitive and noncompetitive immunoassays for the detection of benzothiostrubin using magnetic nanoparticles and fluorescein isothiocyanate-labeled peptides. **C. He, X. Hua**

201. Human photoreceptor protein-graphene hybrid material allowing detection of visible light with human-like spectral sensitivities. **H. Song**

202. An activatable contrast agent for photoacoustic imaging of gingipains associated with periodontal disease. **C. Moore, J.V. Jokerst**

- 203.** Aptamer-based detection of vaspin by phytoplankton-derived biomineral modified electrode. **S. Kim**, O. Nam, E. Jin, M. Gu
- 204.** Sensitive SERS detection of small molecules by photothermal convection based real-time and pin-point colloidal assembly. **K. TaeHo**, I. Seo, H. An, I. Choi
- 205.** Poly(ethylene glycol)-dibromomaleimide as a stabiliser for volatile sulfur compounds. **G. Kirby**, R. Hand, D.M. Haddleton
- 206.** Mirror image fluorogenic aptamer sensor for live-cell imaging of microRNAs. **W. Zhong**, J. Sczepanski
- 207.** Iodide-doped gold/silver hybrid nanorods report reactive oxygen species concentrations via photoacoustic imaging. **Y. Mantri**, J.V. Jokerst
- 208.** Decoration of S,N co-doped graphene quantum dots with ρ -aminothiophenol functionalized AuNPs for molecular imprinted sensing of sofosbuvir in real samples. **M. Mahnashi**, A. Mahmoud, S. Alkahtani
- 209.** Enzyme-based colorimetric biosensor for selective detection of L-DOPA. Y. Chou, I. Wang, C. Shih, **Y. 葉怡均**
- 210.** Novel nanobody-based-electrochemical immunosensor on nylon nanofibrous membranes for detection of 3-phenoxybenzoic acid in human urine. **A. El-Moghazy**, J. Huo, **N. Amaly**, N. Vasylieva, B. Hammock, G. Sun
- 211.** Sensitive electrochemical aptasensor for EpCAM by mesoporous silica nanoparticles and quantum dots signal amplification. L. Zhu, **Y. Liu**, B. Yang, L. Qiao, B. Liu
- 212.** Phosphorylation-mediated single-particle assay of protein kinase activity with dark-field microscopy. **T. Tian**, K. Zhang, Y. Liu, B. Liu
- 213.** Electrogenerated chemiluminescence imaging of a single protein based on functional nanoprobe of Ru@SiO₂ nanoparticles. **Y. Liu**, T. Tian, H. Zhang, J. Liu, B. Liu
- 214.** Basic roles of lysophospholipid receptor signaling studied by compensated interferometric reader (CIR). **M. Ray**, A. Kussrow, K. Nagai, M. Kammer, D. Bornhop, J. Chun
- 215.** Graphene oxide-based paper sensor for enhanced colorimetric sensing of miRNA. **J. Lee**
- 216.** Dual-targeting functionalized graphene films for rapid and highly sensitive fluorescence imaging detection of hepatocellular carcinoma circulating tumor cells. **C. Wu**, P. Li, N. Fan, J. Han, W. Zhang, W. Zhang, B. Tang
- 217.** Screen printed mesoporous carbon electrodes for efficient sensing of dopamine. **Y. Lee**, Y. Chang, H. Chang, M. Yeh, Y. Yeh, Y. Liu
- 218.** Observation of acetylcholinesterase in stress-induced depression phenotypes by two-photon fluorescence imaging in the mouse brain. **X. Wang**, **P. Li**, C. Wu, D. Su, Q. Ding, W. Zhang, B. Tang
- 219.** Specific, *in vivo* two-photon fluorescence imaging of malondialdehyde in mice brains using an easily-prepared nanolight. **D. Su**, P. Li, X. Wang, W. Zhang, Y. Zhang, C. Wu, W. Zhang, Y. Li, W. Tai, B. Tang
- 220.** Using nitric oxide-releasing metal-organic frameworks on the surface of blood-contacting glucose biosensors to reduce biofouling. **A.C. Melvin**, M.M. Reynolds
- 221.** Application of super resolution radial fluctuation (SRRF) single-molecule imaging to measurement of DNA hybridization kinetics. **J. Cooper**
- 222.** Nanobodies and phage-display peptides: Attractive biosensing materials for analytical applications. **N. Vasylieva**, D. Li, Z. Li, B. Barnych, B.D. Hammock
- 223.** Novel aptamer candidates for serotonin and dopamine field-effect transistor neurosensing. **S.T. Mensah**, O. Lukyanova, K. Yang, K.M. Cheung, W. Dai, P.S. Weiss, M.N. Stojanovic, A.M. Andrews
- 224.** Novel microfluidic-chemiluminescence detection coupled with microscale separation: Toward highly sensitive analytical technique. **S.M. Al Kindy**, A. Kadavilpparampu, H. Al Lawati
- 225.** Comparative analysis for PCBs and organochlorine pesticides in plasma samples employing C-18 SPE and functionalized electrospun nanofibers. **D.K. Adeyemi**
- 226.** Functionalized nanopore biosensor for quick and highly sensitive glucose detection in human saliva. **y. miao**
- 227.** Microdialysis: Fluorescence analysis system for vancomycin detection in pharmaceuticals and plasma. **f. mu**

SECTION I

San Diego Convention Center

TBD

Nanozymes for Bioanalysis & Beyond

Cosponsored by BIOL and BIOT

H. Wei, *Organizer*

8:00 - 10:00

228. N and B co-doped graphene: Suitable candidate to substitute natural peroxidase in sensitive and selective bioassays. **J. Lee**, J. Lee

229. Mechanisms of oxidase and peroxidase mimicking activities of nanoceria from first

principles calculations. **W. Zhenzhen**, X. Gao, C. Chen, Y. Zhao

230. Regulating oxidase mimicking activity of platinum by surface modifications. **S. Xiaomei**, X. Gao

231. Molecular mechanisms for the peroxidase-mimicking activities of perovskite nanomaterials. **X. Gao**, X. Wang, H. Wei, X. Gao

232. Novel silk-biomaterials-supported artificial enzymes: Synthesis and applications. **Y. Lin**

SECTION J

San Diego Convention Center
TBD

Zarefest: Symposium in honor of Richard Zare's Love for Science

Cosponsored by PHYS

M. Dulay, A. Orr-Ewing, H. Park, *Organizers*

8:00 - 10:00

233. Teaching through research: Freshman research initiative at the University of Texas at Austin. **R.I. Shear**, K.H. Rogers, S.E. Eichhorn

234. Ultra-narrow linewidth lasers for atom-based devices. **A. Matsko**, A. Savchenkov, D. Eliyahu, S. Williams

235. High sensitivity differential temperature detection. **G.J. Diebold**

236. On-demand drug release from polypyrrole nanoparticulate films. **C. Chamberlayne**, S. Baltasvias, H. Xu, A. Arbabian, J. Annes, R.N. Zare

237. Novel antibody drug conjugates for pancreatic cancer therapy. **J. Huang**, P. Guo, M. Moses

238. Photon-catalyzed photoisomerization of stilbene. **J. Meiser**, **K. Hilsabeck**, J.A. Harrison, R.N. Zare

239. Spectroscopic Investigation of semiconductor halide compounds interaction with silicon dioxide. **S.D. Fleischman**

240. Simple algorithms for some unconventional uses of the method of least squares. **J.B. Tellinghuisen**

241. Using DESI-MSI to identify the genetic basis and tumorigenic mechanism of pheochromocytomas. **S.E. Noll**, N. Armstrong, K. Margulis, V. Shankar, C. Storey, P. Kunz, L. Fishbein, R.N. Zare, J. Annes

242. Can machine learning be used to learn laws of natural science? Illustration for Planck's blackbody radiation. **V. Shankar**, S. Shankar

243. Evanescent-wave cavity-ring-down imaging. **M.A. Everest**

244. Kinetic studies on unimolecular processes in Criegee intermediates. **T.A. Stephenson**, M.I. Lester

245. Solutions for lightweight construction and CO₂ footprint reduction by analysis of surfaces exposed to laser and plasma treatment. **U. Lommatzsch**, K. Thiel, M. Noeske, J. Ihde, R. Wilken

246. Phenotyping macrophages involved in the onset of diabetes type 1 with label-free and quantitative proteomics. F. Sandbaumhüter, G. Christoffersson, **E.T. Jansson**

247. Pulsed triboelectric nanospray ionization for analysis of complex organics. M. Bouza Areces, A. Li, Z.L. Wang, **F.M. Fernandez**

248. Mathematical Knowledge for Teaching to support student learning in chemistry. **L.A. Posey**, K.N. Bieda, P.L. Mosley, C.J. Fessler, V.A. Kuechle, E.N. Thomas

249. Detecting bacteria using an artificial antibody. **M. Dulay**, A.C. Mody, R.N. Zare, C. Da-Silva-Granja

250. Non-cationic and deformable nanolipogels for *in vivo* genome editing of triple negative breast cancer. **P. Guo**, J. Yang, J. Huang, D. Auguste, M. Moses

251. Multiplexed quantitative MALDI MS approach for assessing activity and inhibition of protein kinases based on post-enrichment dephosphorylation of phosphopeptides by MOF-templated porous CeO₂. **Q. Min**, H. Xu, M. Liu, X. Huang, J. Zhu

252. Droplet spray ionization mass spectrometry for solution chemistry: Advances & future trends. H. Zhang, K. Yu, J. He, **J. Jiang**

253. Synchrotron infrared nanospectroscopy at the advanced light source. **H.A. Bechtel**, S.N. Gilbert Corder, M.C. Martin

254. Electronic structure of naturally occurring aromatic carbon. **A.E. Pomerantz**

255. Changing the nature of electroless etching with a syringe pump: ReEtching, MACE and low load MACE. **K.W. Kolasinski**, B.A. Unger, J.D. Swanson, H. Yu, A.T. Ernst, M. Aindow, E. Mäkilä, J. Salonen, K. Tamarov, J. Riikonen, V. Lehto

256. Oncogene MYC regulates lipogenesis essential for neoplastic growth. **K. Margulis**, A. Gouw, N. Liu, D. Felsher, R.N. Zare

257. HPLC column for nanoparticles and nanomedicines. **M. Kato**

258. Solar-driven biohybrid N₂ and CO₂ fixation. **S. Cestellos-Blanco**, Y. Shen, P. Yang

259. Development of new stationary phases for HPLC. **L.A. Colon**, J.R. Ezzo

260. 3-D mapping of the chemical contents of anthropogenic soils by the chemometric analysis of infrared and visible spectra. **D.S. Perry**, A.J. Lopa, A. Cava, T. Matney, L. Barrett, D. Maki

- 261.** Synchronization modulated surface plasmon coupled emission for improving spectral resolution. Y. Zhao, Y. Liu, S. Cao, **Y. Li**
- 262.** Soft ionization and dissociation based on laser activated interfacial photoelectron transfer for mass spectrometry. **H. Zhong**
- 263.** Aesthetic education in chemistry. **H. Zhong**
- 264.** Photoacoustic measurements of single aerosol droplets: Microscopic heat transfer and accelerated photoreactions. **J. Cremer**, P. Covert, E. Parmentier, M. Diveky, S. Roy, R. Signorell

SECTION K

San Diego Convention Center

TBD

Structure at Solid-Liquid Interfaces: Effects of Confinement & Chemical Patterning

Cosponsored by COLL

T. C. Davis, T. R. Hayes, *Organizers*

8:00 - 10:00

- 265.** Large-scale noncovalent functionalization of 2D materials through heated roller Langmuir-Schaefer conversion. **T.R. Hayes**, A.G. Porter, E.N. Lang, S.A. Claridge
- 266.** Effective loading of plasmonic silver nanoparticles into mesopores for SERS applications. **S. Chen**, Y. Chang, H. Hou, W. Chiang, Y. Liu
- 267.** Surface-seeded folding of DNA origami. **H. Cao**, Q. Gu, G.R. Abel, G.V. Gueorguieva, Y. Zhang, W. Nanney, T. Ye
- 268.** Surface chemistry and spectroscopic study of tyrosinase enzyme langmuir monolayer. **s. paudyal**

Theoretical & Experimental Investigations of Water Interactions with Materials

Posters

Sponsored by COLL, Cosponsored by ANYL

MONDAY MORNING – ANYL

SECTION A

Marriott Marquis San Diego Marina

San Diego Ballroom Salon C

Nanotechnology & Single Cell Analysis in Biology & Medicine

Nanoscience

Cosponsored by BIOL, COLL, MPPG and PHYS

X. Xu, *Organizer, Presiding*

- 8:00** **269.** Nanotechnology approaches to cellular therapies. S.J. Jonas, **P.S. Weiss**
- 8:30** **270.** New tools for single-cell genotyping and analysis. **D.T. Chiu**
- 9:00** **271.** Mapping the inner world of cells. **B. Huang**
- 9:30** **272.** Single nanoparticle plasmonic spectroscopy for biomedical applications: From diagnosis to therapy. **X. Xu**, P. Songkiatisak, P. Cherukuri, K. Raut, R.M. Richardson
- 10:00** Intermission.
- 10:10** **273.** Beyond biomarkers: Array-based profiling for diagnostics and geno-/phenotypic screening for precision medicine. **V.M. Rotello**
- 10:40** **274.** Nanoengineered materials and devices to detect DNA hybridization and single nucleotide polymorphisms. K.M. Cheung, H. Cao, N. Nakatsuka, J. Abendroth, P.S. Weiss, **A.M. Andrews**
- 11:10** **275.** Rapid determinations of antibiotic susceptibility phenotypes using label-free cytometry and new adaptive statistic. T. Huang, A. Filbrun, J. Richardson, Y. Tzeng, **R. Dickson**
- 11:40** **276.** Nanostructure imaging mass spectrometry (NIMS) for metabolomics and systems biology. **A. Palermo**, E.M. Forsberg, B. Warth, A.E. Aisporna, E. Billings, E. Kuang, P.H. Benton, D. Berry, G. Siuzdak

SECTION B

Marriott Marquis San Diego Marina

Torrey Pines 3

Structure at Solid-Liquid Interfaces: Effects of Confinement & Chemical Patterning

Cosponsored by COLL

T. C. Davis, T. R. Hayes, *Organizers, Presiding*

- 8:00** Introductory Remarks.
- 8:05** **277.** Advances in chemical lift-off lithography. **K.M. Cheung**, D.P. Goronzy, D.M. Stemer, C. Zhao, T.D. Young, J.N. Belling, T. Base, A.M. Andrews, P.S. Weiss
- 8:25** **278.** Surface confinement: Friend or foe to complex self-assembled DNA architectures?. **T. Ye**, H. Cao, G.R. Abel
- 8:55** **279.** Confined defects formed by chemical lift-off lithography to pattern multi-functional substrates. N. Nakatsuka, H. Cao, P.S. Weiss, **A.M. Andrews**
- 9:25** **280.** Protein structure at the bio/abio interface. **L.J. Webb**
- 9:55** Intermission.
- 10:10** **281.** Surface-mediated peptide self-assembly to modulate surface energy. **Z. Fakhraai**, Y. Lin, M. Skolnick, E. Petersson
- 10:40** **282.** Dynamic organization of complex droplets via chemotactic surface-mediated interaction. C. Meredith, Y. Chiu, J. Groenewold, W. Kegel, **L.D. Zarzar**, A. van Blaaderen, P. Moerman

- 11:10 283.** Uniform, large-area, highly-ordered peptoid monolayer and bilayer films for sensing applications. D. Murray, J. Kim, E. Grzincic, S. Kim, A. Abate, **R.N. Zuckermann**

SECTION C

Marriott Marquis San Diego Marina
Presidio 1

Identification & Design of Catalytic Sites in Electrochemical Reactions

Cosponsored by ORGN

Y. Liang, H. Wang, *Organizers*

C. Liu, *Organizer, Presiding*

- 8:00 284.** Understanding the active sites of structurally dynamic nanomaterials for CO₂ electrocatalysis to multicarbon products. Y. Li, D. Kim, **P. Yang**
- 8:30 285.** Highly active and selective electrochemical CO₂ reduction to formate enabled by structural defects on converted Bi₂O₃ nanotubes. **Y. Li**
- 9:00 286.** Two-dimensional copper nanosheets for electrochemical reduction of carbon monoxide to acetate. **F. Jiao**
- 9:30** Intermission.
- 9:45 287.** One-dimensional core/shell nanocrystals with favorable interfacial synergy for electrocatalysis. **S. Zhang**, Z. Zhang, C. Liu
- 10:15 288.** Synthesizing intermetallic nanoparticle catalysts for enhanced catalytic electro-oxidation. **W. Huang**, Z. Qi
- 10:45 289.** Controllable synthesis of N-doped hollow carbon spheres @ highly dispersed Mo₂C and ultra-low platinum nanoparticles core-shell electrocatalysts: Remarkable active toward PEMFCs hydrogen oxidation. **C. Deng**, Q. Feng, Z. Zhao, Z. Zhang, H. Li, H. Wang
- 11:05 290.** Strain-driven energy electrocatalysis. **S. Guo**

SECTION D

Marriott Marquis San Diego Marina
Presidio 2

Advances in Fluorescence & Bioluminescence Imaging Probes

Cosponsored by PHYS

H. Ai, *Organizer, Presiding*

X. Zhang, *Presiding*

- 8:00** Introductory Remarks.
- 8:05 291.** Rational design of fluorogenic and spontaneously blinking fluorophores for live-cell, super-resolution imaging. **Q. Zheng**, I. Chung, A. Weigel, A. Ranjan, A.X. Ayala, J. Grimm, C. Wu, J. Lippincott-Schwartz, R.H. Singer, L.D. Lavis

- 8:25 292.** Optical sensors for detecting signaling phospholipids. **A. Chandra**, S. Mondal, R. Venkatramani, A. Datta
- 8:45 293.** Multifunctional super-resolution microscopy with solvatochromic and conventional fluorescent probes. **K. Xu**
- 9:05 294.** Fluorescent probes for imaging enzyme activity. **J. Rao**
- 9:25 295.** Imaging of disease targets in cells via stimulus-responsive molecular probes. **R.L. McCarley**
- 9:45 296.** Benzoxanthene probes with inherent pancreatic ductal adenocarcinoma selectivity. **I.R. Munhenzva**, **L. Wang**, **M. Sibrian-Vazquez**, **J. Escobedo**, **R.M. Strongin**
- 10:25** Intermission.
- 10:40 297.** Imaging drug release from biomedical implants via radioluminescence. **G.B. Schober**, J.N. Anker

SECTION E

Marriott Marquis San Diego Marina
Torrey Pines 2

Chemical Forensics

C. Fraga, *Organizer*

C. Åstot, *Presiding*

- 8:00** Introductory Remarks.
- 8:05 298.** Applications of the US EPA's CompTox Chemistry Dashboard to support structure identification and chemical forensics using mass spectrometry. **A.J. Williams**, A. Chao, T. Cathey, T. Transue, E.M. Ulrich, J. Sobus
- 8:25 299.** New evaluation methods for building a seized-drug electron ionization mass spectral library. **W. Ji**, W.E. Wallace, D.V. Tchekhovskoi, S.E. Stein
- 8:45 300.** Towards standardless identification of trichothecene-based mycotoxins. **B.P. Mayer**, M.C. Prieto-Conaway, M. Dreyer, K.E. Mason, T. Corzett, A.M. Williams
- 9:05 301.** Microcystin analysis in biological fluids: Evaluation of 1D and 2D LC-MS/MS methods. **B.J. Garcia-Barboza**, S. Botch-Jones, C. Mallet, M. Lame
- 9:25** Intermission.
- 9:45 302.** Identification of organophosphorus chemical warfare agents (CWAs), precursors, and decomposition products with a fieldable NMR spectrometer using earth's magnetic field. **R.F. Williams**, D. Kaseman, S. Widgeon Paisner, J.L. Yoder, P.E. Magnelind, M.T. Janicke, R. Michalczyk, A.V. Urbaitis, M.A. Espy

- 10:05 303.** Characterization of impurities in gallium alloys via laser-induced breakdown spectroscopy. **A. Rao**, M. Shattan, J.D. Auxier
- 10:25 304.** Enhanced peroxidase-like catalytic assay for the colorimetric aptamer-based biosensing of amphetamine-type stimulants using multi-shaped gold nanoparticle-graphene oxide-hemin hybrid nanozyme. **O. Adegoke**
- 10:45 305.** Authentication of edible oils using vibrational spectroscopy and pattern recognition techniques. **B.K. Lavine**, F. Kwofie, I.S. Uba, M. Bamidele, K.S. Booksh

SECTION F

Marriott Marquis San Diego Marina
San Diego Ballroom Salon A

Advances in Wearable & Implantable Sensors

M. A. Daniele, L. Deravi, M. Yokus, *Organizers, Presiding*

- 8:00 306.** What can conformable decoders do?. **C. Dagdeviren**
- 8:30 307.** Real-time biosensors for continuous measurements of specific biomolecules in live animals. **H.T. Soh**
- 9:00 308.** Light-activated open circuit potentiometry. **J.E. Dick**
- 9:30** Intermission.
- 9:45 309.** Flexible and wearable sensors for human motion analysis. **E. Thostenson**, S. Doshi, A. Chaudhari
- 10:15 310.** Soft wearable systems with physiological monitoring and biochemical sensing capabilities. **R. Ghaffari**
- 10:45 311.** Stretchable conductive nanocomposite for wearable and implantable bioelectronics. **D. Jung**, **D. Kim**
- 11:00 312.** Wearable microfluidic sensing patch for dynamic sweat secretion analysis and regional sweat studies. **H.Y. Nyein**, M. Bariya, A. Javey

Liquid Assets: The Business of Water

Sponsored by SCHB, Cosponsored by ANYL, BMGT and I&EC

Getting to the Bottom: Optical & Electron Imaging of Reactive Chemical Systems

Imaging Plasmon-Coupled Processes

Sponsored by PHYS, Cosponsored by ANYL

SECTION A

Marriott Marquis San Diego Marina
San Diego Ballroom Salon C

Nanotechnology & Single Cell Analysis in Biology & Medicine

Nanoscience

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

- 1:00 313.** Single cell analysis of dynamic signaling activities with fluorescent biosensors. **J. Zhang**
- 1:30 314.** Molecular imaging and cellular reprogramming in single cells. **Y. Wang**
- 2:00 315.** Cellular imaging with genetically encoded RNA-based sensors. **M. You**
- 2:30 316.** Stimulated Raman imaging with chemical probes for subcellular bioanalysis. **L. Wei**
- 3:00** Intermission.
- 3:10 317.** Stimulated Raman scattering: Next frontier of light microscopy. **W. Min**
- 3:40 318.** Quantitative super-resolution microscopy of the mammalian glycocalyx. **L. Möckl**, **K. Pedram**, **A. Roy**, **V. Krishnan**, **A. Gustavsson**, **O. Dorigo**, **C.R. Bertozzi**, **W.E. Moerner**
- 4:10 319.** Variable-angle plasmonic fluorescence microscopy for tracking the endocytic pathway. **M. Chen**, **X. Pan**, **Q. Liu**, **Y. Li**
- 4:40 320.** Augmented fluorescent-free 3D super-resolution microscopy based on wavelength-dependent plasmonic scattering illumination. **S.H. Kang**

SECTION B

Marriott Marquis San Diego Marina
Torrey Pines 3

Structure at Solid-Liquid Interfaces: Effects of Confinement & Chemical Patterning

Cosponsored by COLL
T. C. Davis, T. R. Hayes, *Organizers, Presiding*

- 1:00 321.** Impact of passively and actively confining self-assembled molecular networks in 2D corrals. **S. De Feyter**
- 1:30 322.** Standing, lying, and sitting: Phospholipid striped phases as templates for nanomaterials at interfaces. **S.A. Claridge**
- 2:00 323.** Controlled molecular assembly at solid-liquid interfaces. **G. Liu**, **J. Zhang**, **V.A. Piunova**, **J. Frommer**
- 2:30 324.** Correlating structure and molecular transport at wet and semi-wet interfaces. **D.K. Schwartz**

- 3:00 **325.** Confined growth and transformation of colloidal nanostructures at solid-liquid interfaces. **Y. Yin**
- 3:30 **326.** Impact of fixed chemical patterns on moving surfaces. **M.M. Santore**

SECTION C

Marriott Marquis San Diego Marina
Presidio 1

Identification & Design of Catalytic Sites in Electrochemical Reactions

Cosponsored by ENFL and ORGN

C. Liu, H. Wang, *Organizers*
Y. Liang, *Organizer, Presiding*

- 1:00 **327.** Selective CO₂ reduction on isolated transition metal single atomic sites: From identification to scaling-up. **H. Wang**
- 1:30 **328.** Atomic design of metal nano-catalysts toward activation of energy-related molecules. **Y. Wu**
- 2:00 **329.** Molecular engineering of nickel single-site electrocatalysts. **X. Zhang, Y. Liang**
- 2:20 Intermission.
- 2:35 **330.** Oxygen evolution reaction electrocatalysis on mixed-metal oxyhydroxides. **S.W. Boettcher, M. Burke Stevens**
- 3:05 **331.** *In situ* stimulated Raman spectroscopy shows phosphate assisted cobalt oxide formation. **C.J. Eom, G. Brunin, G. Hautier, J. Suntivich**
- 3:25 **332.** Probing electrochemical reactions under *operando* conditions. **B. Liu**
- 3:55 **333.** *In situ* and *operando* spectroscopy of oxide electrocatalyst surfaces. **K.A. Stoerzinger**

SECTION D

Marriott Marquis San Diego Marina
Presidio 2

Advances in Fluorescence & Bioluminescence Imaging Probes

Cosponsored by PHYS

H. Ai, *Organizer, Presiding*
X. Zhang, *Presiding*

- 1:00 **334.** Multi-component bioluminescence imaging with diverse luciferin architectures. **J.A. Prescher**
- 1:20 **335.** Structure-luminescence relationship of near-infrared firefly luciferin analogues. **Y. Ikeda, Y. Hiruta, D. Citterio**
- 1:40 **336.** ATP-independent bioluminescent reporters for *in vivo* imaging. **H. Ai, H. Yeh**
- 2:00 **337.** SAFE method for luminescence quantum yield determination. **K. Nawara, J. Waluk**

- 2:20 **338.** Novel NanoLuc substrates enable bright and sustained bioluminescence imaging in animals. **J.R. Walker, Y. Park, T.P. Smith, D.C. Wang, M.P. Hall, L.X. Liu, R. Hurst, Y. Su, I.P. encell, N. Kim, K. Casey, T.A. Kirkland, M. Lin**
- 2:40 Intermission.
- 2:55 **339.** Methods for improving the biodetection performances of upconversion nanoprobes. **S. Xu**
- 3:15 **340.** Short-wavelength infrared nanosensors for imaging dopamine neuromodulation in the brain. **J.T. Del Bonis-O'Donnell, A. Beyene, K. Delevich, I. McFarlane, D. Piekarski, R. Page, L. Wilbrecht, M. Landry**
- 3:35 **341.** Near-infrared fluorescent probe for fast and ultrasensitive detection of nitroreductase in live cells. **S. Wan**
- 3:55 **342.** Near-infrared hybrid rhodol dyes with spiropyran switches for sensitive ratiometric sensing of pH changes in mitochondria. **S. Xia, H. Liu**
- 4:15 **343.** Ratiometric near-infrared fluorescent probes for sensitive detection of intracellular pH changes. **H. Liu**
- 4:35 **344.** Withdrawn

SECTION E

Marriott Marquis San Diego Marina
Torrey Pines 2

Metabolomics in Forensics: Applications, Technical Barriers & Emerging Approaches for Chemical Identification Using In Silico Reference Libraries

Cosponsored by COMP

T. E. Metz, *Organizer*
D. Wunschel, *Organizer, Presiding*
T. O. Metz, *Presiding*

- 1:00 Introductory Remarks.
- 1:05 **345.** Metabolomics for forensic analysis. **R. Bull**
- 1:20 **346.** Identification of emerging opioids in clinical samples using high-resolution tandem mass spectrometry. **K.D. Swanson, L. Krajewski, W. Bragg, R. Shaner, E. Hamelin, M. Carter, R. Johnson**
- 1:45 **347.** Studying the metabolome of *Ricinus communis* for attribution. **S. Ovenden**
- 2:10 **348.** Advancement in gas-phase separations for metabolomics. **G. Nagy, A. Li, A.L. Hollerbach, R.D. Smith, Y.M. Ibrahim**
- 2:35 **349.** LC-HRMS data and *in silico* fragmentation for identifying transformation products in environmental matrices. **J. Schollee, K. Kiefer, R. Gulde, H. Singer, J. Hollender, C. McArdeall**
- 3:00 Intermission.

- 3:15** **350.** Tools and databases for *in silico* compound identification. **D.S. Wishart**
- 3:40** **351.** *In silico* metabolite property libraries and quantitative chemical space analysis: Path toward novel molecule identification and false discovery assessment. **R. Renslow**, S.M. Colby, J. Nunez, Y. Yesiltepe, N. Govind, D. Thomas, J.R. Cort, J.G. Teeguarden, K. Wahl, D. Wunschel, T.O. Metz
- 4:00** **352.** Identification of unknown compounds using *in silico* fragmentation algorithms and *in silico* reference libraries. **T. Kind**
- 4:25** **353.** Evaluation of molecular ionization propensities in different ionization modes: Providing evidence for the presence of small molecules in synthetic blinded samples. **J. Nunez**, S.M. Colby, T.O. Metz, J.G. Teeguarden, R. Renslow
- 4:45** **354.** Optimal conformer selection for accurate *in silico* chemical property prediction. **F. Nielson**, D. Thomas, S.M. Colby, Y. Yesiltepe, R. Renslow

SECTION F

Marriott Marquis San Diego Marina
San Diego Ballroom Salon A

Advances in Wearable & Implantable Sensors

M. A. Daniele, L. Deravi, M. Yokus, *Organizers, Presiding*

- 1:00** **355.** Minimally- and non-invasive continuous biosensing: Frontiers for devices and sensors. **J. Heikenfeld**
- 1:30** **356.** Minimally invasive microneedle sensor arrays: New window on the body. **A.E. Cass**, S. Sharma, D. O'Hare
- 2:00** **357.** Rethinking on/in-body biochemical sensing strategies to achieve long-term functionality. **D. Diamond**
- 2:30** **358.** Facilitating collaboration to advanced nanotechnology-enabled wearable and implantable sensors: NNI sensors signature initiative. **S.D. Standridge**
- 3:00** Intermission.
- 3:15** **359.** New antifouling electrochemical aptamer-based sensor. **R.J. White**, S. Hendrickson
- 3:45** **360.** Band-Aid®-like electrochemical and electromechanical sensors for continuous physiological monitoring. M. Chu, L. Lin, E. Chou, J. Zakashansky, A. Hikari Imamura, J. Kim, **M. Khine**
- 4:15** **361.** Implantable aptamer field-effect transistor neuroprobes: Towards *in vivo* neurotransmitter detection. **C. Zhao**, I. Huang, K.M. Cheung, N. Nakatsuka, H. Yang, L. Scarabelli, L. Heidenreich, J. Belling, P.S. Weiss, H.G. Monbouquette, A.M. Andrews

- 4:30** **362.** Inkjet printing electronic materials on textile platforms and processing strategies for wearable electronics. **I. Kim**, Y. Zhou, B. Li, J. Jur
- 4:45** Concluding Remarks.

Eminent Scientist Lecture with Dr. Marya Lieberman

Sponsored by SOCED, Cosponsored by ANYL

Getting to the Bottom: Optical & Electron Imaging of Reactive Chemical Systems

Observing Chemical Processes and Nanostructures In Situ at the Atomic Level

Sponsored by PHYS, Cosponsored by ANYL

MONDAY EVENING – ANYL

SECTION A

San Diego Convention Center
TBD

Sci-Mix

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

8:00 - 10:00

55, 74, 99, 111, 127, 128, 180, 207, 236, 241, 263, 289, 291, 296, 312, 329, 349. See Previous Listings.
368, 369, 416, 458, 477, 537, 538, 557. See Subsequent Listings.

TUESDAY MORNING – ANYL

SECTION A

Marriott Marquis San Diego Marina
Rancho Santa Fe 2

Nanozymes for Bioanalysis & Beyond

Cosponsored by BIOL and BIOT

H. Wei, *Organizer, Presiding*

- 8:00** Introductory Remarks.
- 8:05** **363.** Single atom nanozyme for wound antibacterial applications. **X. Yan**
- 8:45** **364.** Platinum-nickel nanozyme and branched ruthenium nanoparticle catalysts. **R. Tilley**
- 9:25** **365.** Applications of inorganic nanoparticle enzyme mimics. **W. Tremel**
- 10:05** Intermission.
- 10:10** **366.** New strategies for nanozyme-based bioanalysis. **J. Liu**

- 10:50 367.** Ceria-based nanomaterials for therapeutic antioxidants. **T. Hyeon**
- 11:30 368.** Nanozyme based tumor catalytic theranostics. **K. Fan, X. Yan**

SECTION B

Marriott Marquis San Diego Marina
Torrey Pines 3

Structure at Solid-Liquid Interfaces: Effects of Confinement & Chemical Patterning

T. C. Davis, T. R. Hayes, *Organizers, Presiding*

- 8:00 369.** Stabilizing noncovalent monolayers on MoS₂ through edge-on adsorption of multi-chain functional alkanes. **T.C. Davis, S.R. Russell, S.A. Claridge**
- 8:20 370.** Surface microstructure functionalised by multicomponent femtoliter droplets at liquid-solid interface: Fabrication and applications. **M. Li, x. zhang**
- 8:40 371.** Broad probe for function of crystal nucleation by engineered nucleation features with proteins and small molecules in batch and continuous flow crystallization. **A.H. Bond, K. Nordquist, T.L. Kinnibrugh, K.M. Schaab**
- 9:10 372.** Functional chemical patterns as useful analytical devices. **W. Liao, C. Chen, C. Wang**
- 9:40** Intermission.
- 9:55 373.** Relative permittivity in the electrical double layer from nonlinear optics. **F. Geiger, M. Boamah**
- 10:25 374.** Surface chemistry of silica particles in aqueous solution. **A. Marchioro, S. Roke**
- 10:55 375.** Experimental and theoretical study of hydration and dehydration of zeolites. **T. Guo, D. Donadio**
- 11:25** Concluding Remarks.

SECTION C

Marriott Marquis San Diego Marina
Presidio 1

Identification & Design of Catalytic Sites in Electrochemical Reactions

Cosponsored by ENFL and ORGN

C. Liu, H. Wang, *Organizers*
Y. Liang, *Organizer, Presiding*

- 8:00 376.** Probing structure-performance relation for electrocatalysis using multimodal characterization techniques. **D. Su**
- 8:30 377.** Atomically precise metal nanoclusters for electrocatalysis. **D. Jiang**

- 9:00 378.** Identification of active species and mechanisms in non-precious metal oxygen reduction catalysts by poisoning and magnetic measurements. **A.A. Gewirth, A. Esposito**
- 9:30** Intermission.
- 9:45 379.** Understanding the electronic structure and reactivity of carbon monoxide dehydrogenase model systems for carbon dioxide reduction. **J. Panetier**
- 10:15 380.** Cation-mediated evolution of hydrogen on Cu electrodes. **M. Waegle**
- 10:45 381.** High performance electrochemical CO₂ reduction cells based on non-noble metal catalysts. **H. Wang**
- 11:05 382.** Identification of active phase of oxide-derived Cu in electrochemical CO reduction reaction with *operando* surface enhanced spectroscopy. **B. Xu**

SECTION D

Marriott Marquis San Diego Marina
Presidio 2

Mass Spectrometry of Biomolecular Assemblies

Cosponsored by BIOT, BMGT and MEDI

Financially supported by Agilent

J. S. Prell, *Organizer*

M. T. Marty, *Organizer, Presiding*

- 8:00 383.** Role of surface collisions in an MS-based structural biology approach. **V.H. Wysocki**
- 8:30 384.** Ion mobility mass spectrometry to characterize formation and structure of DNA assemblies. **T.L. Pukala, A. Begbie, J. Li**
- 9:00 385.** Pinpointing isomerization sites in long-lived proteins using IMS-MS. **R. Julian**
- 9:30** Intermission.
- 9:45 386.** Multidimensional ion mobility of proteins and protein complexes enabled by modular design. **M.F. Bush**
- 10:15 387.** Fourier transform ion mobility-Orbitrap spectrometer for native mass spectrometry. **J. McCabe, M. Shirzadeh, D.H. Russell**
- 10:45** Intermission.
- 11:00 388.** Tandem-trapped ion mobility/mass spectrometry measurements relates proteoform identity to their tertiary and quaternary structures. **C. Bleiholder, F.C. Liu, T.C. Cropley, M. Chai**
- 11:30 389.** Nanoscale ion emitters in native mass spectrometry for measuring ligand-protein and ligand-DNA binding affinities. **W.A. Donald**

SECTION E

Marriott Marquis San Diego Marina
Torrey Pines 2

Connecting Safety, Education, Training & Productivity in Analytical Laboratories

Cosponsored by CCS, CHAS, CINF and PRES

C. D. Incarvito, J. L. Maclachlan, *Organizers, Presiding*

- 8:00 Introductory Remarks.
- 8:10 **390.** Principles to influence culture and establish practices regarding safe operation of research instrumentation and application development. **E. Robinson**
- 8:30 **391.** Computer-assisted separation modeling in analytical space translated into improved preparative chromatography productivity. **I. Haidar Ahmad**, F. Tsay, R. Bennett, D. Henderson, R. Hartman, B. Mann, I.K. Mangion, E. Regalado
- 8:50 **392.** Generic GC-FID method for high-throughput analysis of residual solvents in pharmaceutical substances. **T. Nowak**, F. Bernardoni, H. Halsey, A.A. Makarov, E. Regalado
- 9:10 **393.** Safe solvent management for LC/MS and GC/MS. **P.A. Reinhardt**, S. Bain
- 9:30 Panel Discussion.
- 10:45 Concluding Remarks.

SECTION F

Marriott Marquis San Diego Marina
San Diego Ballroom Salon A

ACS Sensors Young Investigators

J. Gooding, S. O. Kelley, *Organizers, Presiding*

- 8:00 Introductory Remarks.
- 8:05 **394.** Multi-modal sensing for measuring tissue development and function in microphysiological systems. **M.A. Daniele**, V. Pozdin, K. Rivera, A. Young, P. Erb
- 8:35 **395.** Expanding the scope of biosensors: RNA- and small molecule-generating sensing systems. **B.C. Dickinson**
- 9:05 **396.** Probing and constructing bio-inorganic interfaces within a nanocavity for adaptive single molecule sensing. **S. Huang**
- 9:35 Intermission.
- 9:45 **397.** Not everybody dyes: Leveraging quantum dots and other luminescent nanomaterials for new opportunities in bioanalysis. **W.R. Algar**
- 10:15 **398.** Integration of dielectrophoretic selective single-cell capture at a wireless electrode array with on-chip analysis. M. Li, D. Pagariya, **R.K. Anand**

Getting to the Bottom: Optical & Electron Imaging of Reactive Chemical Systems

Spectroscopy of Reactive Chemical Systems

Sponsored by PHYS, Cosponsored by ANYL

TUESDAY AFTERNOON – ANYL

SECTION A

Marriott Marquis San Diego Marina
Rancho Santa Fe 2

Nanozymes for Bioanalysis & Beyond

Cosponsored by BIOL and BIOT

H. Wei, *Organizer, Presiding*

- 1:00 **399.** Imaging and treatment of multidrug-resistant bacteria and biofilms using bioorthogonal transition metal catalyst nanoparticle “nanozymes”. **V.M. Rotello**
- 1:40 **400.** Peptide-gold clusters as enzyme-like catalyst for *in situ* cell analysis and induce tumor-specific cell apoptosis. **L. Gao**
- 2:20 **401.** e_g occupancy as an activity descriptor for guiding the design of transitional oxide-based peroxidase mimics. X. Wang, X. Gao, L. Qin, C. Wang, L. Song, Y. Zhou, G. Zhu, W. Cao, S. Lin, Q. Zhou, K. Wang, H. Zhang, Z. Jin, P. Wang, X. Gao, **H. Wei**
- 3:00 Intermission.
- 3:05 **402.** Enzyme-mimic metal-bismuth oxyhalide for sensing and antimicrobial applications. **C. Huang**, H. Chang, J. Lai
- 3:45 **403.** Truncated tetrahedral CdTe QDs act as endonucleases for site-selective photoinduced cleavage of DNA. **C. Xu**, M. Sun, H. Kuang, L. Xu, A. Qu
- 4:25 **404.** Withdrawn

SECTION B

Marriott Marquis San Diego Marina
Torrey Pines 3

Analytical Division Awards

K. Agnew-Heard, *Organizer, Presiding*

- 1:00 Introductory Remarks.
- 1:05 **405.** Spectroscopy through the microscope: Chemical analysis at liquid/solid interfaces. **J.M. Harris**
- 1:40 **406.** Structure-activity relationships at complex electrodes from correlative electrochemical multi-microscopy. **P.R. Unwin**

- 2:15** **407.** New nano tools for real-time single molecule imaging of single live cells: From fundamental discoveries to biomedical applications. **X. Xu**
- 2:50** Intermission.
- 3:00** **408.** Building learning & teaching communities in analytical chemistry: From campus to textbook. **C.A. Lucy**
- 3:35** **409.** *In vivo* and intraoperative chemical analysis and tissue diagnosis using the MasSpec Pen technology. **L. Schiavinato Eberlin**
- 4:10** **410.** Atomic ions to intact protein complexes: 25-year quest for structure, dynamics, and thermodynamics. **D.H. Russell**

SECTION C

Marriott Marquis San Diego Marina
Presidio 1

Identification & Design of Catalytic Sites in Electrochemical Reactions

Cosponsored by ENFL and ORGN

Y. Liang, C. Liu, *Organizers*

H. Wang, *Organizer, Presiding*

- 1:00** **411.** Ambient electrochemical activation of small molecules with inorganic and hybrid catalysts. **C. Liu**
- 1:30** **412.** Designing functional sites in framework materials for energy storage devices. **V. Thoi**
- 2:00** **413.** CO₂ reduction by immobilized rhenium bipyridine moieties. **S.C. Marinescu**
- 2:30** Intermission.
- 2:45** **414.** Hydracity as an activity descriptor for molecular hydrogen evolution electrocatalyst design. **J.Y. Yang**, D.W. Cunningham, B. Ceballos
- 3:15** **415.** Phthalocyanine precursors to construct atomically dispersed metal electrocatalysts. **Y. Liang**, Y. Wang, Z. Jiang
- 3:45** **416.** Electrocatalytic oxidation of d⁰-oxo for ambient methane functionalization. **j. deng**, J. Iñiguez, D. Yang, D. Xiang, G. Chan, C. Liu

SECTION D

Marriott Marquis San Diego Marina
Presidio 2

Mass Spectrometry of Biomolecular Assemblies

Cosponsored by BIOL, BIOT and MEDI

Financially supported by Agilent

M. T. Marty, *Organizer*

J. S. Prell, *Organizer, Presiding*

- 1:00** **417.** Temperature-programmed native ESI-MS as a versatile biophysical toolbox to study noncovalent complexes. **R. Zenobi**

- 1:30** **418.** Flying viruses: From biophysical to structural characterisation. **C. Uetrecht**
- 2:00** **419.** Native mass spectrometry: Probing gas-phase or solution-phase protein structures?. **J.A. Loo**
- 2:30** Intermission.
- 2:45** **420.** Role of macroion-droplet interactions in the charge state of macromolecules. **S. Consta**
- 3:05** **421.** Investigation of membrane toxin assemblies with native ion mobility-mass spectrometry and Gábor transform. **J.S. Prell**
- 3:25** **422.** Characterizing oligomerization of biomolecular assemblies within intact membranes using native mass spectrometry and lipoprotein nanodiscs. **M.T. Marty**
- 3:45** Intermission.
- 4:00** **423.** Denaturing and native top-down proteomics using capillary electrophoresis-tandem mass spectrometry. **L. Sun**
- 4:30** **424.** Identifying protein interactions using in-cell protein footprinting coupled with mass spectrometry. **L.M. Jones**

SECTION E

Marriott Marquis San Diego Marina
Torrey Pines 2

Exploration of the Nano-Bio Interface with Analytical Tools

Cosponsored by BIOL and BIOT

W. Zhong, *Organizer, Presiding*

R. Coreas, *Presiding*

- 1:00** **425.** Nanotoxicity and nanomedicines. **Y. Zhao**
- 1:40** **426.** Toxicological profiling of metal and metal oxide nanomaterials in liver cells. **T. Xia**
- 2:10** **427.** Investigation of immune cell responses to engineered metal oxide nanomaterials by quantitative proteomics tools. T. Zhang, M. Gaffrey, B.D. Thrall, **W. Qian**
- 2:40** Intermission.
- 2:50** **428.** Single particle spatiotemporal analysis of transmembrane process of functionalized nanocargos. **Y. He**
- 3:20** **429.** Membrane-protein-hydration interaction of α -synuclein with anionic vesicles in solution probed via angle-resolved second harmonic scattering. J. Dedic, S. Rocha, P. Wittung Stafshede, **S. Roke**
- 3:50** **430.** Toxicological risk assessment of cellulose nanofibrils by using a fluorescent molecular probe. **I. Patel**, J.W. Woodcock, J. Shatkin, S. Stranick, G. DeLoid, P. Demokritou, S. Harper, J.W. Gilman, D. Fox

SECTION F

Marriott Marquis San Diego Marina
San Diego Ballroom Salon A

Biosensing: New Strategies & Latest Development

Cosponsored by BIOL, BIOT and MEDI

Q. J. Cheng, *Organizer, Presiding*

- 1:00** 431. Single hydrogel nanoparticle SPR imaging measurements for biosensing and bioaffinity uptake. **R.M. Corn**
- 1:30** 432. Supramolecular assemblies for chiral molecular sensing. **M. Liu**, L. Zhang
- 2:00** 433. Mirror-image nucleic acid-based sensors for live-cell imaging of RNA. **J. Sczepanski**, B. Young, A. Kabza, W. Zhong
- 2:20** 434. Microfluidic biochip platform incorporating hydrogel-based differential Coulter counting technology for rapid, multiplexed quantification of proteins. T. Cowell, E. Valera, A. Jackelow, J. Park, R. Ding, R. Bashir, **H. Han**
- 2:40** Intermission.
- 2:55** 435. Microscale interfaces for sensitive biosensing and comprehensive identification of biomolecules. **B. Liu**, Y. Wang, H. Zhang, K. Zhang, L. Qiao, J. Liu
- 3:25** 436. Preparation and integration of specifically functionalized biosensors for liquid biopsy. **R. Heer**
- 3:55** 437. New catalytic DNA based biosensors for selective metal ions detection. **J. Liu**
- 4:15** 438. Using gold nanoparticles for diagnostics and sensing in low cost devices. K. Hamad-Schifferli, **C. Rodriguez-Quijada**
- 4:35** 439. Switchable chemical reactivity to multiplex aptamer-field-effect transistor sensing. **O. Lukyanova**, S.T. Mensah, J. Stauber, W. Dai, C. Zhao, K. Cheung, P. Weiss, M.N. Stojanovic, A.M. Spokoiny, A.M. Andrews

WEDNESDAY MORNING – ANYL

SECTION A

Marriott Marquis San Diego Marina
Rancho Santa Fe 2

Nanozymes for Bioanalysis & Beyond

Cosponsored by BIOL and BIOT

H. Wei, *Organizer, Presiding*

- 8:00** 440. Strong candidate graphene based materials to replace natural peroxidase in sensitive and selective bioassays. **J. Lee**
- 8:40** 441. Nanozyme-prodrug therapy. **A. Zelikin**

- 9:20** 442. Bifunctional nanozyme based on modified carbon nitride photocatalyst that mimics glucose oxidase-peroxidase. **W. Choi**, P. Zhang, J. Han, D. Kim
- 10:00** Intermission.
- 10:05** 443. Combat resistant bacteria with nanozymes. **L. Gao**
- 10:45** 444. Biological applications by nucleobase analogues capped gold nanoclusters with peroxidase-like activity. **H. Jiang**, Y. Zheng, L. Liu, X. Wang
- 11:15** 445. Fluorescent C₃N₄-based nanozymes for ratiometric biomedical assays. **X. Wang**, H. Wei

SECTION B

Marriott Marquis San Diego Marina
Torrey Pines 3

From Antibody-Based to Mass Spectrometry-Based Analysis of Emerging Contaminants in Water: Advances & Future Trends

Cosponsored by ENVR

D. S. Aga, R. J. Schneider, *Organizers, Presiding*

- 8:00** Introductory Remarks.
- 8:10** 446. Antibody-based approaches to respond to the environmental analytical challenges. **M. Marco**
- 8:45** 447. Using mass spectrometry to vet microcystin concentrations by enzyme-linked immunosorbent assay. **J. Westrick**
- 9:10** 448. VHH antibodies are versatile tools for monitoring of environmental chemical contamination. **N. Vasylieva**, Z. Li, D. Li, B. Barnych, B.D. Hammock
- 9:35** Intermission.
- 10:00** 449. Improving small molecule annotation in nontargeted soft-ionization GC/LC high-resolution mass spectrometry. **C. Jaeger**, J. Lisec
- 10:25** 450. Ultrasensitive MALDI-TOF quantitation of microcystins in complex matrices by direct on-target analysis of nanobody-captured toxins. M. Pérez-Schirmer, B.M. Brena, **G. Gonzalez**

SECTION C

Marriott Marquis San Diego Marina
Presidio 1

Advances in Electrochemistry

L. A. Baker, *Organizer, Presiding*

- 8:00** 451. Imaging local electrochemistry with ion conductance microscopy. **L.A. Baker**

- 8:25 452.** Using image processing algorithms to treat electrochemical images. **L. Stephens**, N. Payne, S. Skaanvik, D. Polcari, M. Geissler, J. Mauzeroll
- 8:45 453.** Positive and negative feedback theory and experiments in hot-tip scanning electrochemical microscopy. **Z. Zhao**, A. Boika
- 9:05 454.** Bubble nucleation-based electrochemical detection method for perfluorinated surfactants. **R. Ranaweera**, L. Luo
- 9:25** Intermission.
- 9:40 455.** Critical nuclei size and rate of nanobubble nucleation. **M.A. Edwards**, S. German, H. Ren, A. Moreno Soto, H. White
- 10:05 456.** Mechanism of histamine oxidation and electropolymerization at carbon electrodes. **P. Puthongkham**, B.J. Venton
- 10:25 457.** Neurotransmitter detection at near the theoretical performance limit of electroenzymatic sensors. **I. Huang**, M. Clay, H.G. Monbouquette
- 10:45 458.** Single drop fabrication of the cholesterol biosensor based on synthesized NiFe₂O₄ NPs dispersed on PDDA–CNTs. **C. Moonla**, T. Tangkuaram, A. Preechaworapun

SECTION D

Marriott Marquis San Diego Marina
Presidio 2

Interface between Experiments & Modeling in Unraveling the Physical & Chemical Properties of Charged Droplets

Cosponsored by COMP, ORGN and PHYS
S. Consta, S. Xantheas, *Organizers, Presiding*

- 8:00** Introductory Remarks.
- 8:05 459.** Understanding molecular aspects of aqueous interfacial chemistry with clusters. **M.A. Johnson**
- 8:35 460.** Photoemission from charged droplets. **R. Signorell**
- 9:05 461.** Diverse nature of ion speciation at the nanoscale hydrophobic/water interface. E. Zdrali, M.D. Baer, H. Okur, C.J. Mundy, **S. Roke**
- 9:35** Intermission.
- 9:50 462.** Native electrospray ionization: From solution to charged droplets to final ions. **M.F. Bush**
- 10:20 463.** Spectroscopic characterization and computational investigation of anionic clusters generated from charged droplets. **X. Wang**
- 10:50 464.** Vibrating sharp-edge spray ionization (VSSI) for in-droplet hydrogen/deuterium exchange reactions. **S.J. Valentine**, N. Ranganathan, C. Li, X. Li, K. Attanayake, S. Majuta, A. Kiani Karanji, P. Li
- 11:20 465.** Adventures in anion photoelectron spectroscopy. **K.H. Bowen**
- 11:50** Discussion.

SECTION E

Marriott Marquis San Diego Marina
Torrey Pines 2

Exploration of the Nano-Bio Interface with Analytical Tools

Cosponsored by BIOL and BIOT
W. Zhong, *Organizer, Presiding*

- 8:00 466.** Don't forget the lipids: Biomolecular coronas on nanoparticles. **C.J. Murphy**
- 8:40 467.** Pulmonary surfactant corona and nano-bio interactions in the lung. **Y. Zuo**
- 9:10 468.** Protein conformational change induced by nanomaterials elucidated with limited proteolysis. **W. Zhong**, Y. Duan, R. Coreas
- 9:40** Intermission.
- 9:50 469.** Optimized carbon dots: Green imaging agents at the nano-bio interface. **C.L. Haynes**
- 10:20 470.** Fluorescent black carbon surrogates: Probing biological impacts of black carbon while relating form and function in creating fluorescent carbon dots. **C. Sumner**, R.L. McCarley
- 10:40 471.** Characterizing protein coronas with limited proteolysis and lipid coronas with liquid-liquid extractions coupled to liquid chromatography-mass spectrometry. **R. Coreas**, J. Lee, Y. Duan, W. Zhong
- 11:00 472.** Gold nanoparticle-based screening platform to assess protein-carbohydrate interactions. **S. Richards**

SECTION F

Marriott Marquis San Diego Marina
San Diego Ballroom Salon A

Biosensing: New Strategies & Latest Development

Cosponsored by BIOL, BIOT and MEDI
Q. J. Cheng, *Organizer*
R. Heer, M. Liu, *Presiding*

- 8:00 473.** Development of miniature surface plasmon resonance systems and sensor applications. **A. Baba**, S. Nootchanat, C. Lertvachirapaiboon, K. Shinbo, K. Kato, S. Ekgasit
- 8:30 474.** Supported lipid membranes as biosensing interface. **Q.J. Cheng**
- 9:00 475.** Interference effect of silica colloidal crystal films and their applications on biosensing. **W. Qian**, Q. Su, F. Wu, P. Xu, A. Dong, C. Liu, Y. Wan
- 9:20 476.** Electrochemical quantification of bladder cancer biomarkers with a phase-based bioresistor. **E.C. Sanders**, A. Attar, A. Santos, S. Majumdar, R.M. Penner, G.A. Weiss

- 9:40 **477.** Polymeric nanofilter biointerface for potentiometric small-biomolecule recognition. **S. Nishitani**, S. Himori, F. Nishimori, T. Sakata
- 10:00 Intermission.
- 10:15 **478.** Better analysis for proteins with metallic and non-metallic nanoparticle-integrated biosensing platforms. **H. Lee**
- 10:45 **479.** Towards development of fluorescence quenching-based biosensors for drought stress in plants. **T. Guo**, S. Brady
- 11:05 **480.** Oxidative stress imaging using LED-based photoacoustic imaging system. **A. Hariri**, E. Zhao, J.V. Jokerst
- 11:25 **481.** Massively parallel single-molecule detection platform using nano-electronics. **Y. lee**, K.L. Shepard

Theoretical & Experimental Investigations of Water Interactions with Materials

Sponsored by COLL, Cosponsored by ANYL

WEDNESDAY AFTERNOON – ANYL

SECTION A

Marriott Marquis San Diego Marina
Rancho Santa Fe 2

Nanozymes for Bioanalysis & Beyond

Cosponsored by BIOL and BIOT
H. Wei, *Organizer, Presiding*

- 1:00 **482.** *De novo* design of nanomedicine: Large scale molecular simulation of nanoparticle-biomolecule interactions. **R. Zhou**
- 1:40 **483.** Catalytic model bridging computations and experiments for ceria-based nanozymes. **Z. Wang**, **X. Gao**
- 2:20 **484.** Metallic nanostructures for medical diagnostics. **X. Xia**
- 3:00 Intermission.
- 3:05 **485.** Portable sensors incorporating nanomaterials with enzyme-mimetic properties for bioanalysis. **A. Othman**, F. Mustafa, M. Hassan, **E. Andreescu**
- 3:45 **486.** Standardization of nanozyme research. **M. Liang**
- 4:25 **487.** NanoZymes for colorimetric sensing and beyond. **R. Ramanathan**, V. Bansal, P. Weerathunge, N. Karim, M. Singh, P. Mariathomas, S. Hashmi, S. Prasad

SECTION B

Marriott Marquis San Diego Marina
Torrey Pines 3

From Antibody-Based to Mass Spectrometry-Based Analysis of Emerging Contaminants in Water: Advances & Future Trends

D. S. Aga, R. J. Schneider, *Organizers, Presiding*

- 1:00 **488.** Analysis and fate of antimicrobials in animal manure: Challenges and solutions. **D.S. Aga**
- 1:35 **489.** Immobilization of multivalent nanobodies onto bacteria magnetic particles for the rapid detection of tetrabromobisphenol A in the environment. **J. He**, J. Xu, J. Tian, J. Li, S. Gee, B.D. Hammock, Q.X. Li, **T. Xu**
- 2:00 Intermission.
- 2:25 **490.** Analysis of bisphenol A, octyl and nonyl phenol, estrogens, and other selected pharmaceuticals in surface and wastewater by liquid chromatography-negative ion electrospray-tandem mass spectrometry. **g. aborkhees**, **R. Raina-Fulton**, O. Thirunavukkarasu
- 2:50 **491.** Determination of emerging micropollutants in urban waters and wastewater by portable immunoanalytical methods. **P. Carl**, I.I. Ramos, M.A. Segundo, **R.J. Schneider**
- 3:15 Concluding Remarks.

SECTION C

Marriott Marquis San Diego Marina
Presidio 1

Advances in Electrochemistry

L. A. Baker, *Organizer, Presiding*

- 1:00 **492.** Electrochemical and electrokinetic route for dialysate regeneration. **B. Berzina**, R. Anand
- 1:25 **493.** Electrochemical sensors for field detection of explosives. **S. Trammell**
- 1:50 **494.** Electrochemical reduction of carbon dioxide to formate and carbon monoxide on lead-tin alloys. **A. Hailu**, S.K. Shaw
- 2:10 Intermission.
- 2:25 **495.** Proton transfer regulation across soft interfaces of water. **H. Tavassol**, L. Nguyen, C. Mao, K. Asham
- 2:45 **496.** Coherent X-ray diffraction/absorption microscopy for analyzing organic and inorganic materials. **J. Park**
- 3:05 **497.** Influence of electrochemical polymerization protocols on composite conducting polymer films for supercapacitor electrode materials. **A. Al-Betar**

- 3:25 **498.** Determination of betadex (β -cyclodextrin) according to the USP betadex sulfobutyl ether sodium monograph. **M. Aggrawal**, J.S. Rohrer

SECTION D

Marriott Marquis San Diego Marina
Presidio 2

Interface between Experiments & Modeling in Unraveling the Physical & Chemical Properties of Charged Droplets

Cosponsored by COMP, ORGN and PHYS
S. Consta, S. Xantheas, *Organizers, Presiding*

- 1:00 **499.** Ions from solution to the gas phase: Effects of solvent on the final structure. M.J. Hebert, **D.H. Russell**
- 1:30 **500.** Understanding disordered protein conformations in solution as viewed from the gas phase. **P.E. Barran**
- 2:00 **501.** Microsolvation effects on the encapsulation of metal ions by crown ethers. **Y. Inokuchi**
- 2:30 Intermission.
- 2:45 **502.** Charging proteins by electrospray ionization. **R.R. Loo**, J.A. Loo
- 3:15 **503.** Infrared laser spectroscopy of solvated cations. **M.A. Duncan**
- 3:45 **504.** Chemistry driven by electrons: Metastable electronic states and spin-forbidden processes. **K.B. Bravaya**
- 4:15 **505.** Many-body expansion for ion-water clusters: Convergence, size and basis set effects, and solvation structure. **J.P. Heindel**, S.S. Xantheas
- 4:45 Discussion.

SECTION E

Marriott Marquis San Diego Marina
Torrey Pines 2

Study of Circulating, Cell-Free Biomarkers with Analytical Tools

Cosponsored by BIOL, BIOT and MEDI
W. Zhong, *Organizer, Presiding*
G. Adkins, M. P. Trinh, *Presiding*

- 1:00 **506.** Tracking cell-free, circulating nucleic acids from tumors with electrochemical sensors. **S.O. Kelley**
- 1:40 **507.** Lipid-based normalization of quantum dot probes bound to membrane markers on extracellular vesicles in complex biological samples. **T. Hu**
- 2:20 **508.** High-resolution single-vesicle flow cytometry. **J. Nolan**

- 3:00 Intermission.
- 3:10 **509.** Analyzing maternal blood serum preterm birth risk biomarkers in 3D printed microfluidic devices. **A. Woolley**, M. Beauchamp, A.V. Nielson, E.K. Parker, J.B. Nielsen, H.M. Almughamsi, G.P. Nordin
- 3:50 **510.** Chemical operations on a living single cell by open microfluidics. **J. Lin**
- 4:30 **511.** Analysis of extracellular vesicle (EV) enabled by nanostructures. **W. Zhong**, K. Guo, Q. Jiang

SECTION F

Marriott Marquis San Diego Marina
San Diego Ballroom Salon A

Biosensing: New Strategies & Latest Development

Cosponsored by BIOL, BIOT and MEDI
Q. J. Cheng, *Organizer*
B. Liu, R. Ragan, *Presiding*

- 1:00 **512.** Aptamer-functionalized microelectrodes and nanopipettes to sense neurotransmitters in neuronal networks. **N. Nakatsuka**, S. Weaver, D. Eggemann, T. Schlotter, D. Momotenko, J. Vörös
- 1:30 **513.** Stimulus-responsive nanomaterial for highly efficient intracellular sensing and gene therapy. **Y. Liu**, K. Kw Ren, H. Ju
- 2:00 **514.** Illuminating bacterial communities with plasmonic nanoantennas. **R. Ragan**, W.J. Thrift, A.S. Cabuslay, A. Hochbaum
- 2:20 **515.** Single molecule fluorescence counting assay to measure biomolecules. H. Zhang, Y. Liu, K. Zhang, X. Huang, B. Li, B. Liu, **J. Liu**
- 2:40 **516.** Developing aptamer-based biosensor for onsite detection of stress biomarkers in noninvasive biofluids. **S. Dalirirad**
- 3:00 Intermission.
- 3:15 **517.** Detection of antibiotic-resistant bacteria using nanoparticle-mediated microfluidic capture. **C. Nemr**, S.J. Smith, P. Aldridge, W. Liu, A. Mephram, R. Mohamadi, M. Labib, S.O. Kelley
- 3:35 **518.** Paper-based lateral flow immunoassay for detection of traumatic brain injury biomarkers. **K. Curtin**, X. Gao, N. Wu
- 3:55 **519.** Fabrication of wafer-scale metal oxide nanoribbon field-effect transistor biosensors using chemical lift-off lithography. **C. Zhao**, Q. Liu, K.M. Cheung, W. Liu, Q. Yang, X. Xu, A.M. Andrews, C. Zhou, P.S. Weiss
- 4:15 **520.** Thermally carbonized porous silicon for robust label-free DNA optical sensing. **R. Layouni**, M. Choudhury, P.E. Laibinis, S.M. Weiss

- 4:35 521. Duplex electrochemical DNA sensor to detect B.anthraxis CAP and PAG DNA targets based on the incorporation of tailed primers and ferrocene labelled dATP. **I. Magriñá-Lobato**, M. Jauset-Rubio, M. Ortiz, A. Simonova, M. Hocek, C. O'Sullivan

Theoretical & Experimental Investigations of Water Interactions with Materials

Sponsored by COLL, Cosponsored by ANYL

THURSDAY MORNING – ANYL

SECTION A

Marriott Marquis San Diego Marina
Rancho Santa Fe 2

Advances in Spectroscopy

XRF, NMR, & SEM Spectroscopy

E. A. Smith, *Organizer*

R. F. Hirsch, *Presiding*

- 8:00 Introductory Remarks.
- 8:05 522. Detection of toxic metals contamination in cosmetics using MP-AES and X-Ray fluorescence spectroscopy. **S. Alsherari**, A.W. Apblett
- 8:25 523. Low resolution size chromatographs? The potential applications of diffusion ordered spectroscopy NMR in analysis of polymer size distributions. **T.A. Swift**, S. Rimmer
- 8:45 524. Imaging and analysis of ancient decorative metal threads using scanning electron microscope-based X-ray spectroscopies. **A. Popowich**, E. Vicenzi, T. Lam
- 9:05 525. Applications of broadband ^{19}F - ^1H cross-polarization in NMR spectroscopy: Hetero-TOCSY and ASAP-HSQC. **A.A. Marchione**, E. Diaz
- 9:25 Intermission.
- 9:40 526. Advancing innovation and the adoption of emerging technology in pharmaceutical freeze-drying through laboratory research at FDA's office of testing and research. **M. Korang-Yeboah**, L. Hengst, A. Ako-Adounvo, C. Srinivasan, M. Ashraf, C.N. Cruz
- 10:00 527. Simultaneous measurement of metal coatings thickness and composition using x-ray fluorescence (XRF) spectroscopy. **H. Atae-Esfahani**, J. Peters
- 10:20 528. How analytical chemistry is providing basic advances in climate science. **R.F. Hirsch**
- 10:40 529. Calibration transfer between low-field NMR instruments. D. Galvan, E. Danieli, D. Borsato, **M.H. Killner**

SECTION B

Marriott Marquis San Diego Marina
Torrey Pines 3

Advances in Mass Spectrometry

M. F. Bush, *Organizer, Presiding*

- 8:00 530. Electrochemistry-assisted absolute quantitation by mass spectrometry without the use of standards. **H. Chen**, P. Zhao
- 8:25 531. Applications of *in-situ* mass spectrometry, high resolution mass spectrometry, and theoretical methods to the analysis of e-cigarette thermal degradation chemistry. **Y. Li**, A. Burns, T.B. Nguyen
- 8:45 532. Studying reductive reaction of triple bond in microdroplet by extractive electrospray ionization mass spectrometry and *in-situ* Raman spectroscopy. **K. Huang**, W. Chou, Y. Wang, C. Hsu
- 9:05 533. Heteroatom-doped graphene quantum dots enable negative ion laser desorption ionization mass spectrometry for probing and imaging of small biomolecules. **Q. Min**, X. Huang, M. Liu, J. Zhu
- 9:25 534. Multilayered gold-nanoparticle thin film as a sample substrate in SALDI-MS for osteoporosis risk assessment. **Y. Chang**, T. Kuo
- 9:45 Intermission.
- 10:05 535. Ion mobility-mass spectrometry reveals the effect of sialylation on glycoprotein structures. **G. Li**, L. Li
- 10:25 536. Improved profiling of sialylated N-linked glycans by ion chromatography-mass spectrometry. **S. Patil**, J.S. Rohrer
- 10:45 537. Native top-down proteomics for mouse brain proteome with capillary zone electrophoresis-tandem mass spectrometry. **X. Shen**, L. Sun
- 11:05 538. Module-based method development and life cycle method improvement: Two case studies of complex method development, validation, and implementation using automated tandem mass spectrometry to support regulatory science issues. **J. Zhang**, P. Faustino
- 11:25 539. Trace metals in LPG (liquefied petroleum gas) by ICP-MS (inductively coupled plasma mass spectrometry). **S.S. Chudasama**, K. Lehuta
- 11:45 540. Multidimensional fractionation and molecular characterization of lingering oil compounds in coastal sediments: A nine year evolution. **A.M. McKenna**, H. Chen, C.C. Davis, S.F. Niles, C.R. Weisbrod, A. Hou, M.L. Chacon-Patino, Q. Lin, R.P. Rodgers

SECTION C

Marriott Marquis San Diego Marina
Presidio 1

Chemometric Analysis for Aqueous Sample

Cosponsored by COMP and ENVR

Financially supported by The University of Alabama

X. Liang, T. Mako, Y. Xu, X. Yao, *Organizers, Presiding*

- 8:00 Introductory Remarks.
- 8:05 **541.** Unraveling sample matrix effects for multivariate calibration. **J.H. Kalivas**, T. Lemos
- 8:30 **542.** Differential sensing of multiplex MAPK isoforms using expanded SOX-peptide library. **L. Zeng**, D. Zamora-Olivares, T.S. Kaoud, K. Dalby, E.V. Anslyn
- 8:55 **543.** Chemometrics to guide the design of a lignin electrocatalytic reactor. **P.D. Harrington**, Z. Chen, M. Naderinasrabadi, J. Staser
- 9:20 Intermission.
- 9:30 **544.** Temperature-dependent near-infrared spectroscopy for analyzing aqueous samples. **X. Shao**, X. Cui, L. Ma, L. Wang, Y. Sun, M. Wang, W. Cai
- 9:55 **545.** Calibration-based detection and confidence limits are (almost) exact when the data variance function is known. **J.B. Tellinghuisen**
- 10:20 **546.** Multivariate curve resolution and pattern recognition applied to infrared images of paint chips to facilitate the forensic examination of automotive paints. **B.K. Lavine**, F. Kwofie
- 10:45 Concluding Remarks.

SECTION D

Marriott Marquis San Diego Marina
Presidio 2

Interface between Experiments & Modeling in Unraveling the Physical & Chemical Properties of Charged Droplets

Cosponsored by COMP, ORGN and PHYS

S. Consta, S. Xantheas, *Organizers, Presiding*

- 8:00 **547.** Reversed interfacial fractionation of carbonate and bicarbonate evidenced by X-ray photoemission spectroscopy and theory. **R.J. Saykally**, t. pascal
- 8:30 **548.** Quantum mechanical studies of protonated water clusters through their IR spectra. **J.M. Bowman**, Q. Yu
- 9:00 **549.** How can we use machine learning to study droplet catalysis?. **T. Rhone**, C. O'Connor, R. Hoyt, M. Montemore, C. Kumar, C.M. Friend, E. Kaxiras
- 9:30 Intermission.

- 9:45 **550.** Diffusion Monte Carlo approaches for exploring neutral and protonated water clusters. **A.B. McCoy**, R. Dirisio, V. Lee
- 10:15 **551.** Reaction acceleration in charged microdroplets: Scratching the surface. **B.M. Marsh**, K. Iyer, R.G. Cooks
- 10:45 **552.** Highly charged droplets of superfluid helium. **M. Gatchell**, F. Laimer, P. Martini, L. Tiefenthaler, S. Albertini, F. Zappa, P. Scheier
- 11:15 **553.** Ionic strength in systems that violate the electric neutrality. **S. Consta**
- 11:45 Discussion.
- 11:55 Concluding Remarks.

SECTION E

Marriott Marquis San Diego Marina
Torrey Pines 2

Study of Circulating, Cell-Free Biomarkers with Analytical Tools

Cosponsored by BIOL, BIOT and MEDI

W. Zhong, *Organizer, Presiding*

G. Adkins, M. P. Trinh, *Presiding*

- 8:00 **554.** Fluorescent nanomaterials for detection of cell markers and images. **H. Chang**
- 8:40 **555.** Chemiluminescent gold nanoluminophore-based immunoassays for biomarkers of acute myocardial infarction. **H. Cui**
- 9:20 **556.** Ultrasensitive quantification strategy of extracellular vesicles using CuS microgel and filter membrane. **Q. Jiang**, Y. Liu, W. Zhong
- 9:40 **557.** Photocleavable linker for the release of rare cancer biomarkers after microfluidic affinity selection. **T. Pahattuge**, J.M. Jackson, S.A. Soper
- 10:00 Intermission.
- 10:10 **558.** Nanomaterial-assisted extraction and quantification of circulating non-coding RNAs in serum. **M.P. Trinh**, Y. Zheng, W. Zhong
- 10:30 **559.** DNA terminal structure-mediated enzymatic reaction for ultra-sensitive detection of EGFR exon 19 deletion. **M. Zhao**
- 10:50 **560.** Single exosome analysis based on exosomal proteins using flow cytometry. **K. Guo**, W. Zhong
- 11:10 **561.** Characterizing extracellular vesicles using asymmetrical flow field-flow fractionation: Combining traditional nanoparticle characterization techniques with biomolecular probing. **G.B. Adkins**, E. Sun, W. Zhong

SECTION F
Marriott Marquis San Diego Marina
San Diego Ballroom Salon A

Biosensing: New Strategies & Latest Development

Cosponsored by BIOL, BIOT and MEDI

Q. J. Cheng, *Organizer*

A. Lambert, H. Lee, *Presiding*

- 8:00** **562.** Nucleic-acid-functionalized field-effect transistors for biomedical applications. **K.M. Cheung**, N. Nakatsuka, K. Yang, C. Zhao, H. Yang, J.M. Abendroth, P.S. Weiss, M.N. Stojanovic, A.M. Andrews
- 8:20** **563.** SPR-MALDI Biosensing via carbohydrate small molecule probes. **A. Lambert**, C. Chen, Q.J. Cheng
- 8:40** **564.** Microfluidic synthesis and patterning of silver nanoparticles for biomolecular sensing. **Y. Nie**, J. Zhang
- 9:00** **565.** Supported lipid bilayer-based biosensor to detect phospholipase A2 -lipid membrane interaction. **S. Hossain**, K. Pai, M. Piyasena
- 9:20** **566.** Nanobody-based binding assay for the discovery of potent inhibitors in drug development. **N. Vasylieva**, S. Kitamura, J. Dong, B. Barnych, K. Hvorecny, D. Madden, S. Gee, D.W. Wolan, C. Morisseau, B.D. Hammock
- 9:40** Intermission.
- 9:55** **567.** Microfluidic paper-based analytical devices (microPADs) with DVD player: Centrifugally assisted flow acceleration for rapid distance readout assays. **K. Maejima**, Y. Hiruta, D. Citterio
- 10:15** **568.** Chimeric phage as scaffold for rapid detection of pathogenic bacteria. **H. Peng**, I. Chen
- 10:35** **569.** Fully integrated paper microfluidic single-walled carbon nanotubes chemiresistive biosensor arrays for point-of-care diagnostics. **Y. Shen**, A.K. Mulchandani
- 10:55** **570.** Fast interrogation of electrochemical, aptamer-based (E-AB) sensors for the characterization of small molecule-aptamer binding kinetics. **M.S. Santos Cancel**, R. Lazenby, R. White
- 11:15** **571.** Advantages of gallium indium eutectic contacts for In₂O₃ field-effect transistors. **s. Rahimnejad**, L. Stewart, C. Zhao, A. Andrews, P. Weiss
- 11:35** **572.** Using single-molecule RNA: DNA electrical conductance measurements for ultra-sensitive pathogen detection. Y. Li, **J.M. Artes Vivancos**, B. Demir, S. Gokce, H.M. Mohammad, M. Alangari, A. Anantram, E.E. Oren, J. Hihath

Theoretical & Experimental Investigations of Water Interactions with Materials

Sponsored by COLL, Cosponsored by ANYL

THURSDAY AFTERNOON – ANYL

SECTION A
Marriott Marquis San Diego Marina
Rancho Santa Fe 2

Advances in Spectroscopy

Optical Spectroscopy: IR, Fluorescence, Absorption, and Raman Spectroscopy

E. A. Smith, *Organizer*

R. F. Hirsch, *Presiding*

- 1:00** **573.** Development of fluorescent molecular probes for the highly sensitive and selective detection of living substances using magnetic beads. **Y. Suzuki**
- 1:20** **574.** Pump-probe UV resonance Raman spectroscopic analysis of the redox cofactors in photosystem II. **J. Chen**, J. Chen, Y. Liu
- 1:40** **575.** Polymeric microfluidic continuous flow mixer combined with hyperspectral FT-IR imaging for studying rapid biomolecular events. **H. Jang**, A. Pawate, R. Bhargava, P.J. Kenis
- 2:00** **576.** Cyano-derivatized tryptophans, as a novel 2D IR probe-pair for protein dynamics. **F. Chalyavi**, J. Mauro, A. Schmitz, M.W. Fennie, M.J. Tucker
- 2:20** Intermission.
- 2:35** **577.** Adversarial spectroscopy. **G.J. Simpson**
- 3:00** **578.** Microgel nanostructures for surface-enhanced Raman spectroscopy. **S.R. Emory**, A. Silva, J. Lo, S. Olson, **D.A. Rider**
- 3:20** **579.** Investigating the anion-cation intermolecular interactions in imidazolium acetate ionic liquids by Raman spectroscopy and multiple regression analysis. **J. Li**, J.W. Petrich, E.A. Smith
- 3:40** **580.** All-dielectric, mid-infrared metasurfaces for vibrational circular dichroism enhancement. **J. Abendroth**, J. Hu, L. Poulidakos, M. Solomon, M. Lawrence, J. Dionne

BIOL

DIVISION OF BIOLOGICAL CHEMISTRY

P. Bevilacqua and M. Distefano, *Program Chairs*

SUNDAY MORNING – BIOL

SECTION A

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 5

Biomolecular Structure & Function in Liquid-Liquid Phase Separation: Roles for Nucleic Acids

P. Bevilacqua, M. D. Distefano, *Organizers*
C. D. Keating, *Organizer, Presiding*

- 8:00** Introductory Remarks.
- 8:05** **1.** Bioinspired microenvironments generated by phase coexistence in polyelectrolyte solutions. **C.D. Keating**
- 8:40** **2.** Anion-assisted ribozyme catalysis inside complex coacervates. **P. Bevilacqua**, R. Poudyal, C.D. Keating
- 9:15** **3.** Membrane-free coacervate droplets alter enzyme kinetics. **T.D. Tang**
- 9:50** Intermission.
- 10:05** **4.** RNP granules in health and disease. **r. parker**, B. Van Treeck, T. Matheny, A. Khong, D. Tauber, G.A. Tauber, J. Burke, E. Lester, N. Ripin, T.N. Huynh
- 10:40** **5.** RNA controls a switch-like liquid phase transition of low-complexity protein domains. **P. Banerjee**
- 11:15** **6.** Phase transition drives telomere clustering. **H. Zhang**, M. Liu, C. Aonbangkhen, D.M. Chenoweth, R. Greenberg, M. Lampson

SECTION B

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 6

Early Career Investigators in Biological Chemistry

P. Bevilacqua, M. D. Distefano, *Organizers*
M. E. Farkas, *Presiding*

- 8:00** **7.** Biophysical insight into binding of Chlorin p_6 to Sudlow's site II of human serum albumin. **S. Patel**
- 8:20** **8.** Mapping the oxysterol interactome. **A.E. Ondrus**
- 8:40** **9.** HPLC-based method for the analysis of whole-cell sialic acids. **S.M. Levonis**, H. Kim, S.S. Schweiker

- 9:00** **10.** Targeting Dengue virus replication through pharmacologic modulation of ER proteostasis pathways. **L. Plate**, K. Almasy
- 9:20** **11.** Structural disruption of the amyloid- peptide induced by small molecules through nonspecific binding. **C. Liang**
- 9:40** **12.** Small molecule modulation of circadian rhythms in cancer cells. **M.E. Farkas**
- 10:00** **13.** Tryptophan-zippered 'Trojan horse' peptides with anti-tuberculosis specific activity. **A. Simonson**, A. Mongia, M. Aronson, T. Goralski, K. Keiler, **S.H. Medina**
- 10:20** **14.** Structure-performance relationships in cooperative biocatalysis by multi-enzyme assemblies displayed on cell surface. **F. Wen**
- 10:40** **15.** Hydrogen sulfide: Development of selective probes and useful donors through molecular design. **J.C. Lukesh**
- 11:00** **16.** Providing a molecular level view of active DNA demethylation using designer chromatin. **J. Sczepanski**, C. Deckard

Nanotechnology & Single Cell Analysis in Biology & Medicine

Nanoscience, Biology & Medicine

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

Origins & Future of Metabolite & Small Molecule Identification

Sponsored by ANYL, Cosponsored by BIOL, BIOT and MEDI

CRISPR/Gene Editing & RNAi: Utilization for Enhanced Crop Production

Sponsored by AGRO, Cosponsored by AGFD and BIOL

Characterization of Plastics in Aquatic Environments

Sponsored by POLY, Cosponsored by ANYL, BIOL, CEI, ENVR, I&EC, PMSE and PRES

Measuring Protein Conformations & Folding Inside the Cell

Sponsored by ANYL, Cosponsored by BIOL, BIOT and MEDI

SUNDAY AFTERNOON – BIOL

SECTION A

Marriott Marquis San Diego Marina

Marriott Grand Ballroom Section 5

Gordon Hammes Award Lecture

P. Bevilacqua, M. D. Distefano, *Organizers*

A. Schepartz, *Presiding*

- 1:00** Introductory Remarks.
- 1:05** **17.** Sequence conservation and information analysis provide insight into RNA adaptation. **K.A. Leamy**, N. Yennawar, P. Bevilacqua
- 1:20** **18.** Structure elucidation of colibactin and its DNA interstrand cross-link product. **J. Crawford**
- 2:05** **19.** Synthetic biology approaches to bioorthogonal chemistry. **M. Chang**
- 2:50** **20.** Monitoring translation in space and time with ribosome profiling. **J. Weissman**
- 3:35** Introduction of Awardee.
- 3:40** **21.** Molecular machines that make membranes. **D.E. Kahne**

SECTION B

Marriott Marquis San Diego Marina

Marriott Grand Ballroom Section 6

Graduate Student & Postdoctoral Fellow Symposium

P. Bevilacqua, *Organizer*

M. D. Distefano, *Organizer, Presiding*

- 1:00** **22.** Single-chain synthetic glycolipids: Self-assembly properties and applications to artificial cell development. **A. Bhattacharya**, N.K. Devaraj
- 1:15** **23.** Small molecules for functional protein depalmitoylation. **A. Rudd**, R. Brea, N.K. Devaraj
- 1:30** **24.** *De novo* all-atom self-assembly of Alzheimer's A β 25-35 dimers in a lipid bilayer. **A. Smith**, D.K. Klimov
- 1:45** **25.** New tools for sensitivity-enhanced in-cell NMR spectroscopy. **B. Lim**, B. Ackermann, G. Debelouchina

- 2:00** **26.** Bioluminescent studies of quinoline-based amino analogs of firefly luciferin. **B. Huta**, T. Southworth, B.R. Branchini
- 2:15** **27.** Synthetic α -helical peptidomimetic for substoichiometric modulation of membrane bound IAPP aggregation. **D. Maity**, A. Hamilton
- 2:30** **28.** Phosphinate-based rhodol/fluorescein derivatives and their biological application. **Y. Fang**, X. Zhou, C.I. Stains
- 2:45** **29.** Targeted protein degradation as a tool to probe non-kinase roles in myeloid leukemias. **G. Burslem**, A. Schultz, D. Bondeson, J. Song, C. Eide, S. Savage, J. Hines, B. Druker, C.M. Crews
- 3:00** **30.** Probing interactions in methyllysine reader proteins using genetic code expansion. **K.M. Kean**, K.N. Lamb, L.I. James, M. Waters
- 3:15** **31.** Biochemical characterization of cyclopentenyl uracil analogues: Application in the combination antiviral therapy. **Q. Liu**, C. Khosla
- 3:30** **32.** Analysis of pathways from ATCC 31433 and ATCC 31363, two Burkholderiaceae producers of Bulgecin A and sulfazecin-type monobactams. **M. Horsman**, S. Mobashery
- 3:45** **33.** Development of ultrasensitive fluorescence-quenched probes for monitoring lysosomal glycosidase activity in live cells. **R.A. Ashmus**, S. Cecioni, S. Zhu, M.C. Deen, D.J. Vocadlo
- 4:00** **34.** Active site labeling of fatty acid and polyketide-derived acyl-carrier protein transacylase domains. **T.D. Davis**, J.M. Michaud, M.D. Burkart
- 4:15** **35.** Anti-biofilm activity of nanoparticles via self-assembly with bacterial amyloid proteins. **Y. Wang**, N. Kotov, A. Violi, J. VanEpps
- 4:30** **36.** Activation of p66^{shc} in the heart subjected to ischemia/reperfusion injury. H. Xiong, F. McGowan, Jr., **H. He**
- 4:45** **37.** Development of an activity-based probe for cyclooxygenase-2 (COX-2). **A. Yadav**, C.J. Reinhardt, J. Chan

Origins & Future of Metabolite & Small Molecule Identification

Sponsored by ANYL, Cosponsored by BIOL, BIOT and MEDI

Characterization of Plastics in Aquatic Environments

Sponsored by POLY, Cosponsored by ANYL, BIOL, CEI, ENVR, I&EC, PMSE and PRES

SECTION A

San Diego Convention Center

TBD

Current Topics

P. Bevilacqua, M. D. Distefano, *Organizers*

6:30 - 8:30

38. Activation of orotidine 5'-monophosphate decarboxylase by interactions between substrate or activator ribosyl hydroxyls and the side chains from Asp 37 and T100'. J.R. Cristobal, **J.P. Richard**, T.A. Brandao

39. Chemical probes of histidine phosphatase activity. **B.S. McCullough**, A.M. Barrios

40. Modeling of zwitterionic molecule dynamics and their role in protein stabilization. **E. Fazelpour**, C.J. Fennell, A. Erfani, C. Aichele

41. Towards the development of a real-time insulin biosensor: Engineering the insulin receptor. **S. Sen**, G. Speciale, K.N. Gabriel, E.M. Crawley, K. Safronyuk, C.A. Totoiu, J.N. Pham, S. Majumdar, E.L. Botvinick, G.A. Weiss

42. Anion specific effect on protein. **W. Yao**, B.C. Gibb

43. Functionalized spirocyclic heterocycle synthesis and biological evaluations. **K.S. Huang**, **A. Gray**, **J. Mar**, A. Ramsay, **S. Mawugbe**

44. Exosome nanoencapsulation: Bioinspired coating for advanced cancer therapy. **S. Kumar**

45. Molecular origin of dual functionalities of fluorescent RXR agonists, CU-6PMN, which would be a key element for a high-throughput screening system of RXR ligands based on fluorescence intensity assay. **M. Kawasaki**, S. Nakano, T. Motoyama, S. Yamada, M. Watanabe, M. Fujihara, H. Tokiwa, H. Kakuta, S. Ito

46. Optimization of the benzyl moiety in 2-pyridone amins as HIV integrase strand transfer inhibitors (InSTIs). **R. Ferguson**, T. Yu, Y. Zhang, T. Graham, W. Liu, S.T. Waddell, A.W. Stamford, A.M. Walji, I.T. Raheem, J.S. Wai, P.J. Coleman, A. Verras, J. Sanders, M. Xu, J. Grobler, J. Schreier

47. Clickable glutathione approach to identify protein glutathionylation under ischemic stress. **M. Yapa Abeywardana**, G. VanHecke, Y. Ahn

48. Withdrawn

49. Probing the role of the zinc linchpin motif in the DNA repair glycosylase MUTYH. **C. Khuu**, N. Nunez, S.S. David

50. Excision of oxidatively damaged bases in G-quadruplexes by the DNA glycosylases NEIL1 and NEIL3. **E.R. Lotsof**, S. Conlon, B.M. Anderson-

Steele, K.M. Mifflin, A.M. Fleming, C.J. Burrows, S.S. David

51. Multifunctional protein materials based on recombinant protein engineering for anti-inflammatory skin disease. **T. Sha**, S. Kim, Y. Kim

52. Investigation of the origin of strong physisorption between MPA-coated ZAIS{(ZnxAgylnz)S2} and albumin proteins. **Y. Lee**, H. Seo, S. Sul, J. Park, S. Lee, Y. Kim, J. Jung

53. RiboPCR using a cross-chiral RNA polymerase ribozyme. **G. Bare**

54. Steady-state kinetic analysis of the bovine heart mitochondrial enzymes. **D. Kim**, E. Ko, M. Choi, S. Shin

55. Proline-rich peptide inhibitors of sickle cell polymerization. **B.B. Brennan**, L. Steenberge, N. MacDonald, Z. Fletcher

56. Exploring interactions between chromatin and essential chromatin remodeling complex *in vivo*. **S. Chaudhry**, B. Wilkins

57. Role of protamine phosphorylation on DNA packaging and stability in reconstituted sperm chromatin. **E.I. Oikeh**, J.E. Derouchey

58. Investigation on the relationship between cellular uptake efficiency and cytotoxicity of cell penetrating peptide by systematic sequence modulization. **H. Bae**

59. Bypass electron transfer pathways in Co²⁺-loaded 6His-tagged Ca²⁺-depleted MauG. **S. An**, Y. Moon, S. Shin, M. Choi

60. Spatially organized pattern recognition receptor tri-agonists: NOD2 agonist in combination with two TLR agonists. **N. Naorem**, S. Manna, A. Esser-Kahn

61. Lysosomal probing with sensitive and stable fluorescent LysoProbes. **M.S. Nyansa**, L. Bi

62. Dynamic profiling of human RNA decapping protein hDcp2 reveals the regulation of RNA stability by a *cis*-regulatory motif. **Y. Luo**, J. Schofield, M. Simon, S. Slavoff

63. Withdrawn

64. Palmitoylation of the insulin receptor. **J.C. Merritt**, L.R. Frost

65. Analysis of the apo-AI propeptide. **Z. Mitchell**, L.R. Frost

66. Development of cassette-type antibody via combination of supramolecular self-assembly of coiled-coil protein and scFv. **H. Ji**, M.S. Zafar, Y. No, Y. Kim

67. Using lipidomics to identify biomarkers for hyperglycemic onset breast cancer. N. Devanathan, **A.C. Kimble Hill**

68. Identification and characterization of new RNA tetraloop families. **M. Adams**, K.E. Richardson, C.C. Kirkpatrick, D.W. Gohara, B. Znosko

- 69.** Thermodynamics of iron(II) binding to human carbonic anhydrase II. **Z. Fokakis**, J.P. Emerson, K.D. McConnell, D. Wilson
- 70.** Making DNA from RNA: Optimizing the reverse transcriptase activity of an evolved ribozyme. **N. Setterholm**, G.F. Joyce
- 71.** Dysfunctional cellular signaling in Noonan syndrome and cancer. **A. Migliori**, C. Neale
- 72.** Leaving groups or substituents effects on DNA interstrand cross-link formation induced by binaphthalene analogues. **Q. Zhang**, Z. Lin, X. Peng
- 73.** Computational investigation of the mutant p53 DNA-binding domain through Markov state modeling. **M. Rosenfeld**, E. Pécora de Barros, O. Demir, R.E. Amaro
- 74.** Minimal eukaryotic translation system for studies of FMRP. **A. Maloney**, S. Joseph
- 75.** Destabilization of ALS-variant SOD1 via metal transfer to wild-type SOD1. **C.T. Zahler**, K.M. Baumer, B.F. Shaw
- 76.** Coral's response to climate change: Characterization of coral's metabolome under varied temperature and pH conditions. **K. Gubsch**, T. Schock
- 77.** DNA demethylation in reconstituted systems: Effects of higher order chromatin structure on thymine DNA glycosylase. **C.E. Deckard**, J. Sczepanski
- 78.** Chemoenzymatic *in vitro* synthesis of phospholipids. **S. Khanal**, N.K. Devaraj, M.D. Burkart
- 79.** Synergetic effect of zinc pyrithione with or without selective antibiotics on the growth of *Escherichia coli* and *Staphylococcus aureus*. **D. Yagnik**, E. Loizidou, A. Shah
- 80.** Developing novel labeling techniques for the study of proteins. **J. Flores**, N.K. Devaraj
- 81.** Harnessing the anti-cancer natural product nimbolide for targeted protein degradation. **J.N. Spradlin**, X. Hu, T.J. Maimone, D. Nomura
- 82.** Bacterioferritin from *Pseudomonas aeruginosa* PAO1 is assembled from two distinct subunits. **H. Yao**, A. Soldano, S. Lovell, M. Rivera
- 83.** Systematic identification of allosteric inhibition sites on protein tyrosine phosphatases. **R.M. Seifert**, A.C. Bishop
- 84.** Allosteric-site residues govern the stabilities of classical protein tyrosine phosphatase domains. **M.T. Yarnall**, A.C. Bishop
- 85.** Proton couplings of coenzyme Q across membrane mimics. **L. Nguyen**, C. Mao, H. Tavassol
- 86.** Determining the mechanism of activation of linked toll-like receptor agonists synergies. **J. Ajit**, A. Esser-Kahn
- 87.** Design, synthesis, and evaluation of small molecule PROTACs to induce ERK degradation. **C. Massaro**, T. Kauod, K. Dalby
- 88.** Blockade of prostaglandin D2 glyceryl ester catabolism by carboxylesterase 1 inhibitors enhances the anti-inflammatory effects of this lipid mediator. **A. Borazjani**, H. Scheaffer, B. Szafran, M. Ross
- 89.** Effects of stress on hormones. **V. Ngongang**, M. Hugh-Tay
- 90.** Re-engineering a natural product, apocynin, into an NADPH oxidase inhibitor. **P.P. Senevirathne**, H. Zhu, M. Edward
- 91.** Human glutathione synthetase: E-loop effect on catalysis. **L. Haynes**, B.L. Ingle, H. Pham, A. Furgang, T.R. Cundari, M.E. Anderson
- 92.** Small molecule inhibitors of the BfrB:Bfd interaction affect *Pseudomonas aeruginosa* growth by dysregulating iron homeostasis. **A. PUNCHI Hewage**, H. Yao, K. Gnanasekaran, S. Lovell, R.A. Bunce, S. Phaniraj, B.R. Peterson, M. Rivera
- 93.** Disruption of iron homeostasis impairs *Pseudomonas aeruginosa* biofilms. **A. Soldano**, M. Rivera
- 94.** Galactosylated nanovesicles for liver targeting. **M. Johnson**, A. Bhattacharya, R. Brea, N.K. Devaraj
- 95.** Effects of additives and aging on the efficacy of antimicrobial ionic liquids. **B. Maier**, R. Hensley, J. Greene, S. Shuput, D. Fox, A.T. Koppisch, **R.E. Del Sesto**
- 96.** Role of dissolved oxygen and albumin in indocyanine green photobleaching. **E.D. Clutter**, L. Chen, R. Wang
- 97.** Probing pantetheine interactions within bacterial carrier protein systems: New synthetic tool. **B. Sierra**, K. Charov, J.J. La Clair, M.D. Burkart
- 98.** Effect of deuterohemin-AlaHisThrValGluLys on purine metabolism in the perfused mouse heart subjected to ischemia/reperfusion injury. **K. Luo**, T. Meng, H. He
- 99.** The contribution of hops to the effects of beer on cancer cell growth. **A. Gonzales**
- 100.** Electrokinetic mixing (EKM) for improving the kinetics of biomedical and bioanalytical applications in electrode-embedded multiwell plates. **E. Yasun**, M. Mezić, I. Mezić
- 101.** Spider prey-wrapping silk is an α -helical coiled-coil / β -sheet hybrid nanofiber. **D. Stengel**, B. Addison, D. Onofrei, G.P. Holland
- 102.** Synthesis and application of multiresponsive nanogels by RAFT polymerization-induced self-assembly in water. **C. Luo**

103. Effect of hypoxia chemically induced by cobalt chloride on catecholamine biosynthesis in dopaminergic MN9D cell. **J. Adjei**, F. Jafar, V.Q. Le

104. Hierarchical supramolecular structure design by chemical-induced self-assembling peptide building blocks. **D. Park**, E. Kang, Y. Kim

105. Study of behaviour of charged particle-polymer interactions. **K. Nuti**

106. Suppression of oxidative stress by Deuterohemin-AlaHisThrValGluLys in perfused mouse heart subjected to ischemia/reperfusion injury. **T. Meng**, K. Luo, H. He

107. Targeting immune checkpoint inhibitor PD-L1/PD-1 axis via small molecules discovered by artificial intelligence. C. Laggner, K. Kim, R. Turner, R.G. Moore, **R. Singh**

108. Novel nitroxide derivatives combined with low-level laser irradiation for the treatment of acute limb ischemia/reperfusion injury. **C. Hensley**, L. Bi

109. Determining the roles of amino acids that control substrate-induced conformational changes in DNA damage response polymerase DinB. **J. Nasser**, H. Stern, P.J. Beuning

110. NanoLC/MS/MS profiling of advanced glycation end products (AGE) PTM on MHC-II molecules and components of antigen processing pathway in diabetes. **C.C. Clement**, M.P. Negroni, L. Stern, L. Santambrogio

111. Optical control of a nuclear hormone receptor with a photohormone. **K. Hinnah**, J. Morstein, D. Trauner

112. Glutathione-responsive photoacoustic imaging for targeted-drug delivery. **M. Lucero**, J. Chan

113. Salinomycin modulates antitumor immune response by repolarized tumor-associated macrophages toward M1 phenotype. **h. shen**

114. Construction of two-input logic gates using transcriptional interference. A. Escalas Bordoy, **N. O'Connor**, A. Chatterjee

115. On the brink of lability: Stabilization of the nitrogenase P-cluster by a redox-switchable ligand. **H.L. Rutledge**, J. Rittle, L. Williamson, W.A. Xu, F.A. Tezcan

116. F-containing retinoid X receptor (RXR) partial agonist F-CBt-PMN whose tissue transferability is affected by coadministration of another RXR ligand. **Y. Takamura**, O. Shibahara, M. Watanabe, M. Fujihara, M. Akehi, T. Sasaki, H. Kakuta

117. Synthesis and activity spectra of human antimicrobial peptides. **J. Albin**, B.L. Pentelute

118. Conformational activation promotes CRISPR-Cas12a catalysis and resetting of the endonuclease activity. **N. Hatzakis**, S. Stella, P. Mesa, J. Thomsen, B. Paul, P. Alcon, S.B. Jensen, B. Saligram, M.E. Moses, G. Montoya

119. Synthetic cells synthesize therapeutic proteins inside tumors. **A. Schroeder**

120. Detection of cathepsin B activity with caged melanin precursors for photoacoustic imaging. **S. Lokugama Widanelage**, M.D. Pagel

121. Structure and function of yeast pseudouridine synthase 7. **M. Purchal**, R. McNassor, H. Sharma, T. Khan, K. Koutmou, M. Koutmos

122. Tuning the native conformation of amyloid- β by photochemical oxidation. B. Jiang, C. Pennington, R. Prabhakar, **A.A. Marti**

Biosensing: New Strategies & Latest Development

Sponsored by ANYL, Cosponsored by BIOL, BIOT and MEDI

Nanozymes for Bioanalysis & Beyond

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MONDAY MORNING – BIOL

SECTION A

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 5

Frontiers in Interdisciplinary Research: New Paradigms for Integration of Theory & Experiment

Cosponsored by COMP, ORGN and PHYS
P. Bevilacqua, M. D. Distefano, *Organizers*
D. M. York, *Organizer, Presiding*
A. Boal, *Presiding*

- 8:30** Introductory Remarks.
- 8:35** **123.** New experimental approaches to understand control of reaction outcome in iron(II)- and 2-(oxo)-glutarate-dependent halogenases. **A. Boal**
- 8:55** **124.** Understanding the protein's role in substrate positioning and reactivity with simulation: Case of SyrB2/SyrB1. **H.J. Kulik**, R. Mehmood
- 9:15** Q & A.
- 9:25** **125.** An integrated computational and experimental strategy to explore APOBEC-catalyzed mutation. **R.E. Amaro**
- 9:45** **126.** Development of chemical probes to explore APOBEC-catalyzed mutation: An integrated experimental and computational approach. **D.A. Harki**
- 10:05** Q & A.
- 10:15** Intermission.

- 10:30 **127.** Tackling challenging targets in innate immune pathways with integrated biophysics and simulation. **H. Soutter**, I. Kolossvary, K. Marino, S. Sparks, H. Xu, W. Sherman
 11:10 Q & A.
 11:20 Panel Discussion.

SECTION B

Marriott Marquis San Diego Marina
 Marriott Grand Ballroom Section 6

Mid-Career Investigators in Biological Chemistry

P. Bevilacqua, M. D. Distefano, *Organizers*
 W. C. Pomerantz, *Presiding*

- 8:45 Introductory Remarks.
 8:50 **128.** Linking genes to molecules in lichen fungi: Challenges with heterologous expression. **J.L. Sorensen**
 10:00 Intermission.
 10:15 **129.** Acyl carrier protein crosslinking in fatty acid and polyketide synthases. **M.D. Burkart**
 10:50 **130.** Design of selective ligands for bromodomain-containing proteins using protein-observed ¹⁹F NMR. **W.C. Pomerantz**
 11:25 **131.** Integrating ligand receptor interactions and *in vitro* evolution for streamlined discovery of artificial nucleic acid ligands against T-cell receptor-CD3 complex in human T-cells. **P. Mallikaratchy**

Nanotechnology & Single Cell Analysis in Biology & Medicine

Nanoscience

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

Future of Biomacromolecules at a Crossroads of Polymer Science & Biology

Synthetic Cells

Sponsored by POLY, Cosponsored by BIOL, CARB, CELL, COLL, ENVR, MEDI, PHYS and PMSE

2019 ACS International Award for Research in Agrochemicals: Advances in the Physiology & Biochemistry of Insect Control

Sponsored by AGRO, Cosponsored by AGFD, BIOL, MEDI, POLY and PROF

SECTION A

Marriott Marquis San Diego Marina
 Marriott Grand Ballroom Section 5

Frontiers in Interdisciplinary Research: New Paradigms for Integration of Theory & Experiment

Cosponsored by COMP, ORGN and PHYS
 P. Bevilacqua, M. D. Distefano, *Organizers*
 A. Boal, D. M. York, *Organizers, Presiding*

- 1:10 Introductory Remarks.
 1:15 **132.** Water bridges conduct sequential proton transfer in photosynthetic oxygen evolution. **U. Brahmachari**, J. Gontheir, C.D. Sherrill, **B.A. Barry**
 1:35 **133.** Atomic level characterization of millisecond-time scale protein motions through a combined molecular simulations and NMR approach. **J. Juarez-Jimenez**, A. Gupta, G. Karunanithy, A. Mey, C. Georgiou, H. Ioannidis, A. De Simone, P. Barlow, A. Hulme, M. Walkinshaw, A.J. Baldwin, **J. Michel**
 1:55 **134.** Combining experiments with theory to gain insight into ribozyme catalysis. **P. Bevilacqua**
 2:15 **135.** Evaluating hydrogen bonding to the nucleophilic 2'OH in ribozymes as a driving force for catalysis. **A.J. Veenis**, S. Hammes-Schiffer, P. Bevilacqua
 2:35 **136.** Mechanistic strategies in ribozymes and DNA polymerases. **S. Hammes-Schiffer**
 2:55 Q & A.
 3:05 Intermission.
 3:20 **137.** Convergence of theory and experiment defines the catalytic mechanism of the VS ribozyme. **A. Ganguly**, B. Weissman, D.M. York, **J.A. Piccirilli**
 3:40 **138.** Theory and experiment converge to define the active site configuration and catalytic mechanism of the largest known nucleolytic ribozyme. **D.M. York**
 4:00 **139.** RNA-cleavage by DNA and RNA enzymes. **S. Ekesan**, D.M. York
 4:20 Q & A.
 4:30 Panel Discussion.

SECTION B

Marriott Marquis San Diego Marina
 Marriott Grand Ballroom Section 6

Mid-Career Investigators in Biological Chemistry

P. Bevilacqua, M. D. Distefano, *Organizers*
 A. Miller, *Presiding*

- 1:00 Introductory Remarks.

MONDAY EVENING – BIOL

SECTION A

San Diego Convention Center

TBD

Sci-Mix

P. Bevilacqua, M. D. Distefano, *Organizers*

8:00 - 10:00

49, 50, 55, 57, 70, 72, 87. See Previous Listings.

179, 180, 182, 186, 187, 190, 199, 211, 220, 223,

226, 228, 254. See Subsequent Listings.

TUESDAY MORNING – BIOL

SECTION A

Marriott Marquis San Diego Marina

Marriott Grand Ballroom Section 5

Recent Developments in Structural Biology

Cosponsored by MEDI

P. Bevilacqua, M. D. Distefano, C. Strickland, *Organizers*

C. Strickland, *Presiding*

8:00 Introductory Remarks.

8:05 **145.** Hydrogen-deuterium exchange in large complexes: How big can we go and what can we learn?. **E.A. Komives**

8:40 **146.** Studying the molecular organization and function of cells using cryo-electron tomography. **D. Nicastro**

9:15 **147.** Supporting drug discovery and research at Genentech with cryo-EM. **C. Ciferri**

9:50 Intermission.

10:05 **148.** MicroED: Conception, practice, and future opportunities. **T. Gonen**

10:40 **149.** Transient expression of monoclonal antibody and bispecific fragments, and fragment/antigen complexes for pharmaceutical discovery research. **R. Iyer, J. Harlan, K. Walter**

11:15 **150.** Enabling technologies in structural biology for drug discovery. **S.M. Soisson**

11:50 Concluding Remarks.

SECTION B

Marriott Marquis San Diego Marina

Marriott Grand Ballroom Section 6

Global Health: Biology & Chemistry of Waterborne Diseases

Cosponsored by MEDI

F. Calderón, *Organizer*

- 1:05 **140.** Genetically encoded photosensitizer protein facilitates the rational design of a miniature photocatalytic CO₂ reducing enzyme. **J. Wang**
- 1:40 **141.** Substrate activation by tuning of pK_as in flavin-dependent aromatic hydroxylases. **W. Pitsawong, P. Chenprakhon, T. Dhammaraj, D. Medhanavyn, J. Sucharitakul, P. Chaiyen, A. Miller**
- 2:15 **142.** Biochemical and structural characterization of targeted cytotoxic therapeutics for cancer. **C.E. Dann**
- 2:50 Intermission.
- 3:05 **143.** *In vitro* biochemistry of the TET enzymes and their application in a novel bisulfite-free, enzyme-dependent methylome sequencing methodology. **L. Saleh, M.J. Parker, A. Li, E. Tamanaha, R. Vaisvila, L. Williams, V. Ponnaluri, K. Marks, B. Sexton, L. Hunault, M.R. Brown, N.J. Ferraro, E.T. Dimalanta, T.B. Davis**
- 3:40 **144.** Exploring silicateins for the biocatalysis of organosiloxane chemistry. **L. Wong, S. Tabatabaei Dakhili, E.I. Sparkes, S.A. Caslin, N.L. Stephenson, R.A. Kettles**

2019 ACS International Award for Research in Agrochemicals: Advances in the Physiology & Biochemistry of Insect Control

Sponsored by AGRO, Cosponsored by AGFD, BIOL, MEDI and PROF

Nanotechnology & Single Cell Analysis in Biology & Medicine

Nanoscience

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Challenges & Opportunities Facing Early Career Scientists: Early Career Scientist Symposium

Sponsored by AGRO, Cosponsored by AGFD and BIOL

Future of Biomacromolecules at a Crossroads of Polymer Science & Biology

Tissue Engineering

Sponsored by POLY, Cosponsored by BIOL, CARB, CELL, COLL, ENVR, MEDI, PHYS and PMSE

C. C. Aldrich, *Presiding*

- 8:30** Introductory Remarks.
- 8:35** **151.** Identification and characterization of novel therapeutics for the treatment of cryptosporidiosis and shigellosis. **S. Arnold**, R. Choi, M. Hulverson, G. Whitman, L. Rabago, S. Shaheen, L. Barrett, W. Van Voorhis
- 9:20** **152.** From phenotypic screening to lead optimization: Calibr cryptosporidiosis drug discovery. **M.S. Love**, F. Beasley, R. Modukuri, R. Liu, M. Kumar, A. Woods, R. Jumani, C. Huston, S. Joseph, P. Schultz, A.K. Chatterjee, C.W. McNamara
- 10:05** **153.** Drug treatment algorithms for water-borne parasitic pathogens. **U. Singh**
- 10:50** Intermission.
- 11:00** **154.** Antibiotics as anti-filarial drugs. **J. Sakanari**
- 11:45** **155.** Development of a non-invasive lateral flow assay for monitoring onchocerciasis. **K.D. Janda**

Nanozymes for Bioanalysis & Beyond

Sponsored by ANYL, Cosponsored by BIOL and BIOT

2019 ACS International Award for Research in Agrochemicals: Advances in the Physiology & Biochemistry of Insect Control

Sponsored by AGRO, Cosponsored by AGFD, BIOL, MEDI and PROF

Biostimulants in Agriculture: Chemistry & Regulatory Aspects

Sponsored by AGRO, Cosponsored by BIOL, MEDI and TOXI

TUESDAY AFTERNOON – BIOL

SECTION A

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 5

Eli Lilly Award in Biological Chemistry

P. Bevilacqua, M. D. Distefano, *Organizers*
N. K. Devaraj, *Organizer, Presiding*

- 1:00** Introductory Remarks.
- 1:05** **156.** Drug discovery in academia: Anticancer research. **M.E. Jung**
- 1:45** **157.** Synthetic biology approaches to evolving new chemistry. **M. Chang**
- 2:25** Intermission.
- 2:45** **158.** Activity-based proteomics: Protein and ligand discovery on a global scale. **B. Cravatt**
- 3:25** **159.** Peering into the lipid world. **N.K. Devaraj**

SECTION B

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 6

ACS Infectious Diseases Young Investigators Award Symposium

Cosponsored by MEDI
P. Bevilacqua, M. D. Distefano, *Organizers*
C. C. Aldrich, *Organizer, Presiding*

- 1:00** Introductory Remarks.
- 1:05** **160.** Deciphering the human gut microbiota with chemistry. **E.P. Balskus**
- 1:50** **161.** Chemical proteomic tools to identify the targets of peptide signals at the host-microbe interface. **M. Wright**
- 2:30** **162.** Optimizing the immune response by targeting the Sts enzymes. **J.B. French**
- 3:10** Intermission.
- 3:20** **163.** Human milk oligosaccharides: Guiding temporal development of the gut flora. **S.D. Townsend**
- 4:00** **164.** Chemical tools for unraveling parasite biology. **E. Derbyshire**

Nanozymes for Bioanalysis & Beyond

Sponsored by ANYL, Cosponsored by BIOL and BIOT

Mass Spectrometry of Biomolecular Assemblies

Sponsored by ANYL, Cosponsored by BIOL, BIOT and MEDI

Exploration of the Nano-Bio Interface with Analytical Tools

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Biosensing: New Strategies & Latest Development

Sponsored by ANYL, Cosponsored by BIOL, BIOT and MEDI

Biostimulants in Agriculture: Chemistry & Regulatory Aspects

Sponsored by AGRO, Cosponsored by BIOL, MEDI and TOXI

TUESDAY EVENING – BIOL

SECTION A

San Diego Convention Center
TBD

Current Topics

P. Bevilacqua, M. D. Distefano, *Organizers*

6:00 - 8:00

- 165.** Flavonoids inhibit peroxidase activity of cytochrome c bound to cardiolipin. **M. Rice**, B. Wong, A. Sapse, **E.A. Korobkova**
- 166.** New covalent complexes of the acyl carrier protein with two of its partner enzymes shed light on protein-protein interactions in *Escherichia coli* fatty acid biosynthesis. **L.E. Misson**, J.T. Mindrebo, T. Davis
- 167.** Study of a new class of diaryl compounds as bacterial transcription inhibitors for antibacterial agent discovery. **S. Chan**, Y. Qiu, C. Ma
- 168.** Molecular determinants of liquid-liquid phase separation of intrinsically disordered proteins. **S. Mukhopadhyay**, A. Majumdar, P. Dogra, S. Maity, A. Joshi
- 169.** Reprogramming aryl acid adenylation domains for non-native building blocks. **F. Ishikawa**, A. Miyanaga, F. Kudo, T. Eguchi, G. Tanabe
- 170.** Interface analysis of the pyrrolyl carrier protein and adenylation domain in type II nonribosomal peptide synthetases. **J. Corpuz**, L. Podust, M. Jaremko, T. Davis, M.D. Burkart
- 171.** Microscopic characterization of cartilage load-bearing properties. **F. Horkay**, E. Dimitriadis, I. Horkayne-Szakaly, P. Basser
- 172.** Identification and visualization of protein-protein interactions in protein-protein complex structure. **J.C. Lee**, T. You, J. Zhang, R. Gutell
- 173.** Biodegradation of surgical polypropylene meshes. **P.L. Gamage**, Y. Ren, A.C. Wallace, A.K. Fiedler, M.C. Stefan, M.C. Biewer
- 174.** Genetic incorporation of L-dihydroxyphenylalanine (DOPA) biosynthesized by a tyrosine phenol-lyase and its applications. **S. Kim**, H. Lee
- 175.** Engineering a periplasmic binding protein for amino acid sensors with improved binding properties. W. Ko, **S. Kim**, H. Lee
- 176.** Characterization of molecular self-assemblies of thiamine diphosphate-dependent decarboxylases using ion mobility-mass spectrometry. **S. Mahajan**, I.K. Webb, M.J. McLeish
- 177.** Measuring thermodynamic parameters for cobalt (II) and high-valent species of cobalt on lysozyme. **S. Kim**, S. Shin, S. An, M. Choi
- 178.** Esterase B from a soil bacterium *Sphingobium* sp. SM42 exhibits a novel de-arenethiolase activity against cephalosporin antibiotics. **N. Toewiwat**, W. Whangsuk, P. Ploypradith, S. Mongkolsuk, S. Loprasert
- 179.** Engineering biocatalysts for selective C–C bond formation. **L.E. Zetzsche**, J. Yazarians, M.E. Hinze, A.R. Narayan
- 180.** Engineering translational machinery for a semi-synthetic organism. **R.J. Karadeema**, M.P. Ledbetter, F.E. Romesberg
- 181.** Development of small molecule inhibitors for rhomboid intramembrane proteases. **W.H. Parsons**, J.A. Crainic, C.L. Andrews, B.K. Sheehan
- 182.** Regulating the cancer cell cycle with splice modulators. **K. Krug**, M.D. Burkart
- 183.** Blueprint for *de novo* protein design and engineering. **A. Ouald Chaib**, Y. Kipnis, D. Baker, D. Hilvert
- 184.** Evaluating the efficacy of a novel oxime reactivator against nerve agent exposure. **H. Enright**, M. Malfatti, E. Kuhn, S. Hok, V. Lao, N. Be, T. Carpenter, B. Bennion, T. Nguyen, C.A. Valdez
- 185.** Simple preparation of decursin and decursinol angelate from *Angelica gigas* and their evaluations of chronic alcoholic fatty liver damage prevention. **K. Cho**, K. Kim, S. Chang, S. Oh, **J. Park**
- 186.** Using a fatty-acid-binding fluorescent-protein for oxygen-independent live-cell imaging of microbiomes. **H. Chia**, E. Marsh, J.S. Biteen
- 187.** *In vivo* efficacy study of reactive oxygen species (ROS) inducible anticancer agents. **M. Zaman**, H. Fan, A. Campbell, X. Peng
- 188.** Surface-functionalized exosomes for chemophotothermal combination therapy. T. Nguyen Cao, S. Kim, J. Kang, K. Jung, W. Rhee, Y. Ko, **M. Shim**
- 189.** Biophysical characterization and solution-state structure determination using NMR of J2 crystallin: Novel eye lens protein from the box jellyfish. **M. Unhelkar**, D. Khago, J.C. Bierma, S. Sengupta, R. Martin
- 190.** Targeting cross- β -sheet surfaces with small molecule imaging agents. **C.N. Hoffman**, J. Kuret
- 191.** Extraction of essential oil from spices through steam distillation. **M.A. Agyemang**
- 192.** Develop NanoBRET assay to examine small molecule effect on DNMT3A1-UHRF1 interaction in cancer cells. **S. Liu**, M.A. Perdigones, L. Chang, K. Venken, D. Young
- 193.** Using kinetics and small angle X-ray scattering to elucidate the allosteric regulation of SIRT1. **C. Cabrerros**, Y. Lee, J. Huynh, N. Wang
- 194.** Direct depalmitoylation of NRAS as a therapeutic strategy. **H. Vora**, M. Johnson, R. Brea, A. Rudd, N.K. Devaraj
- 195.** Development of a fluorescence polarization assay for the identification and evaluation of inhibitors at the Ω -loop region of the YAP-TEAD protein-protein interface (PPI). **W. Zhou**, Y. Li, J. Song, C. Li
- 196.** Synthesis and functional analysis of triply O-GlcNAc-modified α -synuclein (gT72/75/81). **S. Moon**, M. Pratt

- 197.** Elucidation of product release mechanism associated with structural changes in L-threonine 3-dehydrogenase. **T. Motoyama**, S. Nakano, Y. Yamamoto, H. Tokiwa, Y. Asano, S. Ito
- 198.** Development of clickable photoaffinity probes to identify outer membrane proteins in mycobacteria. **K. Biegas**, H.W. Kavunja, B. Swarts
- 199.** Radical SAM-dependent thioether installation in freyrasin. **T. Precord**, D. Mitchell
- 200.** Developing and optimizing the biological Glaser–Hay bioconjugation. **D.D. Young**
- 201.** Biochemical and molecular approaches to identify the specificity of long non-coding RNA and protein interactions. **A.C. Button**, C.A. McHugh
- 202.** Insulin photoactivated depots incorporating small tags for highly efficient light triggered solubility modulation. **K. Nadendla**, B.R. Sarode, S.H. Friedman
- 203.** S219V mutation on tobacco etch virus (TEV) protease improved its activity. **H. Nam**, D. Choi, S. Kwon, **K. Bang**, S. Shin
- 204.** Withdrawn
- 205.** Identification of the binding mode of diethyl p-nitrophenyl phosphate to phosphotriesterase. **L. El Khoury**, D.L. Mobley, D. Ye, S.L. Rempe
- 206.** Characterization of antimicrobial peptides using an *in vivo* inducible expression system. **R. Islam**, N. Muthunayake, C.S. Chow
- 207.** Withdrawn
- 208.** Using differential scanning calorimetry to study the thermostability of the diiron metalloenzyme AurF. **O.L. Murtagh**, K.D. McConnell, J.P. Emerson
- 209.** Insights from PTP1B/YopH chimeras into the importance of WPD-loop sequence for activity and structure in protein tyrosine phosphatases. **R. Shen**, K. Olsen, A. Tolman, S.J. Johnson, J. Loria, A.C. Hengge
- 210.** Role of zinc and copper in probiotic *Lactobacillus* species. **U. Huynh**, M. Zastrow
- 211.** Elucidating the mechanism of translation regulation by fragile x-related protein 1: Intrinsically disordered RNA-binding protein. **M. Edwards**, S. Joseph
- 212.** Optimization of replication, transcription, and translation in a semi-synthetic organism. **V. Dien**, A. Feldman, R.J. Karadeema, E.C. Fischer, F.E. Romesberg
- 213.** Antifungal defense molecules from bacterial symbionts of North American *Trachymyrmex* ants. **G. Scherer**, E. Van Arnam, K. Rao
- 214.** Novel ROS-initiated self-cyclizing antioxidant protects against UV damage by NOX inhibitor releasing process. **J. Liu**, M. Edward, H. Zhu, K.G. Earnest, G. Premnauth, K. Ana Luisa, S. Abdul Salam
- 215.** Molecular determinants of SHP2 activation. M.L. Bulos, **A.C. Bishop**
- 216.** Biarsenical-induced activation of engineered protein tyrosine phosphatases (PTPs). **B. Plaman**, W. Chan, A.C. Bishop
- 217.** Sonodynamic therapy of human breast cancer cells using nanoparticle-based sensitizers. **N. Wijesiri**, P. Zhang
- 218.** Parthenolide-alkyne pulldown studies to identify molecular targets in glioblastoma and acute myeloid leukemia cells. **K.F. Jones**, J. Widen, H. Skopec, D. Wang, J. Hexum, S. Rathe, D. Largaespada, D.A. Harki
- 219.** Characterization of beryllium ion complexation in the presence of biological buffers using isothermal titration calorimetry. **G.A. Ramirez**, R.K. Gary
- 220.** Next generation catch and release DNA decoys with photochemically responsive pyrimidine mimics. **S.A. Kennelly**, R.E. Eckermann, R. Moorthy, D.A. Harki
- 221.** Delineating KRAS4b HVR membrane association. **K. Podolsky**, N.K. Devaraj
- 222.** Reactive oxygen species enhanced chemotherapy by polyphenols nanomaterials. **Y. Dai**
- 223.** Structure-based drug discovery for HtrA1: Novel age-related macular degeneration target. **J. Jossart**, A. Eneim, K. Frausto, C. Laggner, J. Perry
- 224.** Production of L-asparaginase free of glutaminase and urease: Comparative study using submerged and solid state fermentation techniques. **A. Ashok**, K. Doriya, S.K. Devarai
- 225.** Targeting non-conserved cysteines for allosteric inhibition of SHP2. **L. Kao**, J.Y. Kim, A.C. Bishop
- 226.** Inhibition of protein-tyrosine phosphatases (PTPs) by chemically-induced dimerization. **S. Buck**, A.C. Bishop
- 227.** Guided neurite growth on functionalized carbon nanotube scaffolds. **E.L. Morgan**
- 228.** Direct selection of sandwich binding pairs with modified phage display technology. **A. Santos**, E.C. Sanders, A. Attar, S. Majumdar, S. Schlegel, A. Wheat, G.A. Weiss
- 229.** Synthesis and mechanism cytotoxic activity investigation of novel pyrimidine derivatives. **A.S. Bunev**, T. Tret'yakova
- 230.** Amyloid formation from partially and intrinsically disordered proteins. **M. Bhattacharya**, P. Dogra, S. Mukhopadhyay

231. Oxidative-cyclization inspired prodrug strategies to selectively release a PI3K inhibitor for cancer therapy. **H. Zhu**, R. Mishra, L. Yuan, S. Abdul Salam, J. Liu, M. Wunderlich, J. Garrett, J. Landero Figueroa, M. Edward

232. Thermodynamic characterization of naturally occurring RNA pentaloops. **M. Saon**, B. Znosko

233. Biogenic metallic nanoparticles: From microbiological biofactories to nanometric trojan horses. **D. Medina Cruz**, T.J. Webster

234. Photoactivated quantum dots as treatments for multidrug-resistant bacterial infection. **C.**

McCollum, K. Eller, C. Courtney, M. Levy, P. Nagpal, A. Chatterjee

235. Split-enzyme activation induced by target binding: Applicability to targeted drug delivery and *in vivo* molecular imaging. S. Hatch, A. Dixon, C. Nervig, S. Owen, **S. Kim**

236. Engineering transcriptional interference for NAND and NOR logic behaviors. **N. O'Connor**, A. Escalas Bordoy, A. Chatterjee

237. Stretching and aligning of DNA oligonucleotides by freezing and its application in bioconjugation. **J. Liu**

238. Comparison of force fields for structure and dynamics of carbonic anhydrase isozymes. **S.**

Kumar, D. Seth, P.A. Deshpande

239. Withdrawn

240. Computational perspective on the gating mechanism of β -ketoacyl-ACP synthases. **A. Patel**, J.T. Mindrebo, W.E. Kim, A. Chen, T.G. Bartholow, T. Davis, J.J. La Clair, J. McCammon, J.P. Noel, M.D. Burkart

241. *De novo* formation of natural liposomes in water. **L. Liu**

242. Development of a nanobiosensor for the detection of leptin; biomarker for obesity. **D.**

Abeyasinghe, N. Sirimuthu, R. Perera

243. Cloning strategies and feeding studies to investigate antibiotic biosynthesis. **J. Nicholas**, C. Horta, V.Z. Petukhova, M. Black, L. Sanchez, K. Watts

244. Evaluating amino acid specificity and intermodular interactions of a deconstructed nonribosomal peptide synthase. **G. Pinzon-Betancourt**, C. Cable, A. Chacon, M. Levine, J.P. Oza, K. Watts

245. Assessing and improving specificity of rhodium metallointerstors in targeting MMR deficient cancer. **S. Threatt**, T.W. Synold, J.K. Barton

246. Activating brown and beige adipose tissue with type II myosin small molecule activators. **G. Dempsey**, A. Li, D. Bernard, A. Stahl

247. Substrate requirements for DNA labeling by *E. coli* tRNA guanine transglycosylase. **E.M. Tota**, N.K. Devaraj

Future of Biomacromolecules at a Crossroads of Polymer Science & Biology

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WEDNESDAY MORNING – BIOL

SECTION A

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 5

Pfizer Award in Enzyme Chemistry

P. Bevilacqua, M. D. Distefano, *Organizers*

K. Yokoyama, *Organizer, Presiding*

8:45 Introductory Remarks.

8:50 **248.** Flexibility of ribonucleotide reductases revealed in many ways. **J. Stubbe**, C.L. Drennan, E. Brignole, B. Greene, D.G. Nocera, G. Kang, C. Cui, M. Bennati

9:30 **249.** Biosynthesis of the side-ring system of nosiheptide: Role of NosN, a class C radical S-adenosylmethionine methylase. B. Wang, J. LaMattina, E. Badding, L. Gadsby, T. Grove, S. Marshall, **S.J. Booker**

10:10 Intermission.

10:25 **250.** Radical SAM enzymes in the biosynthesis of sugar-containing secondary metabolites. **H. Liu**

11:05 **251.** Radical-mediated C–C bond formation in natural product and cofactor biosynthesis. **K. Yokoyama**, B.M. Hover, E.A. Lilla

SECTION B

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 6

Early Career Investigators in Biological Chemistry

P. Bevilacqua, M. D. Distefano, *Organizers*

E. V. Pletneva, *Presiding*

8:00 **252.** Drug target residence time affects pharmacokinetic profile and target occupancy over time. **K.S. Lee**, J. Yang, C. Ng, K. Wagner, B.D. Hammock

8:20 **253.** Molecular mechanism of off-target effects in CRISPR-Cas9. **G. Palermo**, C. Gravina Ricci, J.S. Chen, Y. Miao, M. Jinek, J.A. Doudna, J. McCammon

8:40 **254.** RNA-catalyzed polymerization of RNA, DNA, TNA, and ANA. **D.P. Horning**, K. Tjhung, S. Bala, J. Chaput, G.F. Joyce

9:00 **255.** Chemical approaches to illuminate the RNA epitranscriptome. **R. Kleiner**

- 9:20 **256.** mRNA modifications alter translation elongation and fidelity. D. Eyler, M. Franco, T. Khan, Y. Polikanov, **K. Koutmou**
- 9:40 **257.** Antibiotics from ants: Molecular defenses from specialized insect microbiomes. **E. Van Arnam**
- 10:00 **258.** Structure-based design estrogen related receptors α/γ dual agonists for the treatment of heart failure. **B.E. El-Gendy**
- 10:20 **259.** Effects of metal cations on mechanisms of nucleotide addition in DNA polymerase. **D. Roston**, Q. Cui
- 10:40 **260.** Structural characterization and binding studies of polar organizing protein Z from *Caulobacter crescentus* using NMR spectroscopy. **K. Varga**, C. Nordyke, H. Wang, G.R. Bowman
- 11:00 **261.** Structural and dynamic mechanisms of hijacking human phosphoinositide 3-kinase by nonstructural protein 1 of the 1918 Spanish flu virus. Q. Shen, B. Zhao, J. Byrnes, N. Savage, L. Yang, P. Li, **J. Cho**
- 11:20 **262.** Pausing by bacterial RNA polymerase: Mechanistic insights from structural and biochemical studies. **T.V. Mishanina**

Nanozymes for Bioanalysis & Beyond

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Future of Biomacromolecules at a Crossroads of Polymer Science & Biology

Delivery Systems

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Exploration of the Nano-Bio Interface with Analytical Tools

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Biostimulants in Agriculture: Chemistry & Regulatory Aspects

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WEDNESDAY AFTERNOON – BIOL

SECTION A

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 5

Covalent & Non-Covalent Dimers as Therapeutic Agents in Drug Discovery

Cosponsored by MEDI and ORGN

P. Bevilacqua, M. D. Distefano, *Organizers*

J. Cumming, D. Li, *Organizers, Presiding*

- 1:00 Introductory Remarks.
- 1:05 **263.** Antiviral drug discovery: Symmetry in the design of HCV NS5A replication complex inhibitors. **N.A. Meanwell**
- 1:40 **264.** Novel mechanism of S100A4 inhibition: Phenothiazine-induced protein oligomerization. V. Malashkevich, N.G. Dulyaninova, M. Brenowitz, J.M. Backer, S.C. Almo, **A. Bresnick**
- 2:15 **265.** Small molecule homo dimers mimic large peptide hormone and activate natriuretic peptide receptor A (NPRA) for the potential treatment of heart failure. **D. Li**, A. Hruza, B. Myers, J. Tata, Y. Xiong
- 2:50 Intermission.
- 3:10 **266.** Discovery of small molecule STING antagonists: Novel use of small molecule dimers to drug large protein pockets. **T. Siu**, M. Altman, G. Baltus, M. Childers, M. Ellis, H. Gunaydin, H. Hatch, T. Ho, J.P. Jewell, B. Lacey, C. Lesburg, B. Pan, B. Sauvagnat, G. Schroeder, S. Xu
- 3:45 **267.** Enhancing potency of AMPA receptor positive allosteric modulators through the design of dimeric compounds. **B. Pirotte**
- 4:20 **268.** Rational design & directed evolution of small protein dimers: Inhibiting Myc in cancer and PAI-1 in asthma. **J.A. Shin**
- 4:55 Concluding Remarks.

SECTION B

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 6

Graduate Student & Postdoctoral Fellow Symposium

M. D. Distefano, *Organizer*

P. Bevilacqua, *Organizer, Presiding*

- 1:00 **269.** Antibody drug conjugates as enhanced therapeutics against the drug resistant bacteria *Pseudomonas aeruginosa*. **C. Nervig**, S.C. Owen
- 1:15 **270.** Dynamics of Ash1L SET domain in the presence of inhibitors. **H. Li**, J. Deng, J. Grembecka, T. Cierpicki
- 1:30 **271.** Specificity in the mitogen activated protein kinase signalling cascades. **J.M. Torres**, B.E. Turk
- 1:45 **272.** Modulating selective glycation reactivity with short, linear peptides. **J. McEwen**
- 2:00 **273.** Withdrawn

- 2:15** 274. Exploring the dual properties of luminescent lanthanide complexes functionalized with singlet oxygen generators. **K. Johnson**, C.V. Rodrigues, M.O. Rodrigues, V.C. Lombardi, A. De Bettencourt Dias
- 2:30** 275. Activity-guided single cell enzyme mining. **K. Charov**, W.E. Kim, E. Becraft, J. Brown, W.H. Fenical, J.J. La Clair, R. Stepanauskas, M.D. Burkart
- 2:45** 276. Template-assisted click chemistry as a therapeutic strategy for myotonic dystrophy type 1 (DM1). **L. Hagler**, L. Luu, S.C. Zimmerman
- 3:00** 277. Very long chain fatty acids play a functional role during necroptosis. **L.R. Parisi**, N. Li, S. Sowlati-Hashjin, T. Nguyen, K.A. Carter, I.A. Berhane, S.R. Chemler, J. Lovell, S. Cologna, M. Karttunen, G. Atilla-Gokcumen
- 3:15** 278. Window into the black box of quorum sensing: New LuxR-type protein models for the investigation of ligand-receptor and receptor-DNA interactions *in vitro*. **M.J. Styles**, M.E. Boursier, S.A. Early, M.A. McEwan, T. Tuckolski, Y. Ge, H.E. Blackwell
- 3:30** 279. Fluorescent teixobactin analogue. **M. Morris**, M. Malek, M. Hashemian, J.S. Nowick
- 3:45** 280. Multidomain peptide hydrogel accelerates healing of full-thickness wounds in diabetic mice. **N. Carrejo**, A. Moore, T. Lopez Silva, D. Leach, I. Li, D. Walker, J.D. Hartgerink
- 4:00** 281. Indole nucleosides as a versatile scaffold for fluorophore development. **K. Passow**, D.A. Harki
- 4:15** 282. Discovering *de novo* peptide substrates for enzymes using machine learning. **W.E. Kim**, L. Tallorin, J. Wangj, S. Sahu, N.M. Kosa, P. Yang, M. Thompson, M.K. Gilson, P.I. Frazier, M.D. Burkart, N.C. Gianneschi
- 4:30** 283. Chemo-optogenetic control of cytoskeleton function. **X. Chen**, S. Petry
- 4:45** 284. Attribution of function to structure: Which FAD plays which role in bifurcating electron transfer flavoproteins? Spectroscopic, thermodynamic, and computational evidence. **N. Mohamed Raseek**, H. Duan, P. Hildebrandt, M. Mroginiski, A. Miller

Nanozymes for Bioanalysis & Beyond

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Future of Biomacromolecules at a Crossroads of Polymer Science & Biology

Biomaterials

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THURSDAY MORNING – BIOL

SECTION A

Marriott Marquis San Diego Marina

Marriott Grand Ballroom Section 5

Graduate Student & Postdoctoral Fellow Symposium

P. Bevilacqua, *Organizer*

M. D. Distefano, *Organizer, Presiding*

- 8:15** 285. Uncovering the chemoproteomic potential of azetidines. **R. McCloud**, T. Huang, K. Hsu
- 8:30** 286. Probing and exploiting the reactivity of C radicals for selective protein editing. **M. Imiolek**, B.G. Davis
- 8:45** 287. Elucidating glycogen biosynthesis through palladium-mediated enzyme control. **M.A. Gafitescu**, M. Bilyard, H. Bailey, L. Raich, T. Machida, J. Iglesias-Fernandez, S. Lee, C. Spicer, C. Rovira, W.W. Yue, B.G. Davis
- 9:00** 288. Structural dynamics in an intrinsically disordered subunit, PsbO, of the photosynthetic water oxidizing complex. **J. He**, U. Brahmachari, B. Barry
- 9:15** 289. *De novo* design of a mononuclear, unsaturated Fe^{II} active site in a supramolecular protein trimer. **A. Kakkis**
- 9:30** 290. Mechanistic investigation of terpenoid biosynthesis using non-natural substrates. **A.K. Gayen**, R. Hall, G.J. Williams
- 9:45** 291. *O*-acylated trehalose analogues for probing cellular processes and components in *Corynebacterineae*. **N. Banahene**, T.J. Fiolek, H.W. Kavunja, B.M. Swarts
- 10:00** 292. Photoswitchable PROTACs: Visible light activated degradation of the androgen receptor. **E. Fowler**, A. Hock, D. O'Donovan, J. Gorman, G. Fumagalli, R. Friend, D.R. Spring
- 10:15** 293. Thermodynamic and kinetic analysis of amicyanin biogenesis. **S. Jeoung**, S. Shin, M. Choi
- 10:30** 294. Investigation of substrate recognition and biosynthesis in microviridin pathways. **G. Li**

- 10:45 295.** Exploring composition of peptide loops to enhance biophysical properties of antibody fragments for cancer therapeutics. **J. Han**, T.J. Magliery
- 11:00 296.** Protective effect of thymosin alpha 1 on DSS induced colitis in mice by normalizing the gut microbiota and immune response. **O.P. Ifeoma**
- 11:15 297.** Extreme mechanical diversity of human telomeric DNA probed by single-molecule fluorescence-force spectroscopy. **J. Mitra**, M. Makurath, T. Ngo, A. Troitskaia, Y. Chemla, T. Ha
- 11:30 298.** Using of bio-layer interferometry to quantify protein-DNA interactions. **C.J. Weeramange**, M. Fairlamb, L. Swint-Kruse
- 11:45 299.** Controlling liquid-liquid phase separation of Antarctic toothfish crystallins through surface residue mutations. **J.C. Bierma**, K.W. Roskamp, A. Ledray, A. Kiss, C. Cheng, R.W. Martin

Glycans in Context

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THURSDAY AFTERNOON – BIOL

SECTION A

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 5

Graduate Student & Postdoctoral Fellow Symposium

M. D. Distefano, *Organizer*

P. Bevilacqua, *Organizer, Presiding*

- 1:00 300.** Enhancing cytotoxicity of antibody drug conjugates through co-administration of a potentiating antibody conjugate in an ovarian cancer model. **J.R. McCombs**
- 1:15 301.** Nanoencapsulation of Casiopein®, study of its anticancer biological activity and release *in vivo* and *in vitro*. **J.A. Flood**

- 1:30 302.** Gadolinium doping enhances the photoacoustic signal of synthetic melanin nanoparticles: Dual modality contrast agent for stem cell imaging. **J. Lemaster**
- 1:45 303.** Gating mechanism of β -ketoacyl-ACP synthases. **J.T. Mindrebo**, A. Patel, W.E. Kim, T.G. Bartholow, A. Chen, T.D. Davis, J.J. La Clair, J. McCammon, J.P. Noel, M.D. Burkart
- 2:00 304.** Comparison of PSMA levels in salivary glands of mice and rats. **J. Roy**, B. Warner, F. Basuli, K. Wong, A. Ton, J. Chiorini, P. Choyke, E. Jagoda, F. Lin
- 2:15 305.** Dissecting DNA polymerase at the single-molecule level. **K.N. Gabriel**, M. Turvey, C. Lau, K. Pugliese, S. Majumdar, P.G. Collins, G.A. Weiss
- 2:30 306.** Bioorthogonal chemistry approaches to the cellular imaging of PI3K δ inhibitors. **M. Rouah**, A. Rutkowska, Z. Henley, C. Jamieson
- 2:45 307.** Increasing the fluorescence turn-on of the nucleoside analogue 8-diethylamino-tC in duplex nucleic acids using DNA-RNA heteroduplexes. **M.B. Turner**, J. Ceja, B.W. Purse
- 3:00 308.** Structural and functional characterization of threonylcarbamoyl adenosine biosynthesis in bacteria. **N. Paranagama**, A. Luthra, S. Bayooz, Y. Jeon, D. Lyumkis, M.A. Swairjo
- 3:15 309.** Elucidating the role of histone H4 K20 methylation in chromatin compaction. **N. Elathram**, G. Debelouchina
- 3:30 310.** Structural and dynamical basis for the production of unsaturated fatty acids in *Escherichia coli*. **A. Patel**, G.J. Dodge, K. Finzel, J. McCammon, J.L. Smith, M.D. Burkart
- 3:45 311.** Development of fluorescent nucleosides for real-time measurements of single-stranded DNA cytidine deamination by APOBEC enzymes. **R. Moorthy**, J. Baur, S. Schmidt, M.E. Olson, D.A. Harki
- 4:00 312.** Biodegradability and surface engineering of fully metallic stent enabling controllable generation of reactive oxygen species for antirestenosis. **H. Seo**, J. Park, Y. Kim, M. Ok
- 4:15 313.** Developing methods for the discovery and validation of pre-miRNA-protein interactions. **S.L. Rosenblum**, D. Lorenz, T. Kaur, A.L. Garner
- 4:30 314.** Porphyrins: Gift of nature to eradicate cancer? Phototoxic effect on *Tetrahymena thermophila* and human skin carcinoma. **Z. Berhe**, E.C. Ojadi

Glycans in Context

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DIVISION OF BIOCHEMICAL TECHNOLOGY

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

SUNDAY MORNING – BIOT

Origins & Future of Metabolite & Small Molecule Identification

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Measuring Protein Conformations & Folding Inside the Cell

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SUNDAY AFTERNOON – BIOT

Origins & Future of Metabolite & Small Molecule Identification

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SUNDAY EVENING – BIOT

Biosensing: New Strategies & Latest Development

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Nanozymes for Bioanalysis & Beyond

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TUESDAY MORNING – BIOT

Nanozymes for Bioanalysis & Beyond

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Mass Spectrometry of Biomolecular Assemblies

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TUESDAY AFTERNOON – BIOT

Nanozymes for Bioanalysis & Beyond

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Mass Spectrometry of Biomolecular Assemblies

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Exploration of the Nano-Bio Interface with Analytical Tools

Sponsored by ANYL, Cosponsored by BIOL and BIOT

Biosensing: New Strategies & Latest Development

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WEDNESDAY MORNING – BIOT

Nanozymes for Bioanalysis & Beyond

Sponsored by ANYL, Cosponsored by BIOL and BIOT

Exploration of the Nano-Bio Interface with Analytical Tools

Sponsored by ANYL, Cosponsored by BIOL and BIOT

Biosensing: New Strategies & Latest Development

Sponsored by ANYL, Cosponsored by BIOL, BIOT and MEDI

WEDNESDAY AFTERNOON – BIOT

Nanozymes for Bioanalysis & Beyond

Sponsored by ANYL, Cosponsored by BIOL and BIOT

Study of Circulating, Cell-Free Biomarkers with Analytical Tools

Sponsored by ANYL, Cosponsored by BIOL, BIOT and MEDI

Biosensing: New Strategies & Latest Development

Sponsored by ANYL, Cosponsored by BIOL, BIOT and MEDI

THURSDAY MORNING – BIOT

Study of Circulating, Cell-Free Biomarkers with Analytical Tools

Sponsored by ANYL, Cosponsored by BIOL, BIOT and MEDI

Biosensing: New Strategies & Latest Development

Sponsored by ANYL, Cosponsored by BIOL, BIOT and MEDI

BMGT

DIVISION OF BUSINESS DEVELOPMENT AND MANAGEMENT

A. DeMasi, Program Chair

SUNDAY AFTERNOON – BMGT

SECTION A

San Diego Convention Center
Room 29D

Chemical Angel Network

Chemists Investing in Chemical Companies

Cosponsored by PROF and SCHB

Financially supported by CIEC

J. L. Bryant, S. S. White, *Organizers*

M. Vreeke, *Presiding*

- 1:30** Introductory Remarks.
- 1:35** **1.** Updates and news from the Chemical Angel Network (CaN) and its sixth year of supporting chemists and chemistry-based company creation. **S.H. White**
- 2:00** Company Presentations.
- 3:00** Investment Discussion.
- 3:30** Open Forum.
- 4:00** Concluding Remarks.

Pest Management Economics: Present & Future Considerations

Sponsored by AGRO, Cosponsored by BMGT

MONDAY MORNING – BMGT

Liquid Assets: The Business of Water

Sponsored by SCHB, Cosponsored by ANYL, BMGT and I&EC

MONDAY AFTERNOON – BMGT

SECTION A

San Diego Convention Center
Room 29D

Leadership Development: The ACS Commitment Now & for the Future

Cosponsored by PRES

J. L. Bryant, A. DeMasi, C. A. Duane, D. Mason, B. Maye, *Organizers*

L. K. Krannich, *Presiding*

- 1:30** Introductory Remarks.
- 1:45** **2.** Importance of investing in yourself: Argument for leadership development. **T.H. Lane**
- 2:15** **3.** From dream to reality: It took a village. K.M. Schulz, **M. Lester**
- 2:45** **4.** Who learns more: Instructor or students?. **B.A. Sawrey**
- 3:15** Intermission.
- 3:30** **5.** How Indiana section leaders forged a path to successfully serve the ACS. **C. Bodurow**
- 4:00** **6.** Leadership development: Differentiator and skills multiplier in industry (and elsewhere). **L.W. McQuire**
- 4:30** **7.** Enabling the professional development of ACS members into the future. **W.E. Jones**, A. Campbell
- 5:00** Panel Discussion.

TUESDAY MORNING – BMGT

Gerry Meyer: The First 100 Years

Sponsored by SCHB, Cosponsored by BMGT, CHED, ENFL, HIST and SCC

Mass Spectrometry of Biomolecular Assemblies

Sponsored by ANYL, Cosponsored by BIOT, BMGT and MEDI

SECTION A

San Diego Convention Center
Room 29B

**Collaborating for the Greater Good: What Works
& What Doesn't**

Cosponsored by PRES

J. L. Bryant, A. DeMasi, B. Maye, *Organizers*

J. Cho, D. Mason, *Presiding*

- 1:30** Introductory Remarks.
- 1:45** **8.** Industry-university partnering models. **A.M. Boccanfuso**
- 2:05** **9.** Industrial perspective on selection and establishment of strategic partnerships. **J.S. Witzeman**
- 2:25** **10.** One of the longest, single-corporation university-industry centers in the US: Mitsubishi Chemical Center for Advanced Materials at the University of California in Santa Barbara. **L.A. Edwards**
- 2:45** **11.** Creating and cultivating industry relations: Transformational industry partnerships at UNC-Chapel Hill. **J. Cho**

- 3:05** Intermission.
- 3:20** **12.** The co-op program in chemistry at Northeastern University: Century of success. **T.R. Gilbert**
- 3:40** **13.** Academic drug discovery research at Rutgers University, Piscataway, New Jersey. **D.J. Augeri**
- 4:00** **14.** Industry-academic collaborations: Moulder center experiment. **M. Abou Gharbia**
- 4:20** **15.** From the idea to the product: Industrial perspective on critical success factors. **M. Urmann**
- 4:40** **16.** Start-ups and the challenge of transitioning technology from academic laboratories to industrial processes and scale. **W.E. Jones, M. Sedam**
- 5:00** Panel Discussion.

Gerry Meyer: The First 100 Years

Sponsored by SCHB, Cosponsored by BMGT, CHED, ENFL, HIST and SCC

CARB

DIVISION OF CARBOHYDRATE CHEMISTRY

S. Sucheck, *Program Chair*

SUNDAY MORNING – CARB

SECTION A

San Diego Convention Center
Room 29C

Centennial Celebration of ACS Carbohydrate Chemistry: Chairs' Perspective

P. R. Andreana, *Organizer, Presiding*

- 8:55 Introductory Remarks.
- 9:00 1. One hundred years of basic carbohydrate science as growth in human experience: Personal applications to a spectrum of challenges. **J.R. Vercellotti**
- 9:25 Discussion.
- 9:30 2. One hundred years of carbohydrate science underpinning the worldwide sugar industry. **G. Eggleston**
- 9:55 Discussion.
- 10:00 3. Life after CARB chairmanship. **A.D. French**
- 10:25 Discussion.
- 10:30 Intermission.
- 10:45 4. Recognition of DNA and RNA with small, large and intermediate size molecules. **D.P. Arya**
- 11:10 Discussion.
- 11:15 5. Carbohydrate chemistry for RNA interference: Synthesis, structure, and biological activity of amide-linked RNA. **E. Rozners**
- 11:40 Discussion.
- 11:45 6. How sweet it is to work with sugars: Success story of carbohydrates conjugates of sugar-modified RNAs to make life-saving drugs. **M. Manoharan**
- 12:10 Discussion.

SUNDAY AFTERNOON – CARB

SECTION A

San Diego Convention Center
Room 29C

Centennial Celebration of ACS Carbohydrate Chemistry: Chairs' Perspective

P. R. Andreana, *Organizer, Presiding*

- 1:10 7. Nucleosides, sugars, synthesis, and funding: Rollercoaster ride through carboscience and the CARB Division. **D.C. Baker**
- 1:35 Discussion.
- 1:40 8. From carbohydrate chemistry to biology to sugar-based drugs. **W. Priebe**
- 2:05 Discussion.
- 2:10 9. Thio sugars, *exo*-cyclic enones, *spiro*-chromanones and activities within the CARB Division as components of a wonderful adventure. **Z.J. Witczak**
- 2:35 Discussion.
- 2:40 10. Conformational equilibria and dynamics of saccharides using circular statistics. **A.S. Serianni**
- 3:05 Discussion.
- 3:10 Intermission.
- 3:25 11. Incorporation of diverse sugars and diverse scientists into glycochemistry and the academy. **N.L. Pohl**
- 3:50 Discussion.
- 3:55 12. Fighting cancer with a sweet bullet: Development of glycoconjugate-based anticancer vaccines. **X. Huang**, X. Wu, U. Westerlind, M. Finn
- 4:20 Discussion.
- 4:25 13. Past and present carbohydrate chemistry vignettes from the Hanessian group. **S. Hanessian**
- 4:50 Discussion.
- 4:55 14. Synthesis of complex microbial glycan probes. **T.L. Lowary**
- 5:20 Discussion.
- 5:25 Concluding Remarks.

SECTION A

San Diego Convention Center

TBD

General Posters

S. J. Sucheck, *Organizer*

7:00 - 9:00

15. Synthesis of the antibody glycoform with a2,6-linked 3F^{ax}-Neu5Ac. **H. Lo**, L. Krasnova, S. Dey, T. Cheng, H. Liu, T. Tsai, K. Wu, C.Y. Wu, C. Wong
16. Phenols as nucleophiles in the oxidative deamination of *N*-acetyl neuraminic acid. **M.B. Hawsawi, A. Wickramasinghe**, D. Crich
17. Chemical synthesis of syndecan-4 glycopeptide bearing *O*-, *N*-sulfation, and aspartic acids utilizing sulfate ester strategy. **W. Yang**
18. Synthesis of xylosyl ribitol phosphate. **T. Tamura**, J. Tamura
19. Covalent inhibitors target O-GlcNAc transferase in cells. M. Worth, **A. Esteves Davila**, C. Hu, D. Fan, H. Li, D. Zhu, J. Jiang
20. Withdrawn
21. O-GlcNAcylation of α -synuclein forms ribbons that seed monomers into less pathological aggregates. **A. Balana**, S. Cortes, M. Horvath, K. Luk, A.B. Siemer, M. Pratt
22. Chemoenzymatic synthesis of a heparan sulfate glycopeptide mimetic and evaluation of its biological functions. **J. Gao**, Y. Xu, J. Liu, X. Huang
23. Efforts in the development of a metabolic chemical reporter specific for mucin-type glycosylation. **E. Jackson**, M. Pratt
24. Chemical synthesis of heparin-like, head-to-tail multimers. **J. Zhang**
25. α -Selective glycosidation of D-tagatofuranose using 3,4-O-isopropylidene protection. Y. Makura, **A. Ueda**, T. Matsuzaki, T. Minamino, M. Tanaka
26. Localization of growth factor binding and activity via glycocalyx engineering in embryoid bodies using glycosaminoglycan mimetics. **L. Laubach**
27. Formation of *spiro*-chromanones from dihydrolevoglucosenone. N. Jankowski, C. Hager, **Z.J. Witczak**, R. Bielski, D.E. Mencer
28. Preliminary evidence for reversible *O*-acetyl group migration at 9- and 8-carbon position in sialic acids. **Y. Ji**, A. Sasmal, W. Li, S. Srivastava, B. Wasik, H. Yu, S. Diaz, C. Parrish, X. Chen, A. Varki
29. Phase-transfer catalyzed one-pot functionalization of carbohydrates. **K. Kowalska**, H. Koroniak, L. Nordstroem
30. O-GlcNAc modification alters α -synuclein aggregation and neuronal toxicity. **A. Galesic**, P. Levine, A. Balana, M. Pratt
31. Degradation-resistant trehalose analogues block utilization of trehalose by hypervirulent *Clostridioides difficile*. **A. Stothard**, B. Wilson, Q. Dong, N. Danielson, J. Collins, P. Woodruff, R. Britton, B.M. Swarts
32. Chemical inhibition of glycosaminoglycan biosynthesis to suppress differentiation in murine embryonic stem cells. **M. Naticchia**, K. Godula, S. Verespy
33. Selective *in vivo* metabolic cell-labelling-mediated cancer targeting. H. Wang, K. Cai, **Y. Bo**, J. Cheng
34. Synthesis and biological evaluation of ellagic acid glycosides. **S.A. Chambers**, J.A. Gaddy, S.D. Townsend
35. Synthesis of fluorogenic trehalose and trehalose monomycolate analogues for the detection of mycobacteria. **D. Gepford**, B.M. Swarts, N. Banahene, J.M. Groenevelt, Y. Hsu, M. VanNieuwenhze
36. Development of toll-like receptor 7 ligand and α -mannose immobilized gold nanoparticles toward adjuvant immunotherapy. **H. Shinchi**, T. Yamaguchi, T. Moroishi, T. Hayashi, H.B. Cottam, D. Carson, M. Wakao, Y. Suda
37. FRET-based fluorogenic trehalose dimycolate analogue for probing mycomembrane-remodeling enzymes of mycobacteria. **B.D. Vannest, N. Banahene**, N.J. Holmes, C.N. Ramsey, H.W. Kavunja, B. Swarts
38. *In vivo* studies on non-toxic polysaccharide based delivery systems for pancreatic chemotherapy treatment using mice models. **R. Srinivasan**, J. Speshock, D. Edwards, A. James, D. Bocanegro
39. Direct screening of glycan patterns from human sera by chemically functionalized slides. **p. lin**, H. Tu
40. Chemical synthesis of enantiopure azido inositol analogues via ferrier carbocyclization. **J. Snyder**, A. Ausmus, B.M. Swarts
41. Effective lysozyme adsorption based on 4-vinyl pyridine photoinduced graft on cellulose nanofibrous membranes. **N. Amaly, A. ElMoghazy**, Y. Ma, G. Sun
42. Substrate dysregulation reveals a new regulatory role of OGA in cell signaling. **C. Hu**, D. Fan, M. Worth, Z. Chen, J. Huang, L. Li, J. Jiang
43. Interactome study of heparin, piscidins, and copper ions from phagocytes involved in innate

immunity of fish. **S. Kim**, F. Zhang, W. Gong, K. Chen, K. Xia, F. Liu, R.A. Gross, J. Wang, R.J. Linhardt, M. Cotten

44. Octenylsuccinate hydroxypropyl phytoglycogen to enhance the inhibitory activity of curcumin against the biofilm of *Helicobacter pylori*. **J. Chen**, Y. Yao

12:10 54. Myrosinase–glucosinolate system: Enzymatic triggered isothiocyanate for bioconjugate chemistry. **G. Cutolo**, R. Nehme, P. Lafite, W. Fredey, C. Sabot, P. Renard, M. Schuler, T. Lindhorst, A. Tatibouët

Future of Biomacromolecules at a Crossroads of Polymer Science & Biology

Synthetic Cells

Sponsored by POLY, Cosponsored by BIOL, CARB, CELL, COLL, ENVR, MEDI, PHYS and PMSE

MONDAY AFTERNOON – CARB

SECTION A

San Diego Convention Center
Room 29C

Carbohydrate Synthesis for CARB's Next Century

T. L. Lowary, *Organizer*

D. Crich, *Organizer, Presiding*

1:20 55. Tackling the challenge of glycosylation in the syntheses of complex natural glycosides. **B. Yu**

1:50 56. Streamlined synthesis of core disaccharide building blocks from natural polysaccharides for the generation of heparan sulfate libraries. **N. Pawar**, L. Wang, T. Higo, C. Bhattacharya, P.K. Kancharla, F. Zhang, K. Baryal, C. Huo, J. Liu, R.J. Linhardt, X. Huang, L.C. Hsieh-Wilson

2:10 57. Synthesis of trehalose glycolipids. **S. Jana**, **V. Sarpe**, **S.S. Kulkarni**

2:30 58. Synthesis of the hexasaccharide fragment of landomycin A: Using a mild, reagent-controlled approach. **S. Yalamanchili**, C. Bennett, D. Lloyd
Intermission.

3:10 59. Covalent glycosidase inhibitors in glycobiochemistry research: Activity-based profiling of exo- and endoglycosidases. **H.S. Overkleeft**

3:40 60. New methods for the synthesis and activation of thioglycosides. **S. Escopy**, **Y. Singh**, **A. Demchenko**

4:00 61. *N. meningitidis* capsular polysaccharide (CPS) polymerase and its application in chemoenzymatic synthesis. **R. Li**, H. Yu, X. Chen

4:20 62. Glycosyl crotylborinates for the synthesis of diverse glycomimetics. **S. Truong**, D.R. Mootoo

4:40 63. Stereoselective synthesis of 2-amino-2-deoxy- β -mannosides via anomeric O-alkylation. **B.R. Bhetuwal**, F. Wu, S. Meng, P. Acharya, P. Thapa, J. Zhu

MONDAY MORNING – CARB

SECTION A

San Diego Convention Center
Room 29C

Carbohydrate Synthesis for CARB's Next Century

D. Crich, *Organizer*

T. L. Lowary, *Organizer, Presiding*

8:30 45. Synthesis of carbohydrate lipids and their roles in innate immunity. P. van der Peet, T. Nguyen, S. Burugupalli, S. Shah, **S.J. Williams**

9:00 46. Synthesis of sialyl Lewis-x analogues as selectin antagonists for the treatment of vascular occlusions and inflammatory disease. **M. Prévost**, R. Simard, A. Belouin, M. Joyal, W. Maharsy, M. Nemer, Y. Guindon

9:20 47. Studies aiming at the structural modification of cardiac glycosides digoxin, digitoxin and 21-benzylidene digoxin and evaluation of the action mechanism in tumor cells. **S.C. Silva**, S.O. Bajaj, J.A. Ferreira Perez, L.A. de Oliveira Barbosa, G.A. O'Doherty

9:40 48. Chemical synthesis and anti-inflammatory activity of the chondroitin sulfate oligosaccharide chain (24-mer) of bikunin. **S. Ramadan**, T. Li, X. Huang

10:00 Intermission.

10:20 49. Strategies and stereoselective glycosylations for the synthesis of galactofuranose-containing oligosaccharides of pathogenic microorganisms. **C. Gallo-Rodriguez**

10:50 50. Stereoselective catalytic synthesis of glycosides. **R. Jeanneret**, C. Walz, V. Boddu, M. Galan

11:10 51. Towards catalytic activation of glycosyl halides. **Y. Singh**, S. A. Geringer, A. V. Demchenko

11:30 52. Catalyst-controlled regio- and stereoselective glycosylation. **Q. Li**, S.M. Levi, E.N. Jacobsen

11:50 53. Mechanistic investigations of β -mannosylation via Cs_2CO_3 -mediated anomeric O-alkylation and synthesis of complex biologically significant carbohydrate molecules. **S. Meng**, B.R. Bhetuwal, H.P. Nguyen, C. Fang, K. Saybolt, X. Li, P. Liu, J. Zhu

Future of Biomacromolecules at a Crossroads of Polymer Science & Biology

Tissue Engineering

Sponsored by POLY, Cosponsored by BIOL, CARB, CELL, COLL, ENVR, MEDI, PHYS and PMSE

MONDAY EVENING – CARB

SECTION A

San Diego Convention Center

TBD

Sci-Mix

S. J. Sucheck, *Organizer*

8:00 - 10:00

15, 16, 19, 21, 22, 28, 29, 31, 33, 34, 36, 37, 40, 41, 42, 43, 46, 60, 61. See Previous Listings.
110. See Subsequent Listings.

TUESDAY MORNING – CARB SECTION A

San Diego Convention Center

Room 6C

Japanese-American Symposium on Applied & Translational Glycosciences

Y. Ito, *Organizer*

A. Demchenko, *Organizer, Presiding*

- 8:30 64. Synthetic approaches toward functional analysis of glycoconjugates produced in the ER. **Y. Ito**
- 9:00 65. Carbohydrate synthesis for biologically relevant immune constructs. **P.R. Andreana**
- 9:30 66. Stereoselective synthesis of $\alpha(2,8)$ -linked oligosialic acids using bicyclic sialic acids. **N. Komura**, H. Tanaka, A. Imamura, H. Ishida, H. Ando
- 9:45 67. Synthesis of branched inner-core oligosaccharides expressed in lipopolysaccharide and lipooligosaccharide. **T. Ichyanagi**, N. Ohtani, R. Yi
- 10:00 Intermission.
- 10:15 68. Systematic synthesis of biotinylated chondroitin sulfate tetrasaccharides. **J. Tamura**
- 10:45 69. Hydrogen bonding in the conformations of glycans. **D.I. Freedberg**, M.D. Battistel, H. Azurmendi
- 11:15 70. Novel matrix system for reflectron mode MALDI-TOF and TOF/TOF MS analysis of unmodified sialylated oligosaccharides and glycopeptides. **H. Hinou**
- 11:30 71. Functions of *N*-glycan on protein. **Y. Kajihara**

TUESDAY AFTERNOON – CARB

SECTION A

San Diego Convention Center

Room 6C

Japanese-American Symposium on Applied & Translational Glycosciences

A. Demchenko, *Organizer*

Y. Ito, *Organizer, Presiding*

- 1:30 72. Rewriting the synthesis strategy toward sialic acid-containing glycans. **H. Ando**
- 2:00 73. Synthetic studies on deoxy-sugar oligosaccharides. **C. Bennett**
- 2:30 74. Synthesis of oligo-D-arabinofuranosylated probes as the substrate for mycobacterial arabinan degrading enzymes. **A. Ishiwata**, K. Fujita, S. Fushinobu, Y. Ito
- 2:45 75. Characterization of mycobacterial arabinan degrading enzymes from *Micobacterium arabinogalactanolyticum*. **K. Fujita**, A. Ishiwata, S. Fushinobu, Y. Suda, Y. Ito, K. Kitahara
- 3:00 76. Electrochemical synthesis of cyclic oligosaccharides. **T. Nokami**, S.R. Manmode, S. Tanabe, T. Yamamoto, N. Nishikouri, T. Itoh
- 3:30 Intermission.
- 3:45 77. Structural analysis for studying the reaction mechanism of β -L-arabinofuranosidases. **S. Fushinobu**, S. Maruyama, K. Sawano, T. Arakawa, C. Yamada, A. Ishiwata, Y. Ito, K. Fujita
- 4:15 78. Organoboron-catalyzed regio- and 1,2-*cis*-stereoselective glycosylation via S_Ni -type mechanism. **D. Takahashi**
- 4:45 79. Glycosylation reaction using glucosyl fluorides equipped with bridges of varying length. **H. Yamada**, Y. Hirata, H. Shimada, K. Ikeuchi, S. Wakamori
- 5:15 80. From stereocontrolled glycosylation to automated oligosaccharide synthesis. **A. Demchenko**

TUESDAY EVENING – CARB

Future of Biomacromolecules at a Crossroads of Polymer Science & Biology

Sponsored by POLY, Cosponsored by BIOL, CARB, CELL, COLL, ENVR, MEDI, PHYS and PMSE

SECTION A

San Diego Convention Center
Room 5AUncovering the Biological Roles of Protein
O-GlcNAcylation with ChemistryJ. Jiang, *Organizer*M. Pratt, *Organizer, Presiding*

- 9:00** Introductory Remarks.
- 9:05** **81.** Small-molecule inhibitors reveal that O-GlcNAc signaling globally regulates mRNA splicing. **S. Walker**
- 9:35** **82.** Chemogenetics reveals a role for dynamic O-GlcNAcylation in regulating AMPK-signaling and cytoprotection. K. Fahie, R. Henry, C. Mcken, **N. Zachara**
- 10:05** **83.** O-GlcNAcylation of myosin phosphatase target subunit 1 controls the sensitivity of sphingosine-1-phosphate signaling in fibroblasts. **N. Pedowitz**, A. Batt, N. Darabedian, M. Pratt
- 10:25** Intermission.
- 10:45** **84.** Defining O-GlcNAc cycling rates utilizing dynamic isotopic detection of amino sugars with glutamine (IDAWG). **C. Desbiens**, M. Fang, B. Weatherly, L. Wells
- 11:05** **85.** Exploring the substrate specificity of OGT & OGA and developing new generation of OGA inhibitor. **J. Li**
- 11:25** **86.** New pathway linking OGA to cancer. **J. Jiang**
- 11:55** Concluding Remarks.

Future of Biomacromolecules at a Crossroads of
Polymer Science & Biology

Delivery Systems

Sponsored by POLY, Cosponsored by BIOL, CARB, CELL,
COLL, ENVR, MEDI, PHYS and PMSE

SECTION A

San Diego Convention Center
Room 5AUncovering the Biological Roles of Protein
O-GlcNAcylation with ChemistryM. Pratt, *Organizer*J. Jiang, *Organizer, Presiding*

- 2:00** Introductory Remarks.
- 2:05** **87.** Chemical approaches toward a quantitative, systems-level understanding of protein O-GlcNAcylation signaling networks. **L.C. Hsieh-Wilson**
- 2:35** **88.** O-GlcNAcylation of KLHL proteins links nutrient sensing to proteostasis. **M. Boyce**
- 3:05** **89.** Why is OGT essential?. **Z.G. Levine**, C.M. Joiner, G.Q. Fei, S. Walker
- 3:25** Intermission.
- 3:45** **90.** Development of an O-GlcNAc transferase (OGT) degrader for rapid control of OGT homeostasis. **C. Aonbangkhen**, D. Dubeau, C.J. Thomas, S. Walker, C.M. Woo
- 4:05** **91.** Characterization of gatekeeper residues responsible for O-GlcNAc transferase (OGT) substrate specificity. **C.M. Joiner**, Z.G. Levine, C. Aonbangkhen, C.M. Woo, S. Walker
- 4:25** **92.** Chemical control of the O-GlcNAc proteome in cells. **C. Woo**
- 4:55** Concluding Remarks.

Future of Biomacromolecules at a Crossroads of
Polymer Science & Biology

Biomaterials

Sponsored by POLY, Cosponsored by BIOL, CARB, CELL,
COLL, ENVR, MEDI, PHYS and PMSE

SECTION A

San Diego Convention Center
Room 28A

Glycans in Context

Cosponsored by BIOL

H. Azurmendi, D. I. Freedberg, P. C. McCarthy, *Organizers*,
Presiding

- 8:30** Introductory Remarks.
- 8:35** **93.** One-pot multienzyme (OPME)-synthesized carbohydrate probes for structure-function relationship studies of carbohydrate-active enzymes. **X. Chen**
- 9:00** **94.** Probing the enzymatic breakdown of PNAG by DispersinB using acetylation defined substrates. **M.B. Poulin**, S. Wang, A.P. Breslawec
- 9:20** **95.** Chemical tools to elucidate and exploit trehalose metabolism in pathogenic bacteria. **B.M. Swarts**
- 9:40** **96.** Investigating multivalent virus-glycan interactions. **T. Lucas**, C.J. Fisher, M.O. Altman, K. Godula
- 9:55** **97.** GlycoSense™: Simple alternative to existing methods for glycosylation detection and monitoring. **M.J. Saunders**, R.J. Woods, L. Yang
- 10:10** Intermission.
- 10:25** **98.** Polysaccharide secretion: ABC transporter and synthase-dependent secretion mechanisms. **J. Zimmer**
- 10:50** **99.** Novel strategy for probing the activity of the human 6-O-endosulfatases. **B. Timm**
- 11:10** **100.** Discovery of new oligosaccharides in bovine milk and full glycan structural determination with logically derived sequence tandem mass spectrometry. **C.K. Ni**, S. Tsai, W. Weng, C. Liew, H. Hsu, S. Huang, Y. Kuo
- 11:30** **101.** Tools to probe the SAR in the calcium release agents cADPR and cDPR: Conformational analysis of cADPR and cDPR analogs and a route to a cADPR photoaffinity label. W. Lyu, T.J. Perez, I. Serrano, **S.M. Graham**
- 11:50** **102.** Protein engineering of Nudix hydrolases for processing of poly(ADP-ribosyl)ated proteins. **S.B. Gabelli**

SECTION A

San Diego Convention Center
Room 28A

Glycans in Context

Cosponsored by BIOL

H. Azurmendi, D. I. Freedberg, P. C. McCarthy, *Organizers*,
Presiding

- 1:45** **103.** Dendrimer heparan sulfate glycomimetics: Potent heparanase inhibitors for anticancer therapy. **O.V. Zubkova**, J.H. Miller, J.E. Turnbull, I. Vlodayvsky
- 2:10** **104.** Differential recognition of diet-derived Neu5Gc-neoantigens on glycan microarrays by carbohydrate-specific pooled human IgG and IgA antibodies. S. Leviatan Ben-Arye, C. Schneider, H. Yu, S. Bashir, X. Chen, S. von Gunten, **V. Padler-Karavani**
- 2:30** **105.** Sialoglycan recognizing probes (SGRPs): Toolkit for precise probing of the dynamic mammalian sialoglycome. **A. Sasmal**, S. Srivastava, A. Verhagen, B. Wasik, H. Yu, B. Bensing, N. Khan, Z. Khedri, S. Diaz, P. Sullam, N. Varki, X. Chen, C. Parrish, A. Varki
- 2:45** **106.** DNA barcoded soluble glycopolymer microarrays for improving detection of glycan interactions. **A.L. Michalak**, K. Godula
- 3:00** **107.** Identifying glycosidase mechanism by electrospray ionization mass spectrometry. **C. Liew**
- 3:15** Intermission.
- 3:30** **108.** Mapping global changes in glycoconjugate interactions in native cellular environments. E. Joeh, W. Li, R. Hawkins, C. Parker, **M. Huang**
- 3:55** **109.** Investigating the impact of spectator glycocalyx structures on molecular interactions at the cell surface. **D. Honigfort**, K. Godula
- 4:15** **110.** Engineered high-specificity affinity reagents for the detection of glycan sialylation. S. Wu, L. Meng, C. Gerner-Smidt, R.J. Woods, **L. Yang**
- 4:35** **111.** Polysaccharide-lipid interactions: Theoretical and experimental study using molecular dynamics simulations, quantum chemical ¹³C NMR spectra computation and solid-state ¹³C NMR. **A. Schahl**, F. Jolibois, V. Reat, A. Lemassu
- 4:55** **112.** Why humans don't routinely get bird flu: Importance of bidentate glycan binding. Y. Ji, O.C. Grant, W. Peng, R. McBride, J.C. Paulson, **R.J. Woods**
- 5:20** Concluding Remarks.

CATL

DIVISION OF CATALYSIS SCIENCE AND TECHNOLOGY

S. Crossley and A. Savara, *Program Chairs*

SUNDAY MORNING – CATL

SECTION A

San Diego Convention Center
Room 1A

Catalysis at Metal-Support Interfaces

Cosponsored by ENFL

P. Christopher, S. Crossley, *Organizers, Presiding*

- 8:00** 1. Catalysts design from first principles: Modifying oxide reducibility by nanostructuring and metal/oxide interfaces. **G. Pacchioni**
- 8:40** 2. On the identification of the active site of the Cu/ZnO/Al₂O₃ methanol synthesis catalyst. **D. Laudenschleger**, H. Ruland, M. Muhler
- 9:00** 3. Cu-SAC/TiO₂ as heterogeneous catalyst for selective liquid-phase oxidation of sp³ C–H bonds. **C. Nguyen-Sorenson**, H. Anderson, K.J. Stowers
- 9:20** 4. Influence of support acid sites on Cu-catalyzed non-oxidative dehydrogenation of ethanol to acetaldehyde. **P. Christopher**
- 9:40** Intermission.
- 9:50** 5. Tunability of low-temperature strong metal-support interactions (SMSI) for enhanced catalysis. **F. Polo Garzon**, T.F. Blum, M. Chi, Z. Wu
- 10:10** 6. Interface effects with oxide supports on the structure and reactivity of metal particles relevant for catalysis. **K. Neyman**
- 10:50** 7. Creating metal-support interfaces in metal-organic frameworks for efficient methanol synthesis from CO₂. **Y. Zhu**, J. Zheng, Y. Cui, K. Koh, L. Kovarik, D.M. Camaioni, J. Fulton, J.A. Lercher, **O.Y. Gutierrez Tinoco**
- 11:10** 8. Synthesis and activation of a well-defined dioxomolybdenum(VI) site in a MoO₃/SiO₂ olefin metathesis catalyst. **L. Li**, S.L. Scott
- 11:30** 9. Supported Au nanoparticles with *N*-heterocyclic carbene ligands as active and stable heterogeneous catalysts for lactonization. **R. Ye**, A.V. Zhukhovitskiy, D. Toste, G.A. Somorjai

SECTION B

San Diego Convention Center
Room 1B

Future Insights into Syngas Conversion Catalysis: Symposium in honor of Burtron H. Davis

Cosponsored by ENFL, ENVR, INOR and PHYS

B. Demirel, *Organizer*

M. Gnanamani, H. Kung, W. D. Shafer, *Organizers, Presiding*

- 8:00** 10. In memory of a great scientist Dr. Burtron H. Davis. **B. Demirel**
- 8:50** 11. Influence of intraparticle diffusion on effectiveness factor and methane selectivity of a cobalt based Fischer-Tropsch catalyst. **D.B. Bukur**, M. Mandić, B. Todić, N. Nikačević
- 9:15** 12. Fischer-Tropsch synthesis in a carbon nanoreactor: Spillover effects observed in Co@MHCS@Ru. T. Phaahlamohlaka, R. Forbes, L. Jewell, **N.J. Coville**
- 9:40** 13. Computational catalysis for Fischer-Tropsch synthesis: Shape, structure, activity and selectivity of cobalt catalysts. **M. Saeys**
- 10:05** Intermission.
- 10:20** 14. Improved Fischer-Tropsch catalysts guided by learnings from deactivation studies. **S. Soled**, C.E. Kliewer, S. Miseo, G. Kiss
- 10:45** 15. Fischer-Tropsch synthesis over Pt/Co/Al₂O₃ catalyst: Improvement in catalyst stability by activation with diluted CO. **K. Jalama**, W. Ma, G. Jacobs, D. Sparks, D. Qian, B.H. Davis
- 11:10** 16. Fischer-Tropsch synthesis: Direct cobalt nitrate reduction and use of promoters using supports with different interactions. **M. Mehrbod**, M. Martinelli, A. Martino, J. Castro, D.C. Cronauer, A.J. Kropf, C.L. Marshall, **G. Jacobs**

SECTION C

San Diego Convention Center
Room 2

Solvent Effects in Metal-Catalyzed Reactions

Cosponsored by ENFL and PHYS

D. E. Resasco, B. Wang, *Organizers, Presiding*

- 8:00 Introductory Remarks.
- 8:05 17. When the solvent controls the phase and mechanism of reactions on metal nanoparticles: Direct synthesis of H₂O₂ on Pd. **D. Flaherty**
- 8:25 18. Solvent effects in H₂O₂ synthesis and decomposition: Solvent as a co-reactant. **R.M. Rioux**, T. Xie, A. Dasgupta, L. Ruthardt
- 8:45 19. Modeling the selective electroreduction of oxygen to hydrogen peroxide via metal compound electrocatalysts. **J.R. Schmidt**
- 9:05 20. Different kind of solvent: Effects of high adsorbate coverages on Fischer-Tropsch synthesis and C-C hydrogenolysis. A. Almithn, J. Liu, E. Iglesia, **D.D. Hibbitts**
- 9:25 Intermission.
- 9:40 21. Effects of solvent and electrolyte composition on the electrochemical reduction of CO₂. **A.T. Bell**
- 10:20 22. Electrolyte effects in electrocatalytic reactions for sustainable energy conversion. **M. Escudero-Escribano**
- 10:40 23. General model for determining electrochemical barriers from *ab initio* simulations, and some practical applications. **K. Chan**
- 11:00 24. Incorporating the water layer in first principles simulations of hydrogen evolution on 1T-MoS₂. **D. Jiang**
- 11:20 25. Hydrothermal water a solvent, reactant, and catalyst for sustainable catalytic engineering. **J. McGregor**, L.Q. Gomez, G. Davies, M. Konstantinova

SECTION D

San Diego Convention Center
Room 3

Advances in Catalysis with Ceria & Other Reducible Oxides

Model Ceria Catalyst

Cosponsored by ENFL, ENVR, INOR and PHYS
M. Cargnello, F. Wang, Z. Wu, *Organizers, Presiding*

- 8:00 Introductory Remarks.
- 8:05 26. Model catalysis with ceria-based materials: Surface science models for heterogeneous catalysis and electrocatalysis. **J. Libuda**
- 8:35 27. Inverse ceria/metal systems in catalysis. **J. Rodriguez**
- 9:05 28. Controlling Pt dispersion on ceria by surface oxygen content: From metallic nanoparticles to single ion sites. **S. Fabris**
- 9:35 29. Theoretical analysis of adsorption on ceria surfaces. **P.S. Bagus**, C.J. Nelin
- 10:05 Intermission.
- 10:15 30. Interaction of H₂ and CO₂ with ceria surfaces: Adsorption and absorption. **H. Freund**

- 10:45 31. Topographic and spectroscopic investigation of ceria surface by using scanning tunneling microscopy. **T. Komeda**
- 11:15 32. Size dependent oxygen chemistry of CeO₂ nanoparticles. **J. Kullgren**, D. Du, K. Hermansson, P. Broqvist

SECTION E

San Diego Convention Center
Room 4

Ambient Pressure Spectroscopy in Complex Environments

Cosponsored by COLL
A. R. Head, *Organizer*
B. Eren, *Organizer, Presiding*

- 8:00 Introductory Remarks.
- 8:05 33. Infrared absorption spectroscopy for the *in situ* and *operando* study of catalytic reactions. **F. Zaera**
- 8:45 34. Application of polarization modulation infrared reflection absorption spectroscopy (PM-IRRAS) in electrocatalysis and electrochemical promotion of catalysis. E. Monyoncho, **E. Baranova**
- 9:05 35. Adsorption and reactions at the air/liquid/solid interface using PM-IRRAS in ambient conditions. **K.A. Perrine**
- 9:25 36. Elucidating the geometry-reactivity correlations in chemically-active self assembled monolayers. **E. Gross**
- 9:45 Intermission.
- 10:05 37. *In situ* surface spectroscopy and microscopy of zirconia based model catalysts. **G. Rupprechter**
- 10:45 38. Understanding the role of the metal-support interface during ethanol steam reforming on nickel-cerium oxide catalysts. **L. Baker**, Y. Mueanngern, Y. Khalifa
- 11:05 39. Two new PM-IRRAS setups for solid-gas and solid-liquid interface studies. **B. Eren**

Adsorption & Reaction at Surfaces: Symposium in Honor of Charles T. Campbell

Catalysis

Sponsored by COLL, Cosponsored by CATL

Catalysis for Environmental & Energy Applications

Treatment of Gas & Water Pollutants

Sponsored by ENVR, Cosponsored by CATL

SECTION A

San Diego Convention Center
Room 1A

Catalysis at Metal-Support Interfaces

Cosponsored by ENFL

P. Christopher, S. Crossley, *Organizers, Presiding*

- 1:00 40. Why is the characterization of active sites in heterogeneous catalysts so difficult?. **J.A. van Bokhoven**
- 1:40 41. Controlled synthesis and enhanced catalytic activity of well-defined close-contact Pd-ZnO nanostructures using PdZn ordered nanoparticle precursors. **H. Yin**, Q. Li, S. Zhou, H. Yu
- 2:00 42. Why Ni/silicalite-1 catalyst shows high stability and reactivity in dry reforming of methane?. **E. Vovk**, X. Zhou, Z. Liu, C. Guan, Y. Yang, W. Kong, R. Si
- 2:20 43. Synergistic selective oxidation of alcohols using dilute Pd/Au alloys on oxide supports. **C. Wrasman**, A. Hoffman, S. Bare, M. Cargnello
- 2:40 44. Withdrawn
- 3:00 Intermission.
- 3:10 45. Zeolites as a dynamic metal support. **W.F. Schneider**
- 3:50 46. Distinguishing the kinetic relevance of sites at a metal-support interface from promoter effects. **S. Crossley**
- 4:10 47. Bimetallic Pt-Sn catalysts encapsulated in porous silica nanoparticles for propane and butane dehydrogenation. **K.T. Li**, Y. Shieh, C. Yu
- 4:30 48. Ruthenium-iron oxide colloidal heterodimers unravel promotion mechanism in iron-catalyzed CO₂ hydrogenation to hydrocarbons. **A. Aitbekova**, E. Goodman, A. Boubnov, A. Hoffman, S. Bare, M. Cargnello

SECTION B

San Diego Convention Center
Room 1B

Future Insights into Syngas Conversion Catalysis: Symposium in honor of Burtron H. Davis

Cosponsored by ENFL, ENVR, INOR and PHYS

B. Demirel, H. Kung, W. D. Shafer, *Organizers*

M. Gnanamani, *Organizer, Presiding*

N. J. Coville, S. Soled, *Presiding*

- 1:00 49. Influence of physico-chemical properties of titanosilicate supported cobalt catalysts with different pore sizes on Fischer–Tropsch activity. **G. Kamath**, S. Badoga, A.K. Dalai

- 1:25 50. Fischer–Tropsch synthesis: Catalytic performance over ferrous oxalate based iron catalyst. **X. Feng**, Z. Di, Q. Liu, Z. Yang, **M. Luo**
- 1:50 51. Carbon-carbon bond formation during Fe catalyzed Fischer-Tropsch synthesis. **B. Shi**
- 2:15 52. Fischer-Tropsch synthesis over carbon-supported iron catalysts: Effect of support type and promoter amounts. **D. Dadyburjor**, E.L. Kugler
- 2:40 Intermission.
- 2:55 53. Mesoporous bi-metallic oxide catalysts supports in Fischer–Tropsch synthesis for sustainable fuel production. **R. Boyd**
- 3:20 54. Study on kinetic isotopic effects of iron, cobalt, and ruthenium Fischer–Tropsch catalysts based on newly built deuterium tracer coupled with kinetic approach. **W. Ma**, W.D. Shafer, M. Martinelli, D. Sparks, B.H. Davis
- 3:45 55. Catalytically active iron as a potential factor in neurodegeneration: What can we learn from FTS. **U. Graham**, G. Oberdorster
- 4:10 56. Metal organic framework catalysts in perspective. **B.C. Gates**, D. Yang
- 4:35 57. Vapor phase dehydration of 1,5-pentanediol over CeO₂-based catalysts. **M. Gnanamani**, D.C. Cronauer, A.J. Kropf, C.L. Marshall, R. Garcia, G. Jacobs, M. Martinelli, W.D. Shafer
- 5:00 58. Regulation and *in situ/operando* characterization of active structures, reaction intermediate behaviors and degradation factors at catalyst surfaces, and electrodes for developments of selective catalysis. **Y. Iwasawa**

SECTION C

San Diego Convention Center
Room 2

Solvent Effects in Metal-Catalyzed Reactions

Cosponsored by ENFL and PHYS

D. E. Resasco, B. Wang, *Organizers, Presiding*

- 1:00 59. Impact of solvent introduction on carbonyl hydrogenation over Pt and Ru. **J. Bond**, O. Abdelrahman, X. Gao
- 1:20 60. Solvent effects in metal-catalyzed hydrogenation reactions: Combined experimental and theoretical study. **B. Wang**
- 1:40 61. “Co-solvent” effects induced by polymer over-coatings on metal-supported catalysts for liquid-phase hydrogenation reactions. **J. Faria**, M.E. DaSilva, P. Huang, L. Lefferts
- 2:00 62. Correlating structure and function for nanoparticle catalysts. **G.A. Henkelman**
- 2:20 Intermission.
- 2:35 63. Modelling the role of solvents in heterogeneous catalysis. **P. Sautet**

- 3:15 64. Solvent effects in adsorption and diffusion at solid surfaces. **K.A. Fichtorn**
- 3:35 65. Structure of interfacial water on aqueous Pt/TiO₂. B. Wen, **A. Selloni**
- 3:55 66. Encased cantilevers and spiral inpainting: Probes and scan algorithms for ultrasensitive high speed AFM. **P.D. Ashby**, D. Ziegler, A. Nievergelt, J. Sader, T. Meyer, A. Bertozzi
- 4:15 67. Understanding the impact of solvent on the adsorption and reaction on porous catalysts. **B. Xu**
- 4:35 Concluding Remarks.

SECTION D

San Diego Convention Center
Room 3

Advances in Catalysis with Ceria & Other Reducible Oxides

Theory of Ceria Catalysts

Cosponsored by ENFL, ENVR, INOR and PHYS

M. Cargnello, F. Wang, Z. Wu, *Organizers, Presiding*

- 1:00 68. Computational modelling of ceria-based nanocomposite materials for catalysis. **K. Neyman**
- 1:30 69. *In situ* inelastic neutron scattering study of selective alkyne hydrogenation over cerium oxide catalyst. **J. Moon**, Y. Cheng, L. Daemen, M. Li, F. Polo Garzon, A. Ramirez-Cuesta, Z. Wu
- 2:00 70. Nanoscale morphology and improved activity of ceria-based catalysts prepared by mechanical methods. E. Aneggi, A. Mussio, M. Danielis, S. Colussi, N.J. Divins, L. Soler, X. Vendrell, X. Garcia, I. Serrano, J. Llorca, **A. Trovarelli**
- 2:30 71. *In situ* monitoring of chemical processes at cerium oxide model catalyst surfaces using low-energy electron microscopy. **J. Flege**
- 3:00 Intermission.
- 3:10 72. *In situ* and *operando* atomic level observation of lattice oxygen exchange at different surface sites in ceria-based catalytic systems. **P.A. Crozier**
- 3:40 73. Synthesis of high metal loading thermally stable Pt/CeO₂ single-atom catalysts and activation of O₂ on CeO₂ for low temperature CO oxidation. **Y. Wang**, A.K. Datye, X. Pereira Hernandez, D. Kunwar, A. DeLaRiva, V. Muravev, H. Xiong, B. Sudduth, M. Engelhard, L. Kovarik, E. Hensen, E. Peterson, S. Purdy, J. Miller, S. Lin, H. Guo
- 4:10 74. Stabilizing high metal loadings of thermally stable platinum single atoms on an industrial catalyst support. **D. Kunwar**, S. Zhou, E. Peterson, H. Xiong, A. DeLaRiva, S. Lin, H. Guo, Y. Wang, A.K. Datye

SECTION E

San Diego Convention Center
Room 4

Ambient Pressure Spectroscopy in Complex Environments

Cosponsored by COLL

A. R. Head, *Organizer*

B. Eren, *Organizer, Presiding*

- 1:00 75. First hydration layer of hydroxylation and water adsorption on SrTiO₃: Experiment (AP-XPS) & theory. D. Aschaffenburg, S. Kawasaki, S. Choing, S. Pemmaraju, H. Bluhm, **T. Cuk**
- 1:20 76. Early stages of oxidation in NiCr, and NiCrW alloys: Atomic scale to bonding chemistry. **P. Reinke**, C. Volders, W. Blades
- 1:40 77. Investigation of CO₂ hydrogenation on Pt catalysts using ambient pressure X-ray photoelectron spectroscopy. **H. Su**, Y. Ye, K. Lee, J. Zeng, E.J. Crumlin
- 2:00 78. Spectro-kinetic observations of ligand exchanges for single-site supported metal catalysts through the development of QXAS at SSRL. **A. Hoffman**, S.R. Bare, O. Mueller, C. Fang, J. Perez-Aguilar, B.C. Gates
- 2:20 79. Chemistry in confined spaces. **D.J. Stacchiola**
- 2:40 Intermission.
- 3:00 80. About *in situ* and *operando* characterization of catalysts. **J.A. van Bokhoven**
- 3:40 81. X-ray spectroscopy techniques probing active species in homogeneous catalysis: Selective oligomerisation of ethene. **M. Tromp**
- 4:00 82. Theoretical approaches for the interpretation of X-ray spectroscopy of buried interfaces. **D. Prendergast**

Adsorption & Reaction at Surfaces: Symposium in Honor of Charles T. Campbell

Reactions at Surfaces

Sponsored by COLL, Cosponsored by CATL

Catalysis for Environmental & Energy Applications

Oxidative Process for Water Treatment

Sponsored by ENVR, Cosponsored by CATL

SECTION A

San Diego Convention Center
Room 1A

2019 ACS Catalysis Lectureship for the
Advancement of Catalytic Science: Symposium
in Honor of Maria Flytzani-Stephanopoulos &
Charles Sykes

Cosponsored by WCC

P. Christopher, L. Grabow, *Organizers, Presiding*

- 8:00 Introductory Remarks.
- 8:05 **83.** Atomically dispersed supported metal catalysts: Perspective and suggestions for directions of future research. **B.C. Gates**
- 8:30 **84.** Cluster-size effect in catalysis: From sub-nano to extended surfaces. R. Schimmenti, J. Scaranto, D. Duca, **M. Mavrikakis**
- 8:55 **85.** Activation of small molecules using single atom alloy catalysts. **M. Stamatakis**
- 9:20 **86.** Solvent-free growth of oriented HKUST-1 thin films under vacuum. S. Han, B.K. Keitz, **C.B. Mullins**
- 9:45 Intermission.
- 9:55 **87.** NO_x mediated enhancement of rates and alkene selectivity in gas-phase alkane-O₂ reactions. **P. Deshlahra**
- 10:20 **88.** Robust single-atom catalysts for better catalysis. **J. Liu**
- 10:45 **89.** Controlling the local coordination and reactivity of oxide-supported atomically dispersed Pt-group species. **P. Christopher**

SECTION B

San Diego Convention Center
Room 1B

Ambient Pressure Spectroscopy in Complex
Environments

Cosponsored by COLL

A. R. Head, *Organizer*

B. Eren, *Organizer, Presiding*

- 8:00 **90.** Linking oxide surface composition and structure to reactivity. **K.A. Stoerzinger**
- 8:20 **91.** Recent development in XPS and ambient pressure XPS techniques. **L.D. Walczak**, M. Dzierzega, C. Kirschfeld, M. Florek, S. Zuk, A. Stanik, A. Szatkowski
- 8:40 **92.** Conversion of CO₂ and CH₄ on metal-oxide interfaces: *In situ* studies with XPS and XAS. **J. Rodriguez**

- 9:00 **93.** *In situ* probing of catalyst generation and deactivation with ambient pressure x-ray photoelectron spectroscopy. **B. Yildiz**, J. Wang, A.K. Opitz
- 9:20 **94.** Ambient pressure modelling of heterogeneous catalysts. **P. Sautet**
- 9:40 Intermission.
- 10:00 **95.** Dynamic nanocatalysts during CO₂ hydrogenation. **B. Roldan Cuenya**
- 10:40 **96.** Methane oxidation on an IrO₂(110) film. R. Martin, V. Mehar, C. Lee, S. Albertin, U. Hejral, L. Merte, E. Lundgren, **J.F. Weaver**
- 11:00 **97.** Thermal and spectroscopic analysis of ionic liquid solvent mixtures. **J. Wrona**, S.K. Shaw, N. Walker, K. Gudenkauf

SECTION C

San Diego Convention Center
Room 2

Electrocatalysis for Energy Generation & Storage
Fuel Cells

Cosponsored by ENFL

J. Resasco, L. C. Seitz, *Organizers*

A. Holewinski, K. Manthiram, *Organizers, Presiding*

- 8:00 **98.** Fe-Fe₃C@Fe-N-C derived from dual metal-organic frameworks for universal pH oxygen reduction electrocatalysis: Impacts of Fe crystalline particles. **H. Wang**
- 8:20 **99.** Pt-based ordered intermetallic nanoparticles for efficient electrocatalysis. **D. Wang**, M. Gong
- 8:40 **100.** *In situ/operando* same-time and same-view multi-visualization of electrocatalysis in polymer electrolyte fuel cell by time-resolved XAFS/XRD, HR-XANES/XRD/2D XAFS imaging and 3D XAFS-CT/STEM-EDS techniques. K. Higashi, S. Takao, T. Kaneko, T. Uruga, **Y. Iwasawa**
- 9:00 **101.** Electrochemistry at the metal-electrolyte-gas interface of solid-acid proton-conducting electrolytes. **S. Haile**
- 9:35 **102.** On the pH dependence in the hydrogen oxidation reaction on platinum surfaces. **B. Xu**
- 10:00 **103.** Creation of catalytic activity maps for alloy phase diagrams. **L. Cao**, L. Niu, T. Mueller
- 10:20 **104.** Theoretical resolution of the exceptional oxygen reduction activity of Au(100) in alkaline media. **Z. Duan**, G.A. Henkelman
- 10:40 **105.** Electrochemical synthesis of hydrogen peroxide for water treatment. **S. Siahrostami**
- 11:00 **106.** Electrocatalytic production of H₂O₂ by selective oxygen reduction using Earth-abundant cobalt pyrite (CoS₂). **H. Sheng**, E.D. Hermes, X. Yang, D. Ying, A.N. Janes, W. Li, J.R. Schmidt, S. Jin

- 11:20 107.** Three-dimensionally ordered macro-/mesoporous (3DOMm) transition metal oxides for electrically rechargeable Zn-air batteries. **M. Park**, M. Seo, W. Ahn, Z. Chen
- 11:40 108.** Withdrawn

SECTION D

San Diego Convention Center
Room 3

Advances in Catalysis with Ceria & Other Reducible Oxides

Reactions of Ceria Catalysts

Cosponsored by ENFL, ENVR, INOR and PHYS

M. Cargnello, F. Wang, Z. Wu, *Organizers, Presiding*

- 8:00 109.** Metal-ceria interactions and catalytic activity: Theoretical perspective. **M. Ganduglia-Pirovano**, P. Lustemberg
- 8:30 110.** Low temperature restructuring of CeO₂ supported Ru nanoparticles determines selectivity in CO₂ catalytic reduction. **A. Aitbekova**, L. Wu, C. Wrasman, A. Boubnov, A. Hoffman, S. Bare, M. Cargnello
- 9:00 111.** Dry reforming of methane over nickel/Ti-doped ceria catalysts. D.L. Braedt, T.A. Schumacher, Q. Yang, J.H. Holles, **J. Zhou**
- 9:30 112.** Ru/Ceria catalyzes the C-C/C-N bond formation reactions. J. An, **F. Wang**
- 10:00** Intermission.
- 10:10 113.** Ceria-catalyzed transformations of amides, esters, and nitriles. **K. Shimizu**
- 10:40 114.** Heterogeneous and homogeneous hybrid catalyst of CeO₂ and nitriles ~strong base catalyst~. **M. Tamura**
- 11:10 115.** Interfacial interactions in Pd-embedded ceria catalyst prepared by a one-step dry ball-milling method for methane activation and dry reforming. L.E. Betancourt, M. Danielis, S. Colussi, A. Trovarelli, J. Llorca, J. Rodriguez, **S.D. Senanayake**

SECTION E

San Diego Convention Center
Room 4

Catalytic Conversion of Biomass-Derived Oxygenates

Biomass Conversion in Liquid Environments

Cosponsored by ENFL

J. Faria, X. Zhu, *Organizers, Presiding*

S. Crossley, *Presiding*

- 8:00** Introductory Remarks.
- 8:05 116.** Importance of catalyst wettability for selective conversion of biomass. **F. Xiao**

- 8:45 117.** From homogeneous to heterogeneous amine-catalyzed isomerization of glucose to fructose in aqueous media: Understanding the role of amines' microenvironment. S.S. Chen, J. Carraher, G. Tuci, A. Rossin, C.A. Raman, L. Luconi, D. Tsang, G. Giambastiani, **J. Tessonnier**
- 9:10 118.** Controlling the reaction networks in glucose conversion to selectively obtain target products. **C. Hu**
- 10:05** Intermission.
- 10:20 119.** Efficient and reusable solid acid catalysts for the synthesis of 5-hydroxymethylfurfural from dehydration of fructose in water. **S. Dai**
- 10:50 120.** Aqueous-phase phenol and benzaldehyde hydrogenation on carbon-supported platinum group metals. **N. Singh**, C.T. Campbell, J. Fulton, U. Sanyal, O.Y. Gutierrez Tinoco, J.A. Lercher
- 11:15 121.** Efficient direct glycosylation of unprotected and unactivated simple sugars over mesoporous Lewis acid polymer. **F. Zhang**
- 11:40 122.** Al₁ modified SBA-15 supported NiO_x catalysts for the aqueous-phase guaiacol hydrogenolysis at low H₂ pressure. **R. Ma**, P. Deng, Y. Li, X. Lu, W. Zhu

Adsorption & Reaction at Surfaces: Symposium in Honor of Charles T. Campbell

Mechanisms & Kinetics

Sponsored by COLL, Cosponsored by CATL

MONDAY AFTERNOON – CATL

SECTION A

San Diego Convention Center
Room 1A

2019 ACS Catalysis Lectureship for the Advancement of Catalytic Science: Symposium in Honor of Maria Flytzani-Stephanopoulos & Charles Sykes

Cosponsored by WCC

P. Christopher, L. Grabow, *Organizers, Presiding*

- 1:00 123.** Role of Lewis Acid/Brønsted base sites in the formation of C-C bonds. **A.T. Bell**
- 1:25 124.** Electronic structure engineering in heterogeneous catalysis: From simple analytical to machine learnt models of chemisorption on alloys. **S. Linic**
- 1:50 125.** Spectroscopic characterization of the structure and reaction pathways of Pd-Cu(111) and Pd-Ag(111) single-atom alloys. **M. Trenary**

- 2:15** **126.** Elucidating the chemical nature of single-site catalysts from first principles. K. Groden, A. Schilling, N. Ulumuddin, A. Hensley, A. Therrien, R. Zhang, R. Hannagan, A. Hunt, J. Simonovis, G. Giannakakis, A. Sukkar, S. Cao, J. Liu, M. Flytzani-Stephanopoulos, I. Waluyo, E.H. Sykes, **J. McEwen**
- 2:40** Intermission.
- 2:50** **127.** Single-atom species determine the deactivation of supported catalysts. **M. Cargnello**, E. Goodman, F. Abild-Pedersen, S. Bare
- 3:15** **128.** Back-of-the-envelope prediction of single atom alloy stability. K.M. Pham, Q.K. Do, K.K. Rao, **L. Grabow**
- 3:40** **129.** Single-atom alloy catalysts; Part I: Birth and formative years spent in a chilly vacuum; Part II: Coming of age and transition into a fiery reactor. **M. Flytzani-Stephanopoulos, E.H. Sykes**

SECTION B

San Diego Convention Center
Room 1B

Ambient Pressure Spectroscopy in Complex Environments

Cosponsored by COLL

A. R. Head, *Organizer*

B. Eren, *Organizer, Presiding*

- 1:00** **130.** Solid-gas and solid-liquid interfaces under ambient conditions. **M. Salmeron**
- 1:40** **131.** X-ray standing waves and other ways of using photoelectrons to probe buried interfaces. **S. Nemsak**
- 2:00** **132.** Offset droplet: New approach to probing the electrode/electrolyte interface in X-ray photoelectron spectroscopy. **A. Walton**, C. Byrne
- 2:20** **133.** New ambient pressure X-ray photoelectron spectroscopy facilities for liquid-solid investigations: Opportunities and challenges. **Y. Yu**, Y. Han, Z. Liu
- 2:40** Intermission.
- 3:00** **134.** B07: Versatile soft X-ray beamline (VERSOX) at diamond light source. **D.C. Grinter**
- 3:20** **135.** High temperature oxygen intercalation studied by *operando* X-ray spectroscopy. **D.N. Mueller**, T. Duchon, S. Nemsak, C.M. Schneider
- 3:40** **136.** Monitoring the dynamics and chemical state of size-selected cluster catalysts. **B. Lechner**, A. Bourgund, K. Zhang, F. Knoller, M. Huber, T. Kratky, M. Rötzer, M. Krause, C. Büchner, M. Döblinger, H. Bluhm, M. Meier, G. Parkinson, S. Günther, F. Esch, U. Heiz
- 4:00** **137.** Withdrawn

SECTION C

San Diego Convention Center

Room 2

Electrocatalysis for Energy Generation & Storage

Cosponsored by ENFL

A. Holewinski, K. Manthiram, *Organizers*

J. Resasco, L. C. Seitz, *Organizers, Presiding*

- 1:00** **138.** Calculations of the electrochemical reduction of CO₂ and the competing hydrogen formation. **H. Jonsson**
- 1:20** **139.** Formation pathways to three-carbon products from carbon dioxide reduction reactions electrochemically catalyzed by metallic copper surfaces. **Z. Lin**, K. Jiang, A.J. Garza, A.T. Bell, M.P. Head-Gordon
- 1:40** **140.** Surface topology effect of under-coordinated Cu sites on electrochemical CO₂ reduction. **K. Jiang**, A.T. Bell
- 2:00** **141.** Two-dimensional copper nanosheets for electrochemical reduction of carbon monoxide to acetate. **X. Fu, Y. Kang**
- 2:20** **142.** Effect of organic modifiers on the local environment in the electrocatalytic reduction of CO₂ at metallic surfaces. **A.K. Buckley**, M. Lee, T. Cheng, R.V. Kazantsev, D. Larson, W.A. Goddard, D. Toste, F. Toma
- 2:40** **143.** Evaluating sources of trace metal contamination and their effect on product distribution in the Cu-catalyzed electrochemical CO₂ reduction reaction. **K. Leung**, C.C. McCrory
- 3:00** Intermission.
- 3:05** **144.** Modelling and overcoming mass transport limits during electrochemical CO₂ reduction. **D. Raciti**, Y. Wang, M. Mao, J. Park, C. Wang
- 3:25** **145.** Nature of the active sites for the CO₂ reduction reaction on carbon-based electrocatalysts. **P.B. Atanassov**, **T. Asset**, Y. Chen, I. Matanovic, K. Artyushkova
- 4:00** **146.** Nanoporous carbon materials in CO₂ (photo) electrochemical reduction. **W. Li**, T.J. Bandosz
- 4:20** **147.** Development of an aqueous electrocatalyst for reversible CO₂ reduction to formate. **X.S. Wang**, J.Y. Yang
- 4:40** **148.** Achieving highly effective and selective electroreduction of CO₂-to-CO on porous nanostructured ZnO derivatives. **D. Nguyen**, Y. Hwang

Advances in Catalysis with Ceria & Other Reducible Oxides

Reactions and Other Metal Oxides

Cosponsored by ENFL, ENVR, INOR and PHYS

M. Cargnello, F. Wang, Z. Wu, *Organizers, Presiding*

- 1:00** **149.** Controlled synthesis of multicomponent oxide catalysts for oxidation catalysis. **S. Dai**
- 1:30** **150.** Resolving the promotional mechanism in supported vanadium oxide SCR catalysts. **N.R. Jaegers**, J. Lai, Y. He, E.D. Walter, D.A. Dixon, M. Vasiliu, C. Wang, M. Hu, K. Mueller, I.E. Wachs, J. Hu, Y. Wang
- 2:00** **151.** Catalytic materials derived from MOFs for low-temperature VOC remediation. **Q. Wang**, Z. Li, W. Han, K. Yeung
- 2:20** **152.** Catalysis of hydrogen and oxygen abstraction from ethanol and ethanal over $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_{3-x}$. **B. Chen**, A. Savara
- 2:40** **153.** Enhancing the reactivity of oxygen carrier redox catalysts for chemical looping oxidative coupling of methane via a synergistic co-doping strategy. **Z. Cheng**, D.S. Baser, S.G. Nadgouda, L. Qin, L. Qin, L. Fan
- 3:00** Intermission.
- 3:10** **154.** Single site vs crystalline: Promoted WO_3/SiO_2 catalyst design for oxidative coupling of methane (OCM). **J. Baltrusaitis**, D. Kiani, S. Sourav, I.E. Wachs
- 3:40** **155.** Interfacial effects of CeO_2 supported noble metal nanocatalysts in C1 chemistry. **Y. Guo**, Y. Zhang
- 4:00** **156.** Improvement of the hydrodesulfurization activities by adding cerium to $\text{FeZn}/\gamma\text{-Al}_2\text{O}_3$ catalysts. **X. Liu**, X. Zhang, L. Li, B. Shen
- 4:20** **157.** Effects of adsorption on selective transformations of small alcohol molecules on the strontium titanate(100) surface. R.C. Chapleski, **S. Roy**

Catalytic Conversion of Biomass-Derived Oxygenates

Theoretical & Mechanistic Studies of Biomass-Derived Oxygenates

Cosponsored by ENFL

J. Faria, X. Zhu, *Organizers, Presiding*

S. Crossley, *Presiding*

- 1:00** Introductory Remarks.
- 1:05** **158.** Selectivity control in acid-base catalysis for valorization of several biomass derived oxygenates. **B. Xu**
- 1:45** **159.** Aldolization (C-C coupling) of biomass derived C2 and C3 oxygenates. J. Sun, H. Li, A.D. Winkelman, R. Dagle, V. Lebarbier Dagle, **Y. Wang**
- 2:15** **160.** Methyl ketone condensation over tailored metal oxides for biofuel precursor production. **D. Vardon**, X. Huo, V. Vorotnikov, M. Zhou, D. Conklin, A. York, Z. Li, K. Page, R.M. Richards, R. Assary
- 2:40** **161.** Aldol condensation of acetone over single-facet dominant anatase TiO_2 (101) and (001) catalysts. **F. Lin**, **Y. Zhao**, H. Wang, D. Mei, N.R. Jaegers, F. Gao, Y. Wang
- 2:55** Intermission.
- 3:10** **162.** Ru-catalyzed hydrogenolysis of polyols: From molecular understanding toward rational catalyst design. **P. Hausoul**, A.K. Beine, N. Sackers, L. Negahdar, R. Palkovits
- 3:35** **163.** Catalytic reductions of esters with Re and PdRe nanoparticles. C. Berdugo, Y. Yun, **D. Flaherty**
- 4:00** **164.** Life cycle of iron catalyst: CO_2 hydrogenation to olefins using *operando* methodology. **J. Xu**
- 4:25** **165.** Ni-based catalysts for steam reforming of ethanol: *In situ* investigation of C-C and O-H bond scission. **Z. Liu**, S.D. Senanayake
- 4:45** **166.** Calorimetry to explore the kinetics and thermodynamics of phenol hydrogenation by heterogeneous metal catalysts. **R. Kumar**, T. He, A.J. Karkamkar, U. Sanyal, O.Y. Gutierrez Tinoco, J.C. Linehan, D.M. Camaioni, **T. Autrey**

Adsorption & Reaction at Surfaces: Symposium in Honor of Charles T. Campbell

Adsorption & Binding at Surfaces

Sponsored by COLL, Cosponsored by CATL

Charge & Substrate Transport in 3D Electrocatalytic Materials

Sponsored by INOR, Cosponsored by CATL and ENFL

SECTION A

San Diego Convention Center

Room 1A

CATL Division Awards: Symposium in Honor of Francisco Zaera & Yuriy Román-Leshkov

S. Crossley, D. E. Resasco, *Organizers*

A. J. Gellman, J. D. Rimer, *Presiding*

- 8:00 Introductory Remarks.
- 8:05 **167.** Fundamental studies of CO₂ conversion on novel metal-carbide catalysts. **J. Rodriguez**
- 8:20 **168.** Analysis of selectivity trends during the oxidative scission of ketones and keto-acids. **J. Bond**, R. Zhu, B. Liu, S. Wang, A. Chatzidimitriou
- 8:40 **169.** From crystals to glasses at the atomic level in real space. **H. Freund**
- 9:00 **170.** Mechanism and kinetics of light alkane dehydrogenation over metal cations substituted into zeolite MFI. **A.T. Bell**
- 9:20 **171.** Metal nanoparticles on metal oxide nanoparticles (M_{np}/MO_{np}) as model catalysts. **J.C. Hemminger**
- 9:40 Intermission.
- 10:00 **172.** Influence of zeolite framework on Cu ion mobility and the kinetics of selective catalytic reduction of nitrogen oxides with ammonia. **R. Gounder**
- 10:20 **173.** New catalytic insights from *in situ* neutron scattering investigations. **Z. Wu**
- 10:40 **174.** Intermetallics with controlled active site ensembles dictate catalytic semihydrogenation selectivity. **R.M. Rioux**, A. Dasgupta, H. He, R.J. Meyer, M.J. Janik
- 11:00 **175.** Exploring enantioselective reactions on chirally modified surfaces in ultrahigh vacuum. **W.T. Tysoe**
- 11:20 Introduction of Awardee.
- 11:25 **176.** Universal promotion of heterogeneous olefin metathesis catalysts: Story about failure and perseverance during the early career research years. **Y. Roman-Leshkov**

SECTION B

San Diego Convention Center

Room 1B

Future Insights into Syngas Conversion Catalysis: Symposium in honor of Burtron H. Davis

Cosponsored by ENFL, ENVR, INOR and PHYS

H. Kung, *Organizer*

B. Demirel, M. Gnanamani, W. D. Shafer, *Organizers, Presiding*

- 8:00 **177.** Synthetic crude oil refining: Lifetime contribution by Burtron H. Davis. **A. De Klerk**
- 8:45 **178.** New learnings on selectivity drift with catalyst age for Fe-LTFT process. **M. Janse van Vuuren**
- 9:10 **179.** Challenges and opportunities in Fischer-Tropsch/gas to liquids catalyst and process development. **S.C. Leviness**
- 9:35 **180.** Small scale modular system for gas-to-liquid conversion using FT process. **Z. Jia**
- 10:00 Intermission.
- 10:15 **181.** Design of novel catalytic systems for the gas-to-liquid technology. **N.O. Elbashir**
- 10:40 **182.** Dry reforming of methane on Ni based pyrochlore catalysts: Effect of lanthanum amount. **S. Bhattar**, S. Kanitkar, A. Abedin, D. Haynes, D. Shekhawat, J.J. Spivey
- 11:05 **183.** Carbon tolerance of Rh-substituted pyrochlore catalysts under low steam-to-carbon ratio steam reforming conditions. **Y. Zhou**, D.J. Haynes, D.A. Berry, D. Shekhawat

SECTION C

San Diego Convention Center

Room 2

Electrocatalysis for Energy Generation & Storage

Cosponsored by ENFL

K. Manthiram, J. Resasco, *Organizers*

A. Holewinski, L. C. Seitz, *Organizers, Presiding*

- 8:00 **184.** Withdrawn
- 8:20 **185.** Withdrawn
- 8:40 **186.** Water dissociation catalysis. **S.W. Boettcher**, S. Oener
- 9:15 **187.** Accelerated screening of binary and ternary metallic hydroxide electrocatalysts. C. Yu, K. Yang, **H. Chen**
- 9:35 Intermission.
- 9:40 **188.** Engineering electronic structure of single atom catalyst via lattice strain towards rational optimization of highly efficient and stable electrocatalyst. **S. Hu**, W. Li
- 10:00 **189.** Oxygen electro-adsorption kinetics on well-defined oxide surfaces. D. Kuo, **J. Suntivich**
- 10:25 **190.** Structural evolutions in iron perovskites during oxygen evolution electrocatalysis. **J. Vuong**, S. Derakhshan, H. Tavassol
- 10:45 **191.** Constructing and analysis of Tafel plots for homogeneous water oxidation catalysts. **Q. Yin**, Y.V. Geletii, C.L. Hill

- 11:05 192.** Does doping/co-doping of rare earth metal in BiVO₄ system lead to enhanced photoelectrochemical water oxidation: Electrochemical investigation. **J. Prakash**, U. Prasad, B. Azeredo, A.M. Kannan
- 11:25 193.** Understanding and controlling electrochemistry for electrolyzers. **A.A. Gewirth**, X. Chen, T. Hoang

SECTION D

San Diego Convention Center
Room 3

Advances in Catalysis with Ceria & Other Reducible Oxides

Reactions and Other Metal Oxides

Cosponsored by ENFL, ENVR, INOR and PHYS
M. Carnello, F. Wang, Z. Wu, *Organizers, Presiding*

- 8:00 194.** Chemical activity of ceria nanoparticles: Not the shape, the surface matters. **C. Woell**
- 8:20 195.** Conversion of CO₂ on a highly active and stable Cu/FeOx/CeO₂ catalyst: Tuning catalytic performance by oxide-oxide interactions. **L. Lin**, S. Yao, J. Rodriguez
- 8:40 196.** Performance of MOF-derived CeO₂ catalysts for VOCs oxidation. **Y. Li**, Q. Wang, K. Yeung
- 9:00 197.** Ketonization of propionic acid on CeGaO_x catalysts. **X. Zhu**, S. Ding, Q. Ge
- 9:20** Intermission.
- 9:30 198.** Effect of Ce addition on catalytic performance of Cu TiO₂ for CO oxidation. **C. Li**, **W. Xu**, **J. Wang**, **Y. Yang**, **T. Zhu**
- 9:50 199.** Synergistic effect of anions (C and N), cation (Pd) substitution and oxygen vacancies on the oxygen activation capacity of TiO₂. **S. Vangala**, P. Deshpande
- 10:10 200.** New insight into simultaneous removal of NO and Hg⁰ on CeO₂ modified V₂O₅/TiO₂ catalyst: Nitrate pathway for Hg⁰ oxidation. **Y. Yang**, W. Xu, C. Li, J. Wang, T. Zhu
- 10:30 201.** Plant-mediated synthesised Mn₃O₄ catalyst with enhanced acidic sites and low temperature reducibility for benzene abatement. **T. Odoom-Wubah**, Q. Li, Y. Zhou, M. Chen, M. Usha, J. Huang, Q. Li

SECTION E

San Diego Convention Center
Room 4

Catalytic Conversion of Biomass-Derived Oxygenates

Theoretical & Mechanistic Studies of Biomass-Derived Oxygenates

Cosponsored by ENFL
J. Faria, X. Zhu, *Organizers, Presiding*
S. Crossley, *Presiding*

- 8:00** Introductory Remarks.
- 8:05 202.** TiO₂ and ZrO₂ in biomass conversion: Why catalyst reduction helps. **G. Pacchioni**
- 8:35 203.** Hydrodeoxygenation of phenolic compounds on group VIII metals: Reaction mechanism and product selectivity. **Q. Ge**
- 9:00 204.** Elucidating the function of each metal in bimetallic catalysts and the role of water for hydrodeoxygenation reactions. N. Chaudhary, J. Bray, A. Hensley, M. Hawkins, J. Shangguan, Y. Wang, D. Wu, Y. Chin, **J. McEwen**
- 9:25 205.** Theoretical insights into selective C-O bond cleavage of ethers over transition metal catalysts. **D. Mei**
- 9:50** Intermission.
- 10:05 206.** Understanding oxygenate conversion on oxides from first principles. **D. Jiang**
- 10:30 207.** Coverage-dependent *ab initio* microkinetic models for the copper-catalyzed hydrogenation of carbonyl groups: Role of hydrogen, water, and sacrificial alcohols. **M. Saeys**
- 10:55 208.** Disentangling the size-dependent geometric and electronic effects of palladium nanocatalysts for selective oxidation of benzyl alcohol. **H. Wang**, **X. Gu**, **J. Lu**, **W. Li**
- 11:20 209.** Preferential activation of the sterically hindered C-O bond within 2-methyltetrahydrofuran over nickel phosphide catalysts. A. Almithn, M. Witzke, D. Flaherty, **D.D. Hibbitts**
- 11:45 210.** Kinetic insights into the sites requirements and mechanisms of acetic acid hydrodeoxygenation over Pt and PtMo catalysts. **Y. Zheng**, Z. Tang, S. Podkolzin

Adsorption & Reaction at Surfaces: Symposium in Honor of Charles T. Campbell

Electrocatalytic & Liquid Interfaces

Sponsored by COLL, Cosponsored by CATL

Charge & Substrate Transport in 3D Electrocatalytic Materials

Sponsored by INOR, Cosponsored by CATL and ENFL

SECTION A

San Diego Convention Center

Room 1A

CATL Division Awards: Symposium in Honor of Francisco Zaera & Yuriy Román-Leshkov

S. Crossley, D. E. Resasco, *Organizers*

J. Bond, W. T. Tysoe, *Presiding*

- 1:00 211. Where do ALD precursors react?. **P.C. Stair**
- 1:20 212. Revolution in catalysis science: Integration of the Heterogeneous, homogeneous, and enzyme fields. **G.A. Somorjai**
- 1:40 213. Controlling the physico-chemical properties of small pore zeolites for the MTO reaction. **M. Moliner**
- 2:00 214. Dynamic nature of heterogeneous catalysts in reaction conditions. **P. Sautet**
- 2:20 215. Degree of rate control: Powerful tool for catalysis research. **C.T. Campbell**
- 2:40 216. Cooperative catalysis using supported bifunctional amine-acid catalysts. **C.W. Jones**
- 3:00 Intermission.
- 3:20 217. Mitigating the effects of diffusion limitations in zeolite catalysis. **J.D. Rimer**
- 3:40 218. Biological and catalytic strategies for plastics upcycling. **G. Beckham**
- 4:00 219. Structure sensitive enantioselectivity: Quantification across chiral surface orientations vicinal to the low Miller index Cu surfaces. **A.J. Gellman**, B. Karagoz, P. Kondratyuk
- 4:20 220. Non-equilibrium modeling of mass transport between solids and liquids. **C.H. Hendon**
- 4:40 Introduction of Awardee.
- 4:45 221. New nanostructures for increased selectivity and stability in catalysis. **F. Zaera**

SECTION B

San Diego Convention Center

Room 1B

Future Insights into Syngas Conversion Catalysis: Symposium in honor of Burtron H. Davis

Cosponsored by ENFL, ENVR, INOR and PHYS

B. Demirel, M. Gnanamani, H. Kung, W. D. Shafer, *Organizers*

A. De Klerk, U. Graham, *Presiding*

- 1:00 222. Production of syngas with controllable H₂/CO ratio by high temperature co-electrolysis of CO₂ and H₂O over Ni and Co-doped lanthanum

strontium ferrite perovskite cathodes. **U.S. Ozkan**, D.J. Deka, S. Gunduz, J.T. Miller, A. Co

- 1:25 223. Integrated steam-reforming of glycerol with photocatalytic reforming of glycerol and water to produce synthesis gas for high-temperature Fischer–Tropsch synthesis. T.W. Seadira, **C.M. Masuku**, L.T. Biegler
- 1:50 224. Sodium addition promotes C–C scission during ethanol steam reforming on Pt/m-ZrO₂ catalyst. **M. Martinelli**, C.D. Watson, G. Jacobs
- 2:15 225. Co and Zn-based Ziegler type liquid phase catalysts: preparation and evaluation for carbon monoxide hydrogenation. **C. Kappenstein**, J. Goma, A. Choukchou-Braham, J. Barrault
- 2:40 Intermission.
- 2:55 226. Rhodium-based catalysts for the production of oxygenates in CO hydrogenation. N. Mungwe, S. Sewsunker, M. Fadlalla, N. Fischer, **M. Claeys**
- 3:20 227. Copper-zirconia interfaces in UiO-66 for CO₂ conversion to methanol. Y. Zhu, J. Zheng, K. Koh, L. Kovarik, D.M. Camaioni, J. Fulton, O.Y. Gutierrez Tinoco, **J. Lercher**
- 3:45 228. CO and CO₂ hydrogenation catalytic chemistry and formation of hydrocarbons and methanol. **G.A. Somorjai**
- 4:10 229. On the route to elucidating the relationships between zeolite structure and methanol-to-olefins reaction performance. **M.E. Davis**
- 4:35 230. Deactivation of methanol to olefins revisited. **G.L. Haller**
- 5:00 231. Disentangling promoter, support, and particle size effects in methanol synthesis. **R. Beerthuis**, C.E. Pompe, K. De Jong, P. de Jongh

SECTION C

San Diego Convention Center

Room 2

Electrocatalysis for Energy Generation & Storage Emerging Electrocatalytic Materials & Reaction Chemistries

Cosponsored by ENFL

A. Holewinski, L. C. Seitz, *Organizers*

K. Manthiram, J. Resasco, *Organizers, Presiding*

- 1:00 232. Deposition of nickel phosphide Ni₂P on carbon materials forming a versatile and very active electrocatalyst for application in gas diffusion electrodes. **J. Majchel**, N. Wagner, K. Friedrich
- 1:20 233. Next generation all solid-state flexible Zn-Air batteries using hexaiminobenzene metal-organic frameworks. **S.S. Shinde**, N.K. Wagh, D. Kim, J. Lee
- 1:40 234. Confining aluminum in metal-organic framework triggers carbon dioxide reduction

- activity. **M. Lee**, A. De Riccardis, R.V. Kazantsev, J. Cooper, A.K. Buckley, P. Burroughs, D. Larson, G. Mele, F. Toma
- 2:00** **235.** Electrochemical reduction of CO₂ catalyzed by pyrolyzed ZIFs supported on carbon nanotube networks. **Y. Guo**, C. Wang
- 2:20** **236.** Selective electrocatalytic N₂ reduction to ammonia by bimetallic nanocrystal. **B. Talukdar**, C. Kuo
- 2:40** **237.** Promoting reliable electrocatalytic N₂ reduction. **A. Nielander**, J. McEnaney, S. Blair, J. Schwalbe, J. Baker, T.F. Jaramillo
- 3:00** Intermission.
- 3:10** **238.** Asymmetric electrocatalysis. **S. Lin**
- 3:35** **239.** Homogeneous and heterogeneous catalysts for electrochemical production of 2,5-furandicarboxylic acid. B.J. Taitt, A.C. Cardiel, M.T. Bender, **K. Choi**
- 4:10** **240.** Plasmonic Pd, Au, and Au-Pd nanoparticle photoelectrocatalysts for small molecule oxidation. **R.J. Dillon**, J.P. McClure, A.C. Leff, C.A. Lundgren
- 4:30** **241.** Shape-controlled silver nanocrystals with specific facets as the light-harvesting catalysts for plasmon-enhanced hydrogen production. D. Wang, T. Kuo

SECTION D

San Diego Convention Center
Room 3

Hybrid Biological & Chemocatalytic Processes for Biomass Upgrading to Fuels & Chemicals

Cosponsored by ENFL

K. K. Ramasamy, D. Vardon, *Organizers, Presiding*

- 1:00** **242.** Assessment of structural characteristics and upgrading of lignin from lignocellulosic biomass based on various separation methods. **T. Chen**, **X. Zhang**, **J. Wen**, **F. Xu**
- 1:20** **243.** High-efficient conversion of lignocellulosic biomass to 5-hydroxymethylfurfural (HMF): Effect of Keggin-type heteropolyacid/chitin hybrid catalysts. **P. Wang**, F. Lai, F. Yan, Z. Zhang
- 1:40** **244.** Continuous, solvent-free production of a performance-advantaged, infrastructure-compatible biooxygenate diesel blendstock. **N.A. Huq**, X. Huo, G. Hafenstine, S. Tiffit, J. Stunkel, E. Christensen, G. Chupka, L. Fouts, R.L. McCormick, T. Alleman, P. St. John, S. Kim, R. Connaster, M.D. Kass, P. Cherry, C.S. McEnally, L.D. Pfefferle, D. Vardon
- 2:00** **245.** Conversion, stability, and selectivity improvements through catalyst development for the reductive etherification reaction and implications for bioblendstock production from

- waste biomass. **G. Hafenstine**, N.A. Huq, X. Huo, J. Stunkel, S. Tiffit, D. Vardon
- 2:20** **246.** Ethanol conversion to higher alcohols as fuel blend stocks. **S. Subramaniam**, M. Guo, K.K. Ramasamy, M. Gray
- 2:40** Intermission.
- 2:50** **247.** Catalytic upgrading of biomass for for fuels and chemicals. **B. Sels**
- 3:20** **248.** Withdrawn
- 3:40** **249.** Hybrid organic electrosynthesis of bio-based monomers. M.N. Dell'Anna, S. Abdolmohammadi, G. Gupta, J.E. Matthiesen, E.W. Cochran, L.T. Roling, **J. Tessonnier**
- 4:00** **250.** Surface bonding as a predictor of C–C and C–H bond activation events. **K. Goulas**
- 4:20** **251.** Experimental and computational studies of the production of 1,3-butadiene from bio-2,3-butanediol using SiO₂-supported H₃PO₄ derivatives. J. Alegre Requena, **S. Kim**, Y. Guan, X. Huo, J. Stunkel, D. Vardon, R.S. Paton

SECTION E

San Diego Convention Center
Room 4

Catalytic Conversion of Biomass-Derived Oxygenates

Cosponsored by ENFL

J. Faria, X. Zhu, *Organizers, Presiding*

S. Crossley, *Presiding*

- 1:00** Introductory Remarks.
- 1:05** **252.** New insights into hydrogenation and transfer hydrogenation of levulinic acid and methyl levulinate over Cu-ZrO₂ catalysts. **M. Douthwaite**, B. Zhang, I. Orłowski, J. Hirayama, C. Reece, S. Iqbal, P.J. Miedzian, S.F. Parker, J.K. Bartleyjk@cardiff.ac.uk, D.J. Willock, G. Hutchings
- 1:30** **253.** Glycerol hydrogenolysis to 1,3-propanediol over Pt-WO_x catalysts. **X. Ma**, W. Zhou, X. Wang, Y. Zhao
- 1:55** **254.** Efficient chemo-catalytic conversions of glycerol to lactic acid and derivatives. **H. Heeres**, Z. Tang, P. Pescarmona
- 2:20** **255.** Catalytic conversion of bio-glycerol to value added products via vapor and liquid processes. **Y. Hao**
- 2:45** **256.** Selective electrocatalytic oxidation of glycerol to formic acid by Earth-abundant spinel oxides. X. Han, **H. Sheng**, T. Walker, G.W. Huber, S. Jin
- 3:00** Intermission.
- 3:10** **257.** Catalytic transformations of biomass derived furanics to high value chemicals. **Z. Zhang**, Z. Xu, M. Marri, P. Yan

- 3:35 258.** Solid acid foams for continuous dehydration of xylose to furfural in a biphasic extractive media. **F. Neira Dangelo**
- 4:00 259.** Hydrogenolysis of 5-hydroxymethylfurfural via Ru cluster catalysts. **F. Wang, Q. Wang, R. Xu**
- 4:25 260.** Determination of active site in mesoporous oxides for catalytic furfural hydrogenation. **K. An**
- 4:45 261.** Aqueous phase reforming of the waste water derived from lignin hydrothermal liquefaction: From the simplicity of model compounds to the complexity of real streams. **S. Bensaid, G. Pipitone, G. Zoppi, S. Bocchini, A. Rizzo, D. Chiaramonti, R. Pirone**

Charge & Substrate Transport in 3D Electrocatalytic Materials

Sponsored by INOR, Cosponsored by CATL and ENFL

TUESDAY EVENING – CATL

SECTION A

San Diego Convention Center
TBD

General Catalysis

S. Crossley, *Organizer*

7:00 - 9:00

- 262.** High throughput *in silico* reaction screening for tailored catalytic reactivity and selectivity. **T.J. Mustard, T.F. Hughes, A. Bochevarov, L.D. Jacobson, H.S. Kwak, T. Morisato, J.L. Gavartin, S. Pandiyan, M. Halls**
- 263.** Photocatalytic dehydrogenation of formic acid promoted by a superior PdAg@g-C₃N₄ Mott-Schottky heterojunction. **H. Liu, M. Shen, W. Yang, Y. Yu**
- 264.** Ceramic composite systems of Li-Ce-O as potential carbon dioxide (CO₂) scrubbers. **A. Otero-Gonzalez, H. Pfeiffer**
- 265.** Surface reactivity and stability of core-shell solid catalysts from *ab initio* combinatorial calculations. **T.J. Mustard, J.L. Gavartin, A. Fonari, C. Krauter, A. Goldberg, H.S. Kwak, T. Morisato, S. Pandiyan, M. Halls**
- 266.** Surface-supported cluster catalysis: Fluxionality and the importance of ensemble representation. **B. Zandkarimi, H. Zhai, A. Alexandrova**
- 267.** Morphology-enhanced basicity towards highly-efficient hydrogen production from aqueous phase reforming of cellulose. **J. Zhang, Z. An, X. Shu, H. Song, J. He**

- 268.** Growth mechanisms and catalytic efficiency in metal-organic framework (MOF) composites containing enzymes and structural proteins. **B.P. Carpenter, A.F. Ogata, K.W. Roskamp, R.W. Martin, J.P. Patterson**
- 269.** Dynamic structural evolution of catalyst in a CO oxidation process. **J. Wu, H. Wang, P. Hu**
- 270.** High-throughput continuous flow catalysis of organic reactions using metal-organic frameworks. **J. Thai, J.B. Tapia, M.M. Reynolds**
- 271.** New highly active copper(I) catalyst for aerobic oxidation of primary alcohols. **E. Lagerspets, K. Lagerblom, E. Heliövaara, O. Hiltunen, K. Moslova, M. Nieger, T. Repo**
- 272.** Easily magnetic recovered ionic liquid immobilization catalyst for the cycloaddition of CO₂ at normal pressure. **M. Ji, T. Wang, Y. An**
- 273.** Study on catalytic combustion of monoaromatic hydrocarbons VOCs over monolithic catalytic combustion catalyst. **Y. Yang, G. Wang**
- 274.** Reduction of propionic acid using palladium-promoted supported tungsten catalysts. **J. Kammert, G. Brezicki, E. Stavitski, R.J. Davis**
- 275.** Novel integrated system for CO₂ capture and conversion to methanol using alcoholic NaOH/KOH solutions. **R. Sen, A. Goepfert, S. Kar, S.G. Prakash**
- 276.** New insight into metal oxide on zeolite as support for aerobic oxidation of 5-hydroxymethylfurfural into valuable chemicals. **H. Yu, S. Hwang, H. Kim, H. Cha**
- 277.** Estimate of adsorption energy for a series of highly efficient catalysts based on reaction model. **Z. Lai, J. Chen, H. Wang, P. Hu**
- 278.** Rice husk silica supported palladium based magnetically separable and reusable green catalyst for C-C coupling reactions in water. **K. Hasan, N. Elmabrouk, K. Bagudu**
- 279.** Quick evaluation of catalytic activity of hydrogenation catalysts by UV spectra using imidazo[1,5-a]pyridines as probes. **A.S. Lytvynenko, N.A. Ivanitsa, S.A. Sotnik, D.O. Tverdiy, S. Ryabukhin, D.M. Volochnyuk, S.V. Kolotilov**
- 280.** G3 and G4 Buchwald precatalysts: Scale up, QC and application for the semi-automated parallel synthesis. **S.A. Sotnik, S.V. Kolotilov, D. Radchenko, S. Ryabukhin, D.M. Volochnyuk**
- 281.** Vermiculite/Cu²⁺ composite use as heterogeneous catalyst for the Biginelli synthesis. **C.E. Torres, B.J. López**
- 282.** Hybrid NH₂-MIL-125 (Ti) and ZnCr-LDH photocatalyst for improving H₂ production under visible light. **M. Sohail, T. Kim, H. Kim**
- 283.** Mechanism of (*E*)-selective alkene isomerization by a CpRu(PN) catalyst: Combined

- DFT and experimental approach. **T.C. Cao**, A. Cooksy, D. Grotjahn
- 284.** Modeling-guided design of catalytic processes. **K. Gunasooriya**
- 285.** Enhanced visible-light-assisted peroxymonosulfate activation by cobalt-doped mesoporous iron oxide for Orange II dye degradation. **L.A. Achola**, J. Macharia, S.L. Suib
- 286.** Study of surface adsorption of methanol on $Zn_xCe_{1-x}O_{2-y}$ nanoparticles using temperature-programmed desorption and x-ray photoelectron spectroscopy. **K. Gurung**, M.A. Langell
- 287.** Stepwise kinetic study of glucose conversion to ethylene glycol and propylene glycol over Ru/C and AMT catalysts. **B. Liu**
- 288.** Sixty years of Wacker oxidation: Detailed look into the reaction mechanism with density functional theory. **B. Radcliffe**, S. Ghobadi, A.C. Reber, F. Gupton, S.N. Khanna
- 289.** Long range intercrystallite diffusion of Cu^{+2} , Co^{+2} , Ni^{+2} and Pb^{+2} in Zeolite A and ZSM-5 by DRIFT spectroscopy. **S. Nunes**, S. Crawford
- 290.** Effect of catalyst structure on the bis- urea/thiourea mediated ring-opening polymerization of lactones. **U. Inush Kalana**, R. Hewawasam, T. Wright, M. Kiesewetter
- 291.** Bis- and tris- urea H-bond donors for ring-opening polymerization. **R. Hewawasam**, M. Kiesewetter
- 292.** Spectroscopic insights into the origins of selectivity of bimetallic nanocrystal catalysts for hydrodeoxygenation of HMF. **J.D. Lee**, K. Goulas, W. Zheng, J. Lym, S. Yao, D.S. Oh, C. Wang, R.J. Gorte, J.G. Chen, D.G. Vlachos, C.B. Murray
- 293.** Synthesis and reactivity of catalysts containing electron-poor bifunctional ligands. **D. Sattler**, A.L. Rheingold, D. Grotjahn
- 294.** Series of novel Ru(bda) platform complexes by swapping ligands at diaxial positions as potential water oxidation catalysts (WOC). **S. Yazdani**, A.L. Rheingold, D. Grotjahn
- 295.** Multi-layered $Sb-SnO_2/IrTaO_x/TNT$ anode for electrochemical hypochlorous acid production. **Y. Lee**, J. Shin, E. Cho, Y. Park
- 296.** Photoelectrocatalytic degradation of perfluorooctanoic acid by carbon nanosheets modified $g-C_3N_4/BiWO_6$. **P. Shi**
- 297.** Preparation of mesoporous double-layer carbon microsphere-based solid acid catalyst by hydrothermal method and its application in catalytic transesterification of waste frying oil. L. Yang, S. Wang, **H. Yuan**, **H. Liu**
- 298.** Effect of new additives on sulfuric acid catalyzed alkylation of isobutane with C_4 olefins. **J. SiQi**, M. Dong, Y. Hu
- 299.** Biocatalytic synthesis of amino fatty acids. D. Lee, R. Akula, J. Park, **Y. Kwon**
- 300.** Production of 3-hydroxybutanal via aldol addition of acetaldehyde using base catalysis. **g. lee**, H. Lee, J. Kim, S. Jang, N. Kim, S. Byun, J. Joo
- 301.** Unraveling catalytically active Pt-NiO_{1-x} interfacial structure formations on the bimetallic PtNi nanocrystal surface. **T. Kim**, J. Kim, H. Song, J. Shin, R. Ryoo, J. Park
- 302.** Bead-shaped porous oxide adsorbents for adsorption of organic dye. **J. Kim**, N. Kim, H. Lee, G. Lee, S. Byun, S. Jang, J. Joo, I. Park
- 303.** Withdrawn
- 304.** Effect of Mo/Al-MCM-41 on 1-butene self-metathesis. **X. Huo**, **N. Liu***, A. Zhou
- 305.** Cobalt-containing conducting polymers on carbonaceous supports for catalytic hydrogenation of quinoline. **S. Ryabukhin**, V. Asaula, O. Pariiska, Y. Kurys, S.V. Kolotilov, D.M. Volochnyuk
- 306.** DFT study for CO oxidation over Au nanoparticles supported on CeO₂ under catalytic reaction condition. **H. Choi**, H. Kim, H. Ha, K. An, S. Yoon
- 307.** Withdrawn
- 308.** Nitrogen deficient carbon nitride electrocatalysts for Zn-air batteries. **N.K. Wagh**, S.S. Shinde, J. Lee
- 309.** Green synthesis of gold nanoparticles by grape wine residue and their catalytic activities. **H. Liu**
- 310.** Ring closing of aromatic alkynes and gold cavitand substrate selectivity. **L.E. Rusali**, M.P. Schramm
- 311.** *In situ* study of surface reconstruction of cubic Pt₃Co nanoparticles under thermal stimulus using high resolution TEM. **P. Tieu**, W. Gao, Y. Ma, J. Wu, X. Pan
- 312.** Copper catalysts reduce 3-nitrostyrene to 3-vinyl aniline chemoselectively by ammonia borane at ambient conditions. **M. Shen**
- 313.** Pulse plating of copper-tin alloys onto gas diffusion layers for the electroreduction of carbon dioxide. L. Fuller, **S. Sen**
- 314.** Track and quantify the phase transfer catalyst partition between two phases through mass spectra. **B. Xiang**
- 315.** Nickel catalyzed hydrosilylation of carboxylic acids. **C. Gómez Alcántara**, J.J. Garcia
- 316.** Nickel foam and graphene hybrid aerogels supported CeO₂ for VOCs oxidation. J. Luo, W. Chen, **Q. Wang**, K. Yeung
- 317.** Catalytic ethylene/1-hexene copolymerization by Hf/Zr-amine bis(phenolate) and the kinetic and mechanistic study with kinetic modeling. **C.Y. Park**, M. Abu-Omar

- 318.** Determination of phosphoric acid coverage on carbon supported Pt nanoparticles using *in-situ* X-ray absorption spectroscopy. **H. Park**, S. Lee, S. Yoo, J. Jang
- 319.** Exploring the mechanism of Suzuki and Stille coupling via recombinant peptide-directed Pd nanoparticles. **A. Mosleh**, M. Beyzavi, R. Beitle
- 320.** Withdrawn
- 321.** Catalytic properties of immiscible bimetallic catalysts for direct H₂O₂ synthesis. **H. Nam**, D. Kim, Y. Cho, J. Ahn, K. Lee, S. Han, S. Lee
- 322.** Electrocatalytic performance of nanostructured Ni-Cu systems for oxygen evolution reaction. **R.P. Gautam**, C. Barile
- 323.** Solar H₂ production: CuGa_{1-x}Fe_xO₂-carbon nitride as a novel p-n heterojunction for photocatalytic water-splitting. **B. Martinez**, C. Kuo
- 324.** Withdrawn
- 325.** Effect of crystallographic phase of ruthenium nanosponges on arene and substituted arene hydrogenation activity. **S. Ghosh**, B.R. Jagirdar
- 326.** Simultaneous purification of PM and NO_x over 3DOM layered double hydroxide oxide catalysts. **Z. Duan**, J. Liu
- 327.** MOFs in microreactor for organic synthesis. K. He, **O.V. Ezeh**, W. Han, K. Yeung
- 328.** Reductive amination of polypropylene glycol using Ni-CeO₂@Al₂O₃ with high activity, selectivity and stability. H. Chang, G. Lai, C. Lin, C. Lee, C. Chia, C. Hwang, H. Chang, **D. Tsai**

- 8:20** **330.** Single molecule study of heterogeneous catalysis in nanoconfining material. **N. Fang**, B. Dong, Y. Pei, W. Huang
- 8:40** **331.** Role of the solvent in mediating interactions between active sites and the extended surface of zeolites during epoxidation reactions. **D. Flaherty**
- 9:20** Intermission.
- 9:35** **332.** Quantification of rhenium oxide dispersion on zeolite: Effect of zeolite acidity and mesoporosity. **D. Liu**
- 9:55** **333.** Reaction mechanisms and transport effects of methanol-to-olefin (MTO) processes examined by DFT and novel KMC software for zeolites. M. DeLuca, P. Kravchenko, **D.D. Hibbitts**
- 10:35** **334.** Nature and catalytic properties of *in situ* generated Brønsted acid sites on NaY. B. Murphy, J. Wu, **B. Xu**

SECTION B

San Diego Convention Center

Room 1B

Future Insights into Syngas Conversion Catalysis: Symposium in honor of Burtron H. Davis

Cosponsored by ENFL, ENVR, INOR and PHYS
B. Demirel, M. Gnanamani, W. D. Shafer, *Organizers*
H. Kung, *Organizer, Presiding*
N. O. Elbashir, *Presiding*

- 8:00** **335.** Factors that shape the distribution of products obtained from Fischer–Tropsch synthesis. **A.T. Bell**
- 8:45** **336.** Confinements on growth sites of Fischer–Tropsch synthesis: Manifesting in hydrocarbon chain branching. **H. Schulz**
- 9:10** **337.** Fischer–Tropsch synthesis: Comparative study of paraffin to olefin ratio over an iron-based catalyst activated by both syngas and H₂. Y. Yao, X. Liu, J. Fox, D. Glasser, **D. Hildebrandt**
- 9:35** **338.** Fischer–Tropsch: Product selectivity, the fingerprint of synthetic fuels. **W.D. Shafer**, M. Gnanamani, U. Graham, J. Yang, C.M. Masuku, G. Jacobs, B.H. Davis
- 10:00** Intermission.
- 10:15** **339.** Ethylene co-feeding effect on Fischer–Tropsch synthesis to olefin over Co based catalysts. **J. Yang**, C. Ledesma Rodriguez, Y. Qi, A. Holmen, D. Chen
- 10:40** **340.** Effect of promoters (Mn, Mg, Co and Ni) on the Fischer-Tropsch activity and selectivity of KCuFe/mesoporus-alumina catalyst. **S. Badoga**, G. Kamath, A. Dalai
- 11:05** **341.** Oxide decoration of metal particles and its effect on catalysis. **H. Kung**, M. Kung

Catalysis for Environmental & Energy Applications

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WEDNESDAY MORNING – CATL

SECTION A

San Diego Convention Center

Room 1A

Fundamentals of Catalysis in Nanoporous Materials

Cosponsored by ENFL
M. Orazov, *Organizer*
O. Abdelrahman, M. L. Sarazen, *Organizers, Presiding*

- 8:00** **329.** Effect of tight one-dimensional pores on selectivity for C-H activation and C-O bond formation at lattice oxygens of metal oxides. **P. Deshlahra**

SECTION C
San Diego Convention Center
Room 2

Understanding the Role of Water in Solid Acid-Base Catalysis

Cosponsored by ENFL, INOR and PHYS
J. L. White, T. Xu, *Organizers, Presiding*

- 8:00** 342. Interaction of water molecules with protonated zeolites: Ideal Brønsted site structure and beyond. **J. Sauer**
- 8:40** 343. Promoting effect of water on the acid- and base-catalyzed aldol condensation of Cyclopentanone. D. Ngo, T. Bui, G. Li, Q. Tan, B. Wang, **D.E. Resasco**
- 9:10** 344. Illustrating the effects of pH and salinity on water-phase catalysis. **M.S. Wong**
- 9:40** Intermission.
- 9:55** 345. Role of surface and solvent composition in the behavior of adsorbed water in porous and nonporous solid catalysts. **S.L. Scott**, H. Moon, S. Han
- 10:35** 346. Probing by model reactions the effects of water on the surface acidity of some typical solid acids. Q. Dai, T. Lin, **B. Xu**

SECTION D
San Diego Convention Center
Room 3

Catalysis at Metal-Support Interfaces

Cosponsored by ENFL
P. Christopher, S. Crossley, *Organizers, Presiding*

- 8:00** 347. Adhesion energies of metal nanoparticles to catalyst support surfaces: Relationships to metal atom chemical potential, catalyst activity, and lifetime. **C.T. Campbell**
- 8:40** 348. Chemically induced hot electrons at solid/gas and solid/liquid interfaces during hydrogen peroxide decomposition. **S. Lee**, H. Kim, J. Park
- 9:00** 349. Long-ranging metal/oxide interface effects for ZrO₂ supported Pd and Rh particles. **G. Rupprechter**, Y. Suchorski
- 9:20** 350. Understanding the reaction mechanism over active and stable platinum catalyst emerged from tailored perovskite materials. **Y. Jeon**, M. Kothari, D. Miller, J. Irvine
- 9:40** Intermission.

- 9:50** 351. Metal-support interactions and C₁ chemistry on Ni-CeO₂ surfaces. **J. Rodriguez**
- 10:30** 352. STM studies of the surface morphology of metal oxide clusters on metal surfaces. **J. Wang**, K. Goodman, T. Xiao, D.J. Stacchiola, M.G. White
- 10:50** 353. CO₂ hydrogenation on supported metal sulfide/oxide clusters. **Y. Ma**, K. Goodman, J. Wang, M.G. White
- 11:10** 354. Direct detection of hot electrons at metal-oxide interfaces of PtCo bimetallic nanocatalysts. **H. Lee**, J. Lim, K. An, J. Shin, R. Ryoo, Y. Jung, J. Park

SECTION E
San Diego Convention Center
Room 4

Catalytic Conversion of Biomass-Derived Oxygenates

Cosponsored by ENFL
J. Faria, X. Zhu, *Organizers, Presiding*
S. Crossley, *Presiding*

- 8:00** Introductory Remarks.
- 8:05** 355. Catalytic conversion of cellulose and chitin to chemicals. **A. Fukuoka**
- 8:45** 356. Zeolite encapsulated metal nanoparticles for tandem upgrading of biomass derived feedstocks. **B. Xu**
- 9:10** 357. Synthesis of high-density jet-fuel-ranged hydrocarbons using biomass-derived oxygenates. **J. Zou**, L. Pan, G. Nie, X. Zhang
- 9:35** 358. Low temperature aqueous phase hydrogenation of light oxygenates over Ru/TiO₂ catalyst: Study of model compounds. **H. Bergem**, R. Xu, R.C. Brown, G.W. Huber
- 9:55** Intermission.
- 10:10** 359. Catalytic hydropyrolysis: Effect of CoMo loading and support acidity. **A.D. Jensen**, M.Z. Stummann, J. Gabrielsen, A.B. Hansen, P. Jensen, M. Høj
- 10:40** 360. From Kraft lignin to aromatics over molybdenum catalysts: Effect of crystal phases and supports. **K. Wu**, H. Lu, **B. Liang**
- 11:00** 361. Conversion of biomass-derived polyols and carbonyl compounds to valuable products by catalytic reductive etherification. **M.L. Tulchinsky**, J.R. Stutzman, E.J. Molitor
- 11:20** 362. Direct liquid-phase amination of phenols into anilines and cyclohexylamines. **T. Cuypers**, P. Tomkins, D. De Vos

SECTION A

San Diego Convention Center

Room 1A

Fundamentals of Catalysis in Nanoporous Materials

Cosponsored by ENFL

M. L. Sarazen, *Organizer*

O. Abdelrahman, M. Orazov, *Organizers, Presiding*

- 1:00** **363.** Single-site versus single-ion catalysts in metal–organic frameworks. **O.K. Farha**
- 1:40** **364.** NO oxidation in Brønsted acidic chabazite within low and high temperature regimes: Theoretical study. **T. Salavati-fard**, R.F. Lobo, L. Grabow
- 2:00** **365.** Investigation of the active Bronsted acid site for the DME carbonylation reaction in chabazite-type zeolites. **M. Lusardi**, M.E. Davis
- 2:20** Intermission.
- 2:40** **366.** Integrated experiment and modeling of Raman spectra of zeolites. T. Wang, S. Luo, W. Fan, **S.M. Auerbach**
- 3:20** **367.** Interplay between structure and product selectivity of CO₂ hydrogenation over Co₃O₄ catalysts. **C. Yang**, S. Liu, Y. Wang, Z. Zhao, R. Mu, J. Gong
- 3:40** **368.** Encapsulation of molecular catalysts in metal–organic frameworks. **C. Tsung**

SECTION B

San Diego Convention Center

Room 1B

In Situ & Operando Spectroscopy

Cosponsored by ENFL and PHYS

M. Orazov, B. Xu, *Organizers, Presiding*

- 1:00** **369.** *Operando* studies of cobalt oxide by NAP-XPS, XAS and IR: Commercial and model catalysts. **G. Rupprechter**, K. Föttinger, C. Rameshan, L. Lukashuk, N. Yigit, K. Anic
- 1:20** **370.** Simultaneous *operando* FTIR & Raman study (IRRaman) for unraveling the propane ODH mechanism over V-based catalysts. **M. Guerrero-Perez**, J.J. Ternero-Hidalgo, M.A. Banares, R. Portela, P. Bazin, G. Clet, M. Daturi
- 1:40** **371.** Elucidating the molecular origins of the product selectivity of electrocatalytic CO reduction. **M. Waagele**
- 2:10** **372.** Identifying site-dependent reactivity on the surface of single Au and Pt nanoparticles. **E. Gross**
- 2:30** Intermission.

- 2:50** **373.** Adsorption and activation of O₂ over Cu single-site over ceria surface. **F. Wang**
- 3:10** **374.** Tracking CO-induced migration of highly dispersed Pd in Au nanoparticles supported on raspberry colloid-templated silica. **E. Guan**, W. Chen, A. Foucher, T. Shirman, J. Aizenberg, D.J. Stacchiola, C.M. Friend, A. Frenkel
- 3:30** **375.** Role of *in situ* spectroscopy in elucidating the impact of Pd coordination on the catalytic reduction of O₂ to H₂O₂ on bimetallic nanoparticles. **D. Flaherty**
- 4:00** **376.** Spectroscopic characterization of a highly selective NiCu₃/C hydrodeoxygenation catalyst. **J.D. Lee**, K. Goulas, W. Zheng, J. Lym, S. Yao, D.S. Oh, C. Wang, R.J. Gorte, J.G. Chen, D.G. Vlachos, C.B. Murray
- 4:20** **377.** Withdrawn

SECTION C

San Diego Convention Center

Room 2

Understanding the Role of Water in Solid Acid-Base Catalysis

Cosponsored by ENFL, INOR and PHYS

J. L. White, T. Xu, *Organizers, Presiding*

- 1:00** **378.** Impact of water on acid-base catalyzed reactions: From gas-solid to liquid-solid interfaces. **J.A. Lercher**
- 1:40** **379.** Solvent effects on acid-base interactions in zeolites probed by isothermal titration calorimetry. **R.M. Rioux**, Y. Mu, L. Wang, S. Ogozaly
- 2:10** **380.** Stability of zeolite H-BEA in hot H₂O studied by *operando* magic angle spinning NMR. **J.Z. Hu**, N.R. Jaegers, M. Hu, O.Y. Gutierrez Tinoco, M.A. Derewinski, Y. Wang, J.A. Lercher
- 2:40** **381.** Investigation of water interactions with HZSM-5 and impacts on catalyst reactivity. **K. Chen**, M. Abdolrahmani, S. Horstmeier, S. Crossley, D.E. Resasco, I. Hung, Z. Gan, J.L. White
- 3:10** Intermission.
- 3:25** **382.** First-principles kinetic Monte Carlo study of biomass conversion over titania supported ruthenium catalyst. **X. Li**, L. Grabow
- 3:55** **383.** Theoretical investigation of aldol condensation of formaldehyde and acetone on anatase TiO₂(101) surface. **Y. Zhao**, H. Wang, X. Zhu, Q. Ge, D. Mei
- 4:25** **384.** Influence of substrate complexity on the enthalpy-entropy compensation for rate enhancement in molecular sized confinements. **M. Shetty**, H. Wang, O.Y. Gutierrez Tinoco, D.M. Camaioni, J.A. Lercher

SECTION D
San Diego Convention Center
Room 3

Amorphous Materials: Challenges & Opportunities

Cosponsored by ENFL

N. A. Brunelli, A. Kulkarni, *Organizers, Presiding*

- 1:00** **385.** Amorphous catalysts from global optimization and statistical analysis. G. Sun, B. Zandkarimi, A. Alexandrova, **P. Sautet**
- 1:20** **386.** Research opportunities in chemical upcycling of polymers. **P.F. Britt**, G.W. Coates, K.I. Winey
- 1:40** **387.** Dynamic catalytic interfaces: Ensembles of multiple metastable states break the rules of catalysis. **A. Alexandrova**
- 2:00** **388.** Synthesis of biobased lubricants using Pd/CeZrOx catalysts. **T.J. Schwartz**, G. van Walsum
- 2:20** Intermission.
- 2:40** **389.** Modifying catalyst environments in amorphous silica supports via surface functionalization: Spectroscopic and reactivity studies. **I.I. Slowing**
- 3:00** **390.** Accurate modeling of amorphous silica catalyst supports. **K. Johnson**, A. Bagussety, C. Ewing, G. Vesper, D. Lambrecht, J. McCarthy
- 3:20** **391.** Examining structure-function relationships of mesoporous catalytic materials for biomass conversion. **N.A. Brunelli**
- 3:40** **392.** Modeling the preparation and operation of amorphous catalysts. **B. Peters**, S. Khan, C. Vandervelden, S.L. Scott
- 4:00** **393.** Post-synthesis deposition of mesoporous niobic acid with improved thermal stability by kinetically controlled sol-gel overcoating. **Y. Du**, F. Héroguel, X. Nguyen, J. Luterbacher

SECTION E
San Diego Convention Center
Room 4

Catalytic Conversion of Biomass-Derived Oxygenates

Cosponsored by ENFL

J. Faria, X. Zhu, *Organizers, Presiding*

S. Crossley, *Presiding*

- 1:00** Introductory Remarks.
- 1:05** **394.** Deoxygenation of biomass pyrolysis vapors: Linking model compound studies and biomass catalytic fast pyrolysis experiments at multiple scales to inform catalyst development. **J. Schaidle**
- 1:30** **395.** Steam reforming of dimethyl ether over efficient dual-sites copper catalysts. **X. Li**

- 1:55** **396.** Synergetic effect of manganese on the hydrodesulfurization and hydrodeoxygenation properties of nickel-promoted MoS₂/Al₂O₃. **G. Berhault**, A. Lopez-Benitez, I. Vazquez-Garrido, A. Guevara-Lara
- 2:15** **397.** Enhancing the activity of Pd for carbonyl hydrogenation through functionalization of the carbon support. **K. Koh**, U. Sanyal, O.Y. Gutierrez Tinoco, M. Lee, V. Glezakou, R. Rousseau, M.A. Derewinski, A.J. Karkamkar
- 2:30** **398.** Structural effect of Ni/ZrO₂ catalyst on CO₂ methanation with enhanced activity. **X. Jia**, C. Liu
- 2:45** Intermission.
- 3:00** **399.** Visible-light-driven coproduction of diesel precursors and hydrogen from lignocellulose-derived methylfurans. **N. Luo**, F. Wang
- 3:25** **400.** Kinetics-assisted design of carbon supported catalysts for oxidation reactions. **X. Duan**
- 3:50** **401.** Insights into the electrochemical conversion of biomass derivatives to fuels and chemicals. A. Román, J. Hasse, **A. Holewinski**
- 4:10** **402.** Hollow Au-ZnO/CN nanocages derived from ZIF-8 for efficient visible-light-driven hydrogen evolution from formaldehyde alkaline solution. **H. Wang**, H. Yang, X. Zhu, Q. Ge
- 4:30** **403.** Selective oxidation of glucose using Au-Pd NPs immobilized on nanostructured ceria and titania: Influence of bimetallic composition and support morphology. **M. Khawaji**, Y. Zhang, I. Graça, D. Chadwick
- 4:45** **404.** MoO_x-modified Ni catalysts with unique properties for hydrodeoxygenation of m-cresol. **F. Yang**, X. Zhu, D.E. Resasco

Catalysis for Environmental & Energy Applications

Catalysis for Energy Application

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THURSDAY MORNING – CATL

SECTION A
San Diego Convention Center
Room 1A

General Catalysis

S. Crossley, *Organizer, Presiding*

- 8:00** **405.** Automated high throughput *in silico* reaction screening for design and discovery of enhanced reactivity and tailored chemo-, regio-, and stereo-selectivity. **T.J. Mustard**, T.F. Hughes, A. Bochevarov,

- L.D. Jacobson, H.S. Kwak, T. Morisato, J.L. Gavartin, S. Pandiyan, M. Halls
- 8:20 406.** Mechanism informed general strategy for optimizing the quantum efficiency of photoredox hydroamidation catalysis. **Y. Qin**, S. Ruccolo, C. Schnedermann, D.G. Nocera
- 8:40 407.** Nanostirrers for catalytic reactions inside microdroplets. **W. Song**
- 9:00 408.** Acceleration vs. accuracy: Influence of basis set quality on the mechanism and dynamics predicted by *ab initio* molecular dynamics. **S. Yamijala**, Z. Ali, B.M. Wong
- 9:20 409.** Explicit solvation prediction of band edges of transition metal oxide photocatalysts: Optimal methodology for dealing with localized *d* orbitals in aqueous environments. **K. Park**, A.M. Kolpak
- 9:40** Intermission.
- 9:50 410.** Evaluating research catalysts by combined performance, cost, and life-cycle analysis: Application of the free CatCost tool to catalysts for biomass upgrading to fuels. **K.M. Van Allsburg**, F.G. Baddour, J.D. Super, L. Snowden-Swan, E.C. Tan, J.A. Schaidle
- 10:10 411.** Synthesis and design of cobalt complexes combined with frustrated Lewis pairs to study their reactivity with hydrogen. **M. Tsai**
- 10:30 412.** Crystal phase induced enhanced photocatalytic properties of Zn-Fe₂O₄/Au nanocomposite: Experimental and theoretical studies. **C.A. Huerta-Aguilar**, T. Pandiyan, I.A. Reyes-Dominguez, A.A. Ramirez-Alejandre, J.A. Arenas-Alatorre
- 10:50 413.** Morphology and phase control of Ni₂P nanoparticles. **X. Lu**, G. Basina, D. Abdullah Ali Gaber, S. Abdullah Ali Gaber, K. Polychronopoulou, Y. Fowad AlWahedi
- 11:10 414.** Micro/mesoporous Au@SiO₂ core-shell nanoparticles for the selective benzyl alcohol oxidation. **S.R. Saunders**, E. Hammond-Pereira, D. Wu
- 11:30 415.** Revealing electrocatalytic performance of hybrid double helix metal nanowire using atomic resolution electron tomography. **X. Song**, A. Bruefach, M. Scott

SECTION B

San Diego Convention Center
Room 1B

In Situ & Operando Spectroscopy

Cosponsored by ENFL and PHYS

M. Orazov, B. Xu, *Organizers, Presiding*

- 8:00 416.** *Operando* MAS-NMR investigation of Ni/ - Al₂O₃-catalyzed hydrogenolysis of alkyl aryl ether. **A. Chamas**, L. Qi, S.L. Scott

- 8:20 417.** Investigations of CO₂ hydrogenation by high-pressure NMR spectroscopy. **J.C. Linehan**, K. Grubel, A. Preston, A.M. Appel, S.E. Flowers, E.S. Wiedner
- 8:40 418.** *In situ* neutron scattering and kinetic studies of mayenite-electride-supported ruthenium nanoparticles for ammonia synthesis. **J. Kammert**, J. Moon, Y. Cheng, K. Page, L. Daemen, A. Ramirez-Cuesta, J. Tong, Z. Wu
- 9:00 419.** Investigating the role of Ni and Cu in PtNiCu catalysts for the ethanol oxidation reaction using *in situ* electrochemical surface enhanced infrared absorption spectroscopy (SEIRAS). **S. Jilani**, D. Chen, C. Cohen, Y. Tong
- 9:20** Intermission.
- 9:40 420.** Realizing the behavior of metal center during the water oxidation through *operando* X-ray spectroscopy. **H. Chen**
- 10:00 421.** Effects of doping Zr into the ceria support for the methane dry reforming reaction on Ni/CeO₂ catalyst. **F. Zhang**, S.D. Senanayake, J. Rodriguez
- 10:20 422.** Online kinetics study of oxidative coupling of methane over La₂O₃ for C₂ activation. **Y. Yang**, Z. Liu, E. Vovk, X. Zhou, C. Guan, J. Li, S. Li

SECTION C

San Diego Convention Center
Room 2

General Catalysis

S. Crossley, *Organizer, Presiding*

- 8:00 423.** Mo based sulfated hafnia: Novel solid acid catalyst for activation of ethane. **A. Abedin**, S. Kanitkar, S. Bhattar, J.J. Spivey
- 8:20 424.** Breaking the scaling relationship via thermally stable Pt/Cu single atom alloys for propane dehydrogenation. **G. Sun**, Z. Zhao, J. Gong
- 8:40 425.** Methane to methanol conversion facilitated by metal methoxides: Case of FeOCH₃⁺. **N. Khan**, E. Miliordos
- 9:00 426.** Oxidation of cyclohexane: Kinetic studies of a series of To^MMX catalysts. **K. Basemann**, R. Reinig, Z. Weinstein, T.L. Windus, A.D. Sadov
- 9:20 427.** Oxidative carbon-carbon (C-C) homocoupling and C-C cross-coupling reactions using copper-based nanocatalysts. A. Ravi Teja, **M. Andiappan**
- 9:40** Intermission.
- 9:50 428.** Withdrawn
- 10:10 429.** Kinetics analysis of selective organometallic catalysts for alkene isomerization. **A.L. Cooksy**, E.R. Paulson, T.C. Cao, D. Grotjahn
- 10:30 430.** Micellar approaches towards mild biphasic catalytic epoxidation of olefins with hydrogen peroxide. **F. Schmidt**, B. Zehner, A. Jess, M. Cokoja

- 10:50 431.** Feasibility study of chemical looping epoxidation of ethylene. **S. Gabra**, S. Scott, J. Dennis
- 11:10 432.** Analysis of synthesized PtNi, PtCo, and PtNiCo for the ethanol electrooxidation reaction. **C. Cohen**, S. Jilani, Y. Tong
- 11:30 433.** Machine learning catalytic reactions. **T. Rhone**, C. O'Connor, R. Hoyt, M. Montemore, C. Kumar, A. Yacoby, C.M. Friend, E. Kaxiras

THURSDAY AFTERNOON – CATL

SECTION A

San Diego Convention Center

Room 1A

General Catalysis

S. Crossley, *Organizer, Presiding*

- 1:00 434.** Exploring metal-support interactions to immobilize sub-nm co clusters on g-Mo₂N: A highly selective and stable catalyst for CO₂ activation. **S. Yao**, J. Rodriguez
- 1:20 435.** Huge enhancement of CO₂ capture performance in amine solution using acid-base bifunctional catalyst. **X. Zhang**, H. Gao, Z. Liang, M. Fan
- 1:40 436.** Tuning the edge sites of MoS₂ and catalytic performance in sulfur-resistant methanation of syngas. **J. Shen**, M. Li, X. Ma
- 2:00 437.** Design of nanostructured heterogeneous metal catalysts for CO₂ hydrogenation to formic acid. **K. Mori**, T. Sano, H. Yamashita
- 2:20 438.** Layered Zn₂[Co(CN)₆](CH₃COO) double metal cyanide with improved catalytic performance. **C. Marquez**, D. De Vos, T. De Baerdemaeker
- 2:40** Intermission.
- 2:50 439.** Hydrogen evolution reaction on coupled gamma-Mo C/graphene catalysts: Insights from a new first-principles kinetic approach. **T.T. Yang**, W. Al-Saidi
- 3:10 440.** Withdrawn
- 3:30 441.** Roles of surface properties of amorphous TiO₂ in photocatalytic CO₂ reduction. **A. Kharade**, S. Chang
- 3:50 442.** Photocatalysis meets magnetic recovery: Silica-coated MNPs as photocatalytic supports. **J. Terra**, A.H. Moores
- 4:10 443.** Determination of the active sites of bimetallic Pt/Ni catalysts in reverse water gas shift reaction. **A. Ebrahim**, Y. Li, A. Frenkel
- 4:30 444.** Plasmonic hot-carrier-mediated tunable photochemical reactions. **Y. Zhang**, T. Nelson, S. Tretiak, G.C. Schatz

SECTION C

San Diego Convention Center

Room 2

General Catalysis

S. Crossley, *Organizer, Presiding*

- 1:00 445.** Mechanistic investigation of biocatalytic heme carbenoid Si-H insertions. **R. Khade**, **Y. Zhang**
- 1:20 446.** Silica-supported tantalum amido [(Si-O) Ta(=N^tBu)(NMeEt)₂] catalyst designed with well-defined nitrogen-based fragments for hydroamination of alkyne. **M.A. Alrefai Aljuhani**
- 1:40 447.** Applications of heterodonor carbene-N/S ligands in catalysis: From dehydrogenation reactions to asymmetric hydrogenation. **O. Pamies**, M. Albrecht, M. Diéguez
- 2:00 448.** Heterogeneous base-catalyzed transesterification. **C. Zhang**, H. Lamb
- 2:20 449.** Understanding catalytic efficiency and the mechanism of trans-esterification in vitrimer polymers using density functional theory. **S. Bhusal**, G.S. Kedziora, R. Yixin, V. Varshney, D. Nepal, A. Roy
- 2:40** Intermission.
- 2:50 450.** Catalytic esterification of N,N-dialkyl amides by alkoxy-bridged tetranuclear manganese cluster with N,N-bidentate ligand. **H. Nagae**, T. Hirai, D. Kato, S. Soma, S. Akebi, K. Mashima
- 3:10 451.** Catalytic *in situ* upgrading of bio-oil derived from microalgae hydrothermal liquefaction over modified SBA-15 in biphasic solvents. **J. Bian**, C. Li, L. Feng
- 3:30 452.** Continuous production of fuel grade liquid hydrocarbons from fatty acids using Mo-based catalysts. **M.B. Chowdhury**, M. Hossain, A. Jhavar, S.J. Fraser, P. Charpentier
- 3:50 453.** New gold catalysts in the hydrohydrazination of alkynes under ambient condition. **S. Yazdani**, R.F. Jazzar, D. Grotjahn, G. Bertrand
- 4:10 454.** Hollow nanostructured catalysts for carbon-oxygen bonds hydrogenation reactions: Balanced adsorption-diffusion effect. **D. Yao**, Y. Wang, X. Ma
- 4:30 455.** Withdrawn

CCS

COMMITTEE ON CHEMICAL SAFETY

MONDAY MORNING – CCS

Academic Lab Safety

Sponsored by CHED, Cosponsored by CCS and CHAS

MONDAY AFTERNOON – CCS

Academic Lab Safety

Sponsored by CHED, Cosponsored by CCS and CHAS

TUESDAY MORNING – CCS

Connecting Safety, Education, Training & Productivity in Analytical Laboratories

Sponsored by ANYL, Cosponsored by CCS, CHAS, CINF and PRES

TUESDAY AFTERNOON – CCS

Cannabis & Water: Merging the Insoluble

Sponsored by CHAS, Cosponsored by CCS

Chemistry of Disasters

Sponsored by PRES, Cosponsored by CCS, CHAS and I&EC

WEDNESDAY MORNING – CCS

Graduate Students Perspective on Safety Education

Sponsored by CHAS, Cosponsored by CCS

WEDNESDAY AFTERNOON – CCS

Cannabis & Hemp Analytical Science: The Glass is (More Than) Half-Full

Sponsored by CHAS, Cosponsored by CCS

CEI

COMMITTEE ON ENVIRONMENTAL IMPROVEMENT

SUNDAY MORNING – CEI

Chemists Without Borders: Celebrating 15 Years of Scientific/Humanitarian Collaboration

Sponsored by MPPG, Cosponsored by CEI and ENVR

Characterization of Plastics in Aquatic Environments

Sponsored by POLY, Cosponsored by ANYL, BIOL, CEI, ENVR, I&EC, PMSE and PRES

SUNDAY AFTERNOON – CEI

Chemistry & Water: Opening Session

Sponsored by MPPG, Cosponsored by CEI, ENVR and PRES

Characterization of Plastics in Aquatic Environments

Sponsored by POLY, Cosponsored by ANYL, BIOL, CEI, ENVR, I&EC, PMSE and PRES

MONDAY MORNING – CEI

Current Advances in Water Analysis: From Citizen Scientists to Laboratory Breakthroughs

Sponsored by ENVR, Cosponsored by AGRO and CEI

Green & Sustainable Chemistry Theory & Practice: Chemistry & Water

Sponsored by CHED, Cosponsored by CEI and I&EC

MONDAY AFTERNOON – CEI

Holistic Approaches to Sustainability in Chemical Businesses

Sponsored by SCHB, Cosponsored by CEI

Nanomaterials & Sustainability

Sponsored by ENVR, Cosponsored by CEI

Green Chemistry & the Environment

Sponsored by ENVR, Cosponsored by CEI

TUESDAY MORNING – CEI

Going with the Flow of Water: Career Paths & Journeys

Going with the flow of water: career paths and journeys

Sponsored by YCC, Cosponsored by CEI

State of the Art: Diversity & Inclusion in Chemistry Education

Sponsored by CHED, Cosponsored by CEI and PROF

Nanomaterials & Sustainability

Sponsored by ENVR, Cosponsored by CEI

TUESDAY AFTERNOON – CEI

Environmental Chemistry through the Transformative Power of Film: A Showcase of CEI-ENVR Environmental Film Competition Awardees

Sponsored by MPPG, Cosponsored by CEI and ENVR

Nanomaterials & Sustainability

Sponsored by ENVR, Cosponsored by CEI

TUESDAY EVENING – CEI

Green Chemistry & the Environment

Sponsored by ENVR, Cosponsored by CEI

Nanomaterials & Sustainability

Sponsored by ENVR, Cosponsored by CEI

Safeguarding Water Quality in a Climate of Change

Sponsored by ENVR, Cosponsored by CEI

WEDNESDAY MORNING – CEI

Safeguarding Water Quality in a Climate of Change

Sponsored by ENVR, Cosponsored by CEI

WEDNESDAY AFTERNOON – CEI

Safeguarding Water Quality in a Climate of Change

Sponsored by ENVR, Cosponsored by CEI

THURSDAY MORNING – CEI

Safeguarding Water Quality in a Climate of Change

Sponsored by ENVR, Cosponsored by CEI

CELL

DIVISION OF CELLULOSE AND RENEWABLE MATERIALS

W. Thielemans and G. Larkin, *Program Chairs*

SUNDAY MORNING – CELL

SECTION A

Marriott Marquis San Diego Marina
Rancho Santa Fe 1

Lignin Based Bioproducts

G. Beckham, E. L. Hegg, J. Luterbacher, M. Nejad, M. Paleologou, *Organizers*
D. Hodge, *Organizer, Presiding*
N. A. Rorrer, *Presiding*

- 8:30 Introductory Remarks.
- 8:35 1. Recent progress in the generation of lignin based water soluble polymers. **P. Fatehi**
- 9:00 2. Lignin-based thermoplastic blends: Biorefinery willow lignin and polylactic acid (PLA). **M.J. Ovadias**, B. Bujanovic
- 9:25 3. Polymers from biphenyl-linked lignin dimers. **N.A. Rorrer**, J. Anderson, J. Miscall, M. Price, G. Beckham
- 9:50 Intermission.
- 10:05 4. From trees to plastics: High-performance polymers from lignin-rich feedstocks. **T.H. Epps**
- 10:30 5. Radical polymerization of lignin materials. **J. Jimenez**, E. Ford
- 10:55 6. Recyclable and smart thermoset from lignin biophenols. **M.M. Abu-Omar**, S. Zhao, K. Hanson

SUNDAY AFTERNOON – CELL

SECTION A

Marriott Marquis San Diego Marina
Rancho Santa Fe 1

Lignin Based Bioproducts

G. Beckham, D. Hodge, J. Luterbacher, M. Nejad, *Organizers*
E. L. Hegg, M. Paleologou, *Organizers, Presiding*

- 1:00 Introductory Remarks.
- 1:05 7. Characterization and catalytic upgrading of acetal-functionalized lignin. **J. Luterbacher**
- 1:30 8. Insights into the isolation and structural changes of lignin in inorganic ionic liquid. **X. Pan**

- 1:55 9. Oxidative deconstruction of lignin for the production of renewable chemicals and products. **J.K. Mobley**, M. Meier, Z. Fang, M. Crocker, Y. Song, A. Morris, M. Weisenberger, S. Sorensen
- 2:20 Intermission.
- 2:35 10. Lignin modification and/or selection for application in wood adhesives. **F. Monteil-Rivera**
- 3:00 11. Polyurethanes from unmodified technical lignin fractionated by sequential precipitation. **Y. Wang**, P. Sengupta, Y. Pu, C.E. Wyman, C.M. Cai, A.J. Ragauskas
- 3:25 12. Lignin as a polyol replacement in polyurethane applications. **M. Nejad**, M. Alinejad

SUNDAY EVENING – CELL

SECTION A

San Diego Convention Center
TBD

General Posters

G. M. Larkin, *Organizer*

- 7:00 - 9:00
13. Chemoenzymatic synthesis of carboxy-terminated maltooligosaccharides as cross-linking agent. **H. Chigita**, K. Yamamoto, J. Kadokawa
14. Synthesis of 2-deoxyamyloses by phosphorylase-catalyzed enzymatic polymerization. **S. Nakamura**, K. Yamamoto, J. Kadokawa
15. Detoxification of sugarcane bagasse hydrolysate by atmospheric cold plasma to enhance bioethanol production. T. Kuo, H. Wang, **K. Cheng**
16. Production of bacterial cellulose by treating sugarcane bagasse hydrolysate with atmospheric cold plasma. **S. Huang**, K. Cheng
17. Preparation of chitin nanofiber-based composite/hollow particles by Pickering emulsion polymerization. **S. Noguchi**, K. Yamamoto, J. Kadokawa
18. Synthesis of mixed chitin esters in ionic liquid. **H. Hirayama**, K. Yamamoto, J. Kadokawa

- 19.** Dissolution and functionalization of chitin using deep eutectic solvents. **S. Idenoue**, K. Yamamoto, J. Kadokawa
- 20.** Removal of water toxins via ligand-functionalized cellulose-based membranes. **M.A. Khan**, D.G. Drueckhammer, B.S. Hsiao, S.K. Sharma
- 21.** Withdrawn
- 22.** Improving the fouling resistance of nanocellulose membranes for ultrafiltration. **M. Yang**, P. Hadi Myavagh, H. Ma, H. Walker, B.S. Hsiao
- 23.** Increased adsorption capacity for heavy metal ions via sequential oxidation of carboxycellulose nanofibers from raw wood. **M.C. Nolan**
- 24.** Facile synthesis of vanillin from kraft lignin. **R. Zhang**, T. Repo
- 25.** Analyzing the degree of branching in lignins: Theoretical and experimental results. **E. Terrell**, E. Bartolomei, Y. Le Brech, A. Dufour, M. Garcia Perez
- 26.** Dissolution of lignin-rich microfiber from organosolv assisted with catalysts and its regeneration. H. Choi, **J. Lee**, T. Eom
- 27.** Sustainable pathways to increase lignin reactivity for resin applications. **M. Arefmanesh**, E. Master, M. Nejad
- 28.** Lignin-derived carbon nanocomposites as sodium-ion battery anodes. **K. Jiang**, X. Tan, Z. Li
- 29.** Withdrawn
- 30.** Building wind turbines from renewable and recyclable composites. J.R. Dorgan, **B. Tan**, H. Bambhania, D. Cousins

properties. **S. Kumar Singh**, A. Savoy, Z. Yuan, B. Bals, E.L. Hegg, **D. Hodge**

- 10:30** **35.** Chemical funneling of lignin derived monomers into aromatic chemicals. **N. Yan**
- 10:55** **36.** Exploiting the phase behavior of lignin with renewable aqueous solvents: Enabling higher-value applications. **M.C. Thies**, A.A. Ogale

Future of Biomacromolecules at a Crossroads of Polymer Science & Biology

Synthetic Cells

Sponsored by POLY, Cosponsored by BIOL, CARB, CELL, COLL, ENVR, MEDI, PHYS and PMSE

MONDAY AFTERNOON – CELL

Future of Biomacromolecules at a Crossroads of Polymer Science & Biology

Tissue Engineering

Sponsored by POLY, Cosponsored by BIOL, CARB, CELL, COLL, ENVR, MEDI, PHYS and PMSE

MONDAY EVENING – CELL

SECTION A

San Diego Convention Center
TBD

Sci-Mix

G. M. Larkin, W. Thielemans, *Organizers*

8:00 - 10:00

16, 20, 22, 23, 24, 25, 26, 27, 28, 29, 30. See Previous Listings.

TUESDAY MORNING – CELL

SECTION A

Marriott Marquis San Diego Marina
Rancho Santa Fe 1

Advances in Characterizing Modified & Degraded Wood

M. Aro, G. M. Larkin, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 **37.** Thermal conversion chemistry of wood: Consequences for quality control of heat treated wood products. **W. Willems**

MONDAY MORNING – CELL

SECTION A

Marriott Marquis San Diego Marina
Rancho Santa Fe 1

Lignin Based Bioproducts

G. Beckham, E. L. Hegg, D. Hodge, J. Luterbacher, M. Nejad, M. Paleologou, *Organizers*

G. Bauer, M. Nejad, *Presiding*

8:30 Introductory Remarks.

8:35 **31.** Redefining and redesigning lignin. **J. Ralph**, H. Kim

9:00 **32.** Alkaline enzymes for lignin valorization. **A. Mialon**

9:25 **33.** Biomimetic cleavage of β -O-4 bonds using small organic thiols. **E.L. Hegg**, G.E. Klinger, J.E. Jackson

9:50 Intermission.

10:05 **34.** Evaluating the impacts of two-stage alkaline-oxidative pretreatment of hybrid poplar on lignin

- 8:30** **38.** Integrating multi-scale studies of chemically modified wood. J.E. Jakes, **N. Plaza**, C.R. Frihart, C.G. Hunt, D.J. Yelle, L. Lorenz
- 8:55** **39.** Quantification of wood thermal treatment by electron paramagnetic resonance spectroscopy. **J.A. McVay**, S.M. Berry
- 9:20** **40.** Formulated feedstocks for biorefining: Monitoring key biomass chemical characteristics. **T.G. Rials**, N. Labbé, N. Andre, C. Hamilton, J. McCord
- 9:45** Intermission.
- 10:00** **41.** Probing nanostructural changes in chemically modified wood cell walls with small angle neutron scattering. **N. Plaza**, J.E. Jakes, C.G. Hunt, S. Pingali, C.R. Frihart, D. Stone, L. Lorenz, D.J. Yelle
- 10:25** **42.** Beech wood thermal treatment level characterization by different treatment level markers. **W. Willems**, M. Altgen
- 10:50** **43.** Use of X-ray scattering to understand the mechanisms behind the moisture and decay resistance of epoxybutene modified wood. R.E. Ibach, **N. Plaza**
- 11:15** Discussion.

TUESDAY EVENING – CELL

Future of Biomacromolecules at a Crossroads of Polymer Science & Biology

Sponsored by POLY, Cosponsored by BIOL, CARB, CELL, COLL, ENVR, MEDI, PHYS and PMSE

WEDNESDAY MORNING – CELL

SECTION A

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 8

Materials Advances in Nanocellulose Research for Engineered Functionality

Cosponsored by PMSE and POLY
H. Jameel, L. A. Lucia, *Organizers*
L. Pal, P. Sharma, *Organizers, Presiding*

- 8:00** Introductory Remarks.
- 8:05** **44.** Nitro-oxidized carboxycellulose nanofibers. **P. Sharma**, S.K. Sharma, B.S. Hsiao
- 8:30** **45.** Nitro-oxidized carboxy nanocellulose derived from agave for effective removal of lanthanides from water. **S. Sharma**, P. Sharma, B.S. Hsiao
- 8:55** **46.** Developing hydrophobic cellulosic membrane for membrane distillation. **R. Joshi**, T. Lindstrom, B.S. Hsiao

- 9:20** **47.** Designing cellulose nanocrystal films for superhydrophobicity without the use of fluorine-based chemicals. **A. Cordova**, R. Alimohammadzadeh, **I. Sanhueza**, A. Svedberg, A. Horvath
- 9:45** Intermission.
- 10:05** **48.** Carbonized nanocellulose as low-cost 1D carbon nanomaterials for energy storage. **Z. Li**, T. Thundat
- 10:30** **49.** Nanocellulose reinforced polymer composites as flexible mechanical energy harvesters. **K. Shanmuganathan**, F. Ram
- 10:55** **50.** Cellulose nanofibers biotemplated metal nanoparticles as a water dispersible SERS substrate. **C. Rusin**, Y. Boluk, M.T. McDermott
- 11:20** **51.** High performance of PET coated with bionanomaterials in oxygen barrier and optical properties in digital age. **T.H. Thang**, S. Hwang, J. Park, D. Oh
- 11:45** Concluding Remarks.

Future of Biomacromolecules at a Crossroads of Polymer Science & Biology

Delivery Systems

Sponsored by POLY, Cosponsored by BIOL, CARB, CELL, COLL, ENVR, MEDI, PHYS and PMSE

WEDNESDAY AFTERNOON – CELL

Future of Biomacromolecules at a Crossroads of Polymer Science & Biology

Biomaterials

Sponsored by POLY, Cosponsored by BIOL, CARB, CELL, COLL, ENVR, MEDI, PHYS and PMSE

THURSDAY MORNING – CELL

SECTION A

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 8

Materials Advances in Nanocellulose Research for Engineered Functionality

Cosponsored by PMSE and POLY
H. Jameel, L. Pal, *Organizers*
L. A. Lucia, *Organizer, Presiding*

- 8:00** Introductory Remarks.

- 8:05** **52.** Barrier performance of cellulose nanocrystal (CNC) films for high barrier packaging applications. **M. Nuruddin**, R. Chowdhury, J.P. Youngblood, J.A. Howarter
- 8:30** **53.** Spherical cellulose nanoparticles (CNPs) for magnetic resonance imaging (MRI) and X-ray computed tomography (CT). **S. Chakravarty**, F.J. Buchanan, J.M. Hix, E.M. Shapiro
- 8:55** **54.** Superabsorbent from cellulose nanofibers for oil and chemical spill responses. **O. Laitinen**, H. Liimatainen
- 9:20** **55.** Removal of chromium (VI) from aqueous solutions by cationic nanostructured cellulose. **X. Huang**, G. Dognani, P. Hadi Myavagh, B.S. Hsiao
- 9:45** Intermission.
- 10:00** **56.** Bioactive nanocellulose for bacterial capture and anti-adhesion. H. Dong, J. Terrell, J.P. Jahnke, M. Hurley, **D.N. Stratis-Cullum**, T. Zu
- 10:25** **57.** Improved dispersion and interfacial bonding between nanocellulose and poly(lactic acid) using solvent infiltration and ball milling methods. **M. Li**, Y. Pu, Y. Deng, K. Nelson, A.J. Ragauskas
- 10:50** **58.** Redispersible chitin nanocrystals extracted through electron beam irradiation followed by high pressure homogenization. **H. Lee**, J. Shin
- 11:15** **59.** Fabrication of high-strength antimicrobial chitosan-nanocellulose composite coatings. P. Tyagi, L.A. Lucia, M.A. Hubbe, H. Jameel, **L. Pal**
- 11:40** Concluding Remarks.

CHAL

DIVISION OF CHEMISTRY AND THE LAW

K. Bianco and K. McIntyre, *Program Chairs*

SUNDAY MORNING – CHAL

Nothing New Under the Sun: The Practical Challenges of Patent Novelty Searching

Sponsored by CINF, Cosponsored by CHAL and CPRM

SUNDAY AFTERNOON – CHAL

SECTION A

San Diego Convention Center
Room 30B

Strengthening Your Patent Rights in Light of Recent Federal Circuit Court Decisions

X. Pillai, *Organizer, Presiding*

- 2:00 1. Strengthening your future patent rights in light of recent Federal Circuit court and USPTO decisions. X. Pillai, R. Bone

MONDAY MORNING – CHAL

SECTION A

San Diego Convention Center
Room 30B

Protecting Your Inventions

J. Gledhill, J. Landells, *Organizers*
D. Weingarten, *Presiding*

- 9:00 2. Inventor or contributor? A U.S. perspective. D. Weingarten
- 9:30 3. Navigating patent term adjustment (PTA) and patent term extension (PTE). M. Garcia
- 10:00 4. Uncovering the secrets of “on-sale bar” in Australia, New Zealand, and Southeast Asia. J. Gledhill

- 10:30 5. Securing priority dates for patents in Australia, New Zealand, and Southeast Asia. J. Landells
- 11:00 6. Protecting inventions through litigation in the United States: What every chemist needs to know. J. Smyth

MONDAY AFTERNOON – CHAL

SECTION A

San Diego Convention Center
Room 30B

Evolution of the Chemistry Legal Landscape

R. Smith, *Organizer, Presiding*

- 2:00 7. Blunt talk about cannabis patents. V. Capuano
- 3:00 8. What your competitors don't know can hurt you: Strategies to avoid secret sales from invalidating your patent. V. Norton
- 3:30 9. Layers upon layers of layer complexity: simple chemistry made complex by patent laws. R. Smith
- 4:00 10. Antibody purification is sometimes not quite so obvious. R. Prince

MONDAY EVENING – CHAL

SECTION A

San Diego Convention Center
TBD

Sci-Mix

K. E. Bianco, K. McIntyre, *Organizers*

- 8:00 - 10:00
11. Chocolate: Food of the gods. H.M. Peters, S.B. Peters
12. National Inventors Hall of Fame 2019. H.M. Peters, S.B. Peters

TUESDAY MORNING – CHAL

SECTION A

San Diego Convention Center
Room 30C

Beyond the Bench: Non-Traditional Careers in Chemistry

Cosponsored by PROF and YCC

J. L. Kennedy, *Organizer*

K. McIntyre, *Presiding*

- 9:30 13. Beyond the bench: Nontraditional careers in chemistry. **K. McIntyre, R. Bone**

TUESDAY AFTERNOON – CHAL

SECTION A

San Diego Convention Center
Room 30C

The Many Faces of CHAL: Where Chemistry Meets the Law

K. E. Bianco, *Organizer*

K. McIntyre, *Organizer, Presiding*

K. A. Rubino, *Presiding*

- 1:00 14. How to allocate resources to IP as a start-up in the chemical fields. **K.A. Rubino**
- 1:30 15. Intellectual indexing makes the difference. **E.N. Cheeseman, M. McBride**
- 2:00 16. Protecting innovations: Multi-prong approach to intellectual property. **H. Oh**
- 2:30 17. Visualization of latent fingerprints by copper nanoclusters with variable fluorescent. **R. Huang, D. Peng, J. Yang**
- 3:00 18. Cr- and Sb-doped TiO₂ nano-pigment for the latent and bloody fingermark enhancement on various surfaces. **D. Peng, J. Yang, R. Huang**

THURSDAY AFTERNOON – CHAL

Legal Challenges & Landmark Lawsuits in Agrochemicals

Sponsored by AGRO, Cosponsored by CHAL

CHAS

DIVISION OF CHEMICAL HEALTH AND SAFETY

D. Decker and J. Pickel, *Program Chairs*

SUNDAY AFTERNOON – CHAS

SECTION A

Marriott Marquis San Diego Marina
Rancho Santa Fe 3

Division of Chemical Health & Safety Awards

Cosponsored by PROF
K. J. Brown, *Organizer*
K. Brown, *Presiding*

- 1:30 Introductory Remarks.
1:50 1. Seeking the promised land of chemical safety. **K.P. Fivizzani**
2:20 2. Safety-culture growth catalyzed by an undergraduate laboratory safety course. **E.M. Huston, K.M. Duval**
2:50 3. What can we learn from Lemony Snicket?. **S.B. Sigmann**
3:20 Intermission.
3:35 4. Leading from the front: Thoughts for the next generation of safety (and CHAS) leaders. **H.J. Elston**
4:05 5. Rasmussen's risk management framework applied to academic laboratory safety. **S.J. Sommer**
4:35 Concluding Remarks.

MONDAY MORNING – CHAS

SECTION A

Marriott Marquis San Diego Marina
Rancho Santa Fe 3

Connecting Professionalism, Safety & Ethics: Opportunities & Challenges

Cosponsored by CINF
K. M. Lopez, *Organizer*
C. I. Nitsche, R. Stuart, *Presiding*

- 8:30 Introductory Remarks.
8:35 6. Safety for one, safety for all: Overcoming challenges to sharing chemical incident data. **K.M. Kulinowski**

- 8:55 7. Learnings from a community safety data sharing experiment. **C.I. Nitsche**, G. Whittick, M. Manfredi
9:15 8. Global Chemists' Code of Ethics: Connecting safety, security, and responsible practices in the chemical sciences. **L. Brown**
9:35 9. Safety: International chemical society approach. **B.S. Chance**
9:55 Intermission.
10:10 10. Introducing a safety guidance chapter in the fourth edition of the ACS Style Guide. **S.B. Sigmann**, L.R. McEwen, S.R. Goode
10:30 11. Why metrics matter. **S.I. Addlestone**
10:50 12. Withdrawn
11:10 Panel Discussion.

Academic Lab Safety

Sponsored by CHED, Cosponsored by CCS and CHAS

MONDAY AFTERNOON – CHAS

SECTION A

Marriott Marquis San Diego Marina
Rancho Santa Fe 3

Connecting Professionalism, Safety & Ethics: Opportunities & Challenges

Cosponsored by CINF
K. M. Lopez, *Organizer*
C. I. Nitsche, R. Stuart, *Presiding*

- 1:30 Introductory Remarks.
1:35 13. Backing into safety culture. **P.A. Reinhardt**
1:55 14. Professionalism, safety and ethics: Improving safety culture. **R.M. Izzo**
2:15 15. Engaging senior management to improve the safety culture of a chemical development organization thru the SPYDR (safety as part of your daily routine) lab visit program. **V.W. Rosso**
2:35 16. Understanding the dimensions of risk. **R. Stuart**
2:55 Panel Discussion.

SECTION A

Marriott Marquis San Diego Marina
Rancho Santa Fe 3

CHAS 40th Anniversary Symposium

Cosponsored by HIST
R. Stuart, *Presiding*

- 3:30** Introductory Remarks.
- 3:35** **17.** PubChem LCSS. **J. Zhang**, P. Thiessen, A. Gindulyte, E. Bolton, L.R. McEwen, R. Stuart
- 3:55** **18.** Evolution of “safety” within the ACS world. **R. Stuart**
- 4:15** **19.** 40 years as an environment, health and safety professional. **M.B. Koza**
- 4:35** **20.** CHAS at 40: Twenty years of editor’s insight on professional safety communication. **H.J. Elston**
- 4:55** **21.** From YCC to SCC: Fun times in the Division of Chemical Health and Safety. **D.M. Decker**

Academic Lab Safety

Sponsored by CHED, Cosponsored by CCS and CHAS

MONDAY EVENING – CHAS

SECTION A

San Diego Convention Center
TBD

Sci-Mix

J. M. Pickel, *Organizer*

8:00 - 10:00

- 22.** Capitalizing on teachable moments to enhance a culture of safety. **M.C. Box**, M.T. Gallardo-Williams
- 23.** Safe and economical handling of bulk low-density nanomaterials. **V. Gangoli**, P. Raja, A.R. Barron
- 24.** Multispectral imaging for examination of laboratory contamination. **D.R. Kuespert**, K.J. Brown
- 25.** Division of chemical health and safety information posters. **J.M. Pickel**

TUESDAY MORNING – CHAS

SECTION A

Marriott Marquis San Diego Marina
Rancho Santa Fe 3

Cannabis Production: Streamlining the Flow

T. R. Towle, *Organizer, Presiding*

- 8:30** Introductory Remarks.
- 8:40** **26.** Front end engineering, quality by design, HACCP, GMP, OSHA, and cannabis. Industry jargon or hidden treasures? What they all have in common and why you should care. **D. Vaillencourt**
- 9:05** **27.** Establishing successful and sustained employee engagement for quality cannabis production. **K. Peña**
- 9:30** **28.** Scaling up production for a GMP cannabis facility. **S. Maletich**
- 9:55** Intermission.
- 10:10** **29.** Raising the bar for cannabis extraction methods: Introducing a novel, safe, efficient, and environmentally friendly approach to extracting high quality cannabis resins. **T.R. Towle**
- 10:35** **30.** Fundamental chemistry research from a collaborative cannabis research venture. **M. Roggen**
- 11:00** **31.** AuditPROhbx: Automating the compliance process. **E.M. Pryor**
- 11:25** **32.** Comparison of methods for complete removal of terpenes during extraction. **G. Ray**

Connecting Safety, Education, Training & Productivity in Analytical Laboratories

Sponsored by ANYL, Cosponsored by CCS, CHAS, CINF and PRES

TUESDAY AFTERNOON – CHAS

SECTION A

Marriott Marquis San Diego Marina
Rancho Santa Fe 3

Cannabis & Water: Merging the Insoluble

Cosponsored by CCS
N. Arora, *Organizer, Presiding*

- 1:30** Introductory Remarks.
- 1:35** **33.** Cannabis product critical safety attributes and critical quality attributes and good distribution practices. **A. Samann**

WEDNESDAY AFTERNOON – CHAS

SECTION A

Marriott Marquis San Diego Marina
Rancho Santa Fe 3

Cannabis & Hemp Analytical Science: The Glass is (More Than) Half-Full

Cosponsored by CCS
T. Astill, *Presiding*

- 1:30 Introductory Remarks.
- 1:35 46. Investigation of matrix effects in cannabis-infused chocolates. **D.D. Dawson**
- 2:00 47. Chemistry of vaping concentrates: Current issues and harm reduction. **R.M. Strongin**
- 2:25 48. Degradant formation in cannabis concentrate aerosols. **J. Meehan-Atrash**, **R.M. Strongin**
- 2:50 49. Building in-process analytics to support cannabis LPs in their production optimization needs. **M. Roggen**
- 3:15 Intermission.
- 3:30 50. Alternative sensor for the screening of cannabinoids with a hand-held device. **L. Tay**, **E. Jorgenson**, **S. Poirier**, **J. Hulse**
- 3:55 51. HPLC method development strategies for achieving baseline resolution of 17 cannabinoids. **M.J. Wilcox**, **E. Franklin**
- 4:20 52. Combined LC-DAD-MS/MS and FT-IR platform for the analysis of Cannabis and Cannabis-related products. **L. Mercolini**, **M. Protti**, **V. Brighenti**, **L. Anceschi**, **R. Mandrioli**, **F. Pellati**
- 4:45 Panel Discussion.

Keeping Water Safe

Sponsored by I&EC, Cosponsored by CHAS and PRES

- 2:00 34. Transformation and removal efficacy of common cannabinoids in engineered aquatic systems. **N.B. Saleh**, **T. Karanfil**, **O. Apul**
- 2:25 35. Controlling cannabis formulations. **M. Roggen**
- 2:50 Intermission.
- 3:05 36. How to create a consistent water soluble cannabinoid bulk ingredient. **H. Han**
- 3:30 37. Cannabis decoctions: The time has come!. **J. Abrams**, **A. Samann**
- 3:55 38. Homogeneity, formulation, and shelf life of cannabis-infused beverage emulsions. **M. Vanden Eynden**, **D. Thireault**, **S. Riefler**
- 4:20 Panel Discussion.

Chemistry of Disasters

Sponsored by PRES, Cosponsored by CCS, CHAS and I&EC

WEDNESDAY MORNING – CHAS

SECTION A

Marriott Marquis San Diego Marina
Rancho Santa Fe 3

Graduate Students Perspective on Safety Education

Cosponsored by CCS
K. Miller, **R. Stuart**, *Presiding*

- 8:30 Introductory Remarks.
- 8:35 39. Safety communication is about respect as well as numbers. **R. Stuart**
- 9:00 40. How to train with nothing. **S. George**, **H. Davis-Russell**, **J. de la Rosa Ducut**
- 9:25 41. Development of a short course for collateral duty safety advisors in academic research laboratories. **M.C. Wasson**, **M. Blayney**
- 9:50 42. Secrets to success: Show up, do. **J.A. Martin**
- 10:15 Intermission.
- 10:30 43. Safety minutes: Consistent way to promote and sustain the commitment to research safety. **L. Redfern**, **M. Blayney**
- 10:55 44. GAs are EHS @ USD. **C.M. Karki**
- 11:20 45. Graduate student laboratory safety education programs. **K.A. Miller**

CHED

DIVISION OF CHEMICAL EDUCATION

I. Black, P. Daubenmire and L. Wang, *Program Chairs*

SUNDAY MORNING – CHED

SECTION A

Marriott Marquis San Diego Marina
Mission Hills

Chemistry Teacher's Day

S. C. Rukes, *Organizer*

S. G. Sogo, *Presiding*

- 8:30** Introductory Remarks.
- 8:35** **1.** But I'm a science teacher! Leveraging the engineering embedded in the NGSS for student achievement. **T. Kinner**
- 9:15** **2.** Incorporating current nomenclature, terminology, and symbols in the high school curriculum. **M.D. Mosher**, M. Weinrich
- 9:35** **3.** Engineering in the high school chemistry classroom. **S.G. Sogo**
- 10:15** Intermission.
- 10:25** **4.** Teacher's toolbox for lab safety. **J. Bishoff**, M.U. Gmurczyk
- 11:05** **5.** Growing the periodic table: How are elements discovered, verified and named?. **M.C. Cesa**
- 11:35** **6.** IYPT, National Chemistry Week, and AACT. **S.C. Rukes**

SECTION B

Marriott Marquis San Diego Marina
Balboa

Adapting Authentic Research to the Teaching Lab: Challenges & Rewards

D. Wood, *Organizer*

B. J. McFarland, *Organizer, Presiding*

- 8:30** Introductory Remarks.
- 8:50** **7.** Building an undergraduate laboratory course on cross-disciplinary research practices. **J. Burkett**
- 9:10** **8.** Developing a 3-week mini-research project for first year chemistry undergraduate students to quantify microplastic pollution in local soil. **L.A. Rowe**, A.M. Kubalewski, R. Clark, E. Statza, T.E. Goynes, K. Leach, J.R. Peller

- 9:30** **9.** Genome annotation: Authentic research project for entry-level community college students. **T. Beagley**
- 9:50** Intermission.
- 10:10** **10.** Inorganic chemistry course as research: My experience with CUREs. **J.K. Pagano**
- 10:30** **11.** Advanced experimental physical chemistry course: Research based follow-up to the modified classical experimental physical chemistry course. **B.H. Milosavljevic**
- 10:50** **12.** Project for the advanced physical chemistry lab: Kinetics of silver nanoparticle aggregation. **K.I. Peterson**, D.P. Pullman, C. Tachell, P. Yadao
- 11:10** Panel Discussion.

Immersive Virtual Reality for Molecular Design

Sponsored by COMP, Cosponsored by CHED, CINF and COMSCI

SUNDAY AFTERNOON – CHED

SECTION A

Marriott Marquis San Diego Marina
Mission Hills

Chemistry Teacher's Day

S. C. Rukes, *Organizer*

S. G. Sogo, *Presiding*

- 1:30** Introductory Remarks.
- 1:35** **13.** Chemical engineering for middle and high school. **J.A. Smith**
- 2:15** **14.** Bonding, dissolving, and precipitation: Concept inventories that measure student thinking using multiple representations and Johnstone's domains. **S. Bretz**
- 3:10** Intermission.
- 4:00** **15.** Minimizing chemical waste costs in the teaching labs with solid-state reactions and micro-scale experiments. **J. Noveron**

- 4:40 16. Using green chemistry to remedy environmental problems. **S.P. Kosmas**, M. Ruprecht, K. Anderson
- 5:05 Concluding Remarks.

SECTION B

Marriott Marquis San Diego Marina
Balboa

Adapting Authentic Research to the Teaching Lab: Challenges & Rewards

D. Wood, *Organizer*

B. J. McFarland, *Organizer, Presiding*

- 1:30 Introductory Remarks.
- 1:50 17. Unnatural chemical biology: Implementable, scalable, and tunable chemical biology undergraduate lab course. **K.M. Kean**, K. van Zee, R.A. Mehl
- 2:10 18. Solar Army: Incorporating real-time research experiences into the curriculum. **J.D. Schuttlefield Christus**
- 2:30 19. Proline biosynthesis in *Agrobacterium*: Collaborative course based authentic research across disciplines. **D. Wood**
- 2:50 Intermission.
- 3:10 20. Lessons from 16 years of synthesizing recombinant proteins in the teaching lab. **B.J. McFarland**
- 3:30 21. Electrochemical and spectrophotometric analysis of chocolate to increase student understanding in quantitative analysis. **L.A. Hiatt**, H.B. Musgrove, W.M. Ward
- 3:50 22. Teaching research: Using advanced 2D NMR techniques to characterize alpha-hydroxynitrates of terpenes. **R. LaLonde**, E. McKnight
- 4:10 Panel Discussion.

SECTION C

Marriott Marquis San Diego Marina
Carlsbad

Undergraduate Research Papers

J. V. Ruppel, N. Snyder, *Organizers*

C. V. Gauthier, *Organizer, Presiding*

- 1:30 Introductory Remarks.
- 1:35 23. Formation of extrudates using commercial silica doped aluminas. **J. Small**, B. Huang, B. Woodfield

- 1:45 24. Photocurable poly(ethylene glycol) diacrylate resins with variable silica nanoparticle loading. **A. Hocken**, K. Kline, Y. Yang, T. Piper, F.L. Beyer, M. Green
- 1:55 25. 3D-printable high efficiency upconverting polymer blends. **J. Park**, J. Kim
- 2:05 26. REU summer examining 3D printed microfluidic devices for preterm birth risk biomarker analysis. **D. Topham**, A.V. Nielson, A. Woolley
- 2:15 Intermission.
- 2:30 27. Machine learning analysis of quasiclassical direct dynamics trajectories for thermal deazetization. **N. Rollins**, S. Pugh, R. Carlsen, J. Jenkins, D.H. Ess
- 2:40 28. Molecular dynamics study of pH low insertion peptides in multi-component lipid bilayers. **B. Bogart**, T. Elsen, A. Panahi
- 2:50 29. Optimization of polarizing agents for liquid scalar Overhauser dynamic nuclear polarization at 14.1 T. **N. Harmon**, T. Dubroca, E. Megiel, J. van Tol, S. Hill
- 3:00 30. Application of principle component analysis (PCA) based methodology in characterization of single molecule dynamics. **H. Weatherspoon**, W. Harris, K. Rodriguez, A. Apkarian
- 3:10 31. Learning chemistry nomenclature: Comparing the use of an electronic game versus a study guide approach. **J. Wood**, D. Donnelly
- 3:20 Intermission.
- 3:35 32. Surface hydroxylation of display glass analyzed by time-of-flight secondary ion mass spectrometry. **A. Ralph**, C. Cushman, L. Fisher, J. Banerjee, N. Smith, M.R. Linford
- 3:45 33. Small molecule ratiometric probes for sensing reactive oxygen species (ROS) and peroxidase activity. **A. Hinojosa**, R. Mehta, E.L. Que
- 3:55 34. Synthesis and reactivity of new fluorenofluorene-based hydrocarbons. **K. D'Ambrosio**, H. Hashimoto, A. Hacker, D.K. Frantz
- 4:05 35. Dirhodium carboxylate complexes encapsulated in metal-organic frameworks for the C-H functionalization of alkanes. **E.H. Adillon**, **J. Byers**
- 4:15 36. Antibacterial activity against *Erwinia carotovora*: Synergism interactions between different phytochemical substances present in potato wound tissues. **M. Perez Rodriguez**, K. Dastmalchi, R.E. Stark
- 4:25 Concluding Remarks.

SECTION A

San Diego Convention Center

TBD

General Posters

P. L. Daubenmire, *Organizer*

7:00 - 9:00

- 37.** Biennial conference on chemical education: Place to share information about the teaching and learning of chemistry. **J.M. Sophos**, J. Carmel, R.S. Cole, D.I. Del Carlo, S.J. Donnelly, I.J. Levy, S.R. Moor-ing, B. Murray, M. Orgill, A. Putti, C. Sorensen-Un-ruh, D.G. Sykes, V.M. Williamson
- 38.** Green Chemistry Commitment. **I.J. Levy**, A.S. Cannon
- 39.** Applying psychological constructs and student supports to improve the education of students in STEM (SHAPE STEM): Year 1. **S.P. Wathen**, J. Lindstrom, H. Moody, P. Roussel, J. Tsuji
- 40.** Building a tiered participation model for STEM teacher recruitment. **P.G. Jasien**, R. Chen, C. De Leone, L.M. Holt
- 41.** PhDs enhanced for prospects erasmus plus (PEPUP) approach. **F. Popowycz**
- 42.** Burg Foundation Graduate Student Teaching Fellowship: Unique classroom experience as a valuable opportunity for pursuing a faculty career. **A. Nazarova**
- 43.** Online chemistry education platform. **E. Biro**, A. Peragovics, P. Szakacs
- 44.** Open-ended research laboratory course at community college. **R. Shakya**
- 45.** Analysis of text easability markers in undergraduate electronic and traditional chemistry textbooks. **D. Gomez**, **J. Mendoza**, **C. Cerrato**, J. Ross
- 46.** Hierarchy of attitude effect toward the subject of chemistry in introductory-level college courses. **E. Guerra**, **S. Gonzalez**, J. Ross
- 47.** ChemPAL: Providing a model for impactful and personal chemistry mentorship within a large public university. M. Du, M. Edwards, A.J. Mantanona, **A.L. Michalak**, C. Seitz
- 48.** Investigating trends in chemistry education research instrument publication and use. **A. Corrales**, **S. Wang**, J. Barbera, J. Harshman, R. Komperda
- 49.** Citation patterns of concept inventory development papers as indicators of impact on research community. **A. Leontyev**
- 50.** Chemistry workshops to promote learning and retention in introductory general chemistry. **G.M. Smeureanu**, **K. Grant**
- 51.** “Crystal clear”: Inquiry-based learning of crystal structures in General Chemistry. **S. Sun**, J.E. Headrick
- 52.** Motivating students to learn chemistry with Molecule of the Week. **C. Chen**, F. Manyanga
- 53.** Role-playing a reaction: Clarifying kinetics through active learning. **D.L. Lair**, J.M. Leslie
- 54.** Near-peer tutoring: Chemistry center designed to increase success of a diverse student body in STEM. **S. Bidwell**, **H. Harb**, S. Baker, **J.M. Leslie**, H.P. Hratchian
- 55.** Problem-solving in organic chemistry: Mechanistic analysis of an “unknown” reaction. **C. Nemr**, A. Dicks
- 56.** Comparing long-term retention of organic chemistry using individual and group active learning. **L.G. Habgood**, J. Patrone, J.S. Queen
- 57.** Enantiomeric excess game and experiment. **N. Sanguantrakun**
- 58.** Hydroboration-oxidation reactions as a pathway for transformative learning and development of critical thinking skills in the undergraduate chemistry laboratory. **D.E. Martyn**
- 59.** Probing students’ understanding of experimental design and process through laboratory practical experiences. **J. DeYoung**, L. Kelly, S.K. Shaw
- 60.** Flipping the quantitative analysis/analytical chemistry classroom. **J. Haan**
- 61.** Incorporating Jupyter and Python into analytical chemistry. **E.J. Menke**
- 62.** Withdrawn
- 63.** Cyclic voltammetry in the undergraduate teaching laboratory: Determining cholesterol and cholesterol derivative concentrations in aqueous solution using carbon screen-printed electrodes. **D.E. Martyn**, S.K. Buehler
- 64.** Montebello water filtration plant-I in Baltimore: Engaging students in physical chemistry, a STEM approach. **B. Salazar**, R. Nuss
- 65.** Construction and practice of core course “Surface Physical Chemistry” for the cultivation of full-time application-oriented graduates. **Z. Yao**, S. Hao, P. Cong, C. Li, Z. Jiang, Y. Huang

SECTION A

Marriott Marquis San Diego Marina
Carlsbad

Academic Lab Safety

Cosponsored by CCS and CHAS

S. D. Wiediger, *Organizer, Presiding*

- 8:30 Introductory Remarks.
- 8:45 66. Strategic directions in chemical safety education for the ACS. **R. Stuart**
- 9:10 67. American Chemical Society safety resources. **M.U. Gmurczyk**
- 9:30 68. Leadership and safety education. **S.M. Shih**
- 9:50 69. Integrating safety science instruction. **D.C. Finster**, S.B. Sigmann
- 10:10 Intermission.
- 10:25 70. Academic lab safety at the intersection between green chemistry, ethics, and safety. **G.M. Bodner**
- 10:45 71. CPT's role in enhancing safety education for undergraduates. **R.W. Schwenz**
- 11:05 72. Continued conversation on graduate student laboratory safety education from the 2019 ACS Safety Summit. **K. Miller**
- 11:25 Discussion.
- 12:05 Concluding Remarks.

SECTION B

Marriott Marquis San Diego Marina
Mission Hills

Assessment & Measurement in Research & Practice

K. A. Marek, T. C. Pentecost, J. R. Raker, J. M. Trate,
Organizers

K. L. Murphy, *Organizer, Presiding*

- 8:30 Introductory remarks.
- 8:35 73. Evaluating the development of transferable skills in an organic chemistry laboratory curriculum. **C.L. Stanford**, T. Bethke, M. Brown, N. Evans
- 8:55 74. Characterizing students' abilities to reason about "why" on organic chemistry assessments. **J.M. Deng**, N.E. Bodé, A.B. Flynn
- 9:15 75. Reaction coordinate diagram inventory: Measuring general chemistry and organic chemistry students' thinking and confidence. **M.B. Atkinson**, M. Croisant, M. Popova, S. Bretz

- 9:35 Intermission.
- 9:50 76. Minding the gap: Development of identity measures for use in chemistry courses. **J. Barbera**, K. Hosbein
- 10:10 77. Withdrawn
- 10:30 78. How do I design a chemical reaction to do useful work, and how does my reaction impact society? A case study in reimagining general chemistry. **K.M. Van Heuvelen**, G.W. Daub, L. Hawkins, A.R. Johnson, H. Van Ryswyk, D.A. Vosburg
- 10:50 79. Learning evaluation in P–Chem lab sequence that (a) prepares students for and (b) involves them in authentic research. **R. Baker**, B.H. Milosavljevic
- 11:10 Concluding remarks.

SECTION C

Marriott Marquis San Diego Marina
Balboa

Green & Sustainable Chemistry Theory & Practice: Chemistry & Water

Cosponsored by CEI and I&EC

E. J. Brush, J. E. Wissinger, *Organizers, Presiding*

- 8:30 Introductory Remarks.
- 8:40 80. Teaching students to think about what it means to be "green". **D.A. Laviska**, W.R. Murphy, C.E. Marzabadi, R.L. Augustine, S. Tanielyan
- 9:00 81. Organic laboratory experiments in water. **D.A. Vosburg**
- 9:20 82. Edible water capsules: Hydrogels with a sustainable purpose. **J.E. Wissinger**, E. Corcoran, C. Knutson, M.C. Enright
- 9:40 Intermission.
- 9:55 83. Engaging chemists through the UN sustainable development goals. **D. Constable**
- 10:35 84. Chemical leasing and the implementation of a Moore's Law for chemistry. **M.W. George**, M. Poliakoff, P. Licence
- 10:55 85. UN sustainable development goals as a framework to foster the use of high impact practices for integrating and scaffolding green and sustainable chemistry in the curriculum. **E.J. Brush**
- 11:15 86. Implementing green chemistry in high school chemistry curriculum. **C. Knutson**
- 11:35 Discussion.

SECTION A

Marriott Marquis San Diego Marina
Carlsbad

Academic Lab Safety

Cosponsored by CCS and CHAS
S. D. Wiediger, *Organizer, Presiding*
R. Stuart, *Presiding*

- 1:30** Introductory Remarks.
- 1:35** **87.** Anaphylaxis induced by peptide coupling agents: Lessons learned from prolonged exposure to HATU, HBTU, and HCTU. **K. McNelly**, J.S. Nowick
- 1:55** **88.** Risk assessment for research students: When to get help. **D.R. Kuespert**, N.J. Leon
- 2:15** **89.** Chemical health and safety information in PubChem. **S. Kim**, J. Zhang, P. Thiessen, A. Gindulyte, E. Bolton
- 2:35** **90.** Is this chemical safe? What do I really need to know and how do I find out. **L.R. McEwen**
- 2:55** Intermission.
- 3:10** **91.** Periodic table of the elements of safety. **R.M. Izzo**
- 3:30** **92.** Preparing for a safe workplace culture: Learning and modeling behavior. **M.A. Thomson**
- 3:50** **93.** Withdrawn
- 4:10** **94.** Developing rubrics for assessing safety education case studies. **S.D. Wiediger**
- 4:30** Concluding Remarks.

SECTION B

Marriott Marquis San Diego Marina
Mission Hills

Engaging Students in Physical Chemistry

Cosponsored by PHYS
D. E. Gardner, C. M. Teague, *Organizers*
A. Grushow, *Presiding*

- 1:30** Introductory Remarks.
- 1:35** **95.** PSI4Education: Graphical computational chemistry labs using free software. **R.C. Fortenberry**, **A. Ringer McDonald**, B.B. Magers, D.D. Sherrill
- 1:55** **96.** Beyond the analytical solution: Using mathematical software to enhance understanding of physical chemistry. **A. Ringer McDonald**, J.P. Hagen
- 2:15** **97.** Implementing python-based computational guided inquiry exercises in thermodynamics and quantum chemistry courses. **G.Y. Stokes**, T.L. Guasco, S. Neshyba, P. Rowe, W.C. Pflanzgraff, A.L. Mifflin

- 2:35** **98.** Molecular dynamics simulations of epoxy resin systems: Experiences from three years of undergraduate research. **L.D. Crosby**
- 2:55** Intermission.
- 3:15** **99.** Map for a problem-solving guide for thermodynamics in physical chemistry. **K.E. Murphy**
- 3:35** **100.** Implementation of specifications grading for a junior/senior physical chemistry sequence: Reflections after year one. **K. Mardis**
- 3:55** **101.** Using a POGIL framework for the keto-enol NMR experiment. **A. Grushow**
- 4:15** **102.** Making physical chemistry real!. **J. Selco**
- 4:35** Concluding Remarks.

SECTION C

Marriott Marquis San Diego Marina
Balboa

Programs Designed to Promote Greater Retention in STEM & Chemistry

J. Schwartz-Poehlmann, *Organizer*
C. Cox, *Organizer, Presiding*

- 1:30** Introductory Remarks.
- 1:35** **103.** Videos to enhance the introductory chemistry workshop experiences. **K. Grant**, **G.M. Smeureanu**
- 1:55** **104.** Toward an effective Hispanic serving chemistry curriculum. **E.J. Menke**, L. Reimer, J.M. Leslie, S. Bidwell, C. Isborn, D.L. Lair, B.J. Stokes, H.P. Hratchian
- 2:15** **105.** P3-STEM: Promoting STEM transfer student success at multiple minority serving/Hispanic serving institutions. **K.R. Cousins**, **J. Mallari**
- 2:35** **106.** STEM persistence effects of teaching through research: Freshman Research Initiative at the University of Texas at Austin. **R.I. Shear**, S. Engelman, E. Tallman, K.H. Rogers, S.E. Eichhorn
- 2:55** Intermission.
- 3:10** **107.** Do intensive STEM courses help? Comparison of introductory chemistry tracks. **N. Lapeyrouse**, J. Donnelly, A. Eugster, C. Yestrebky
- 3:30** **108.** Incorporation of peer mentors and an introduction to research into a UNIV 101 course. **D.B. King**, J. Stanford, D. Murasko
- 3:50** **109.** Using open-ended topics as learning communities' focal points to enhance student engagement and retention. **P. Tandler**, J.A. Lupica
- 4:10** **110.** Collaborative professional development program for science faculty and graduate students in support of education reform at two-year, Hispanic-serving institutions: Graduate student's perspective. **M. Edwards**, S. Brydges, D.R. Brown, S.M. Lo

- 4:30 **111.** Assessment of achievement gaps and equity in introductory chemistry courses. **C.E. Brown**
- 4:50 **112.** Talking about POGIL instead of talking about leaving. **B.M. Fetterly**
- 5:10 Concluding Remarks.

SECTION D
San Diego Convention Center
TBD

Undergraduate Research Posters

Analytical Chemistry

N. Di Fabio, D. Hendricks, *Organizers*

2:00 - 4:00

- 113.** REU summer research experience examining sticky paper spray ionization for analysis of powdered analyte grains. **M.S. Laikupu**, P. Hettikananange, G. Klingler, D.E. Austin
- 114.** Quantitative analysis of short chain fatty acid benzyl ester mixtures by proton nuclear magnetic resonance spectroscopy. **J. Mancuso**, N.M. Wachter, R.P. D'Amelia
- 115.** Accurate, precise, and affordable light emitting diode spectrophotometer for diabetes testing in Honduras. **D. Decius**, C.J. Land, B.M. Summers, B. Pietrini, T.R. Lozano, J.F. Gomez-Marquez, M.W. Prairie, S.H. Frisbie
- 116.** Enantiomer migration order reversal of tetrahydrozoline in capillary electrophoresis. **T. Basiashvili**, T. Maisuradze, A. Gogolashvili, B. Chankvetadze
- 117.** Sensing of single bacteria using blocking electrochemical collisions and the dependence of current transients on supporting electrolyte concentration. **S. Jenkins**, S.N. Thorgaard
- 118.** Check out my mixed vape: Chemical analysis of e-cigarette emissions. **A. Burns**, Y. Li, T. Nguyen
- 119.** Spectrophotometric analysis of anthocyanins and other juice components. **D. Crite**, S.D. Wiediger
- 120.** Gold nanoparticle-decorated nickel foam electrodes for the non-enzymatic detection of glucose. **G. Jimenez-Porfirio**, **D. Thrush**, E. Gillette
- 121.** Characterization of spider silks using NMR amino acid analysis. **M. King**, S.K. Davidowski, J.L. Yarger
- 122.** Investigations of the impact of experimental error on the spectrophotometric determination of an equilibrium constant. **T. Kawagoe**, C.C. Langley
- 123.** Photoactivation investigation of the meso-tetra(N-methyl-2-pyridyl) and meso-tetra(N-methyl-3-pyridyl) porphyrins under different light intensities. **L. Sanz**, M. Ballester, V. Castro, V. Hoozen, K. Chamarti

SECTION D

San Diego Convention Center
TBD

Undergraduate Research Posters

Biochemistry

N. Di Fabio, D. Hendricks, *Organizers*

2:00 - 4:00

- 124.** Structural determination of ¹⁹F labeled KIX via disulfide tethering. **R. Reilly**, W.C. Pomerantz, P. Ycas
- 125.** Investigation of conformational changes in histone methyltransferase PRDM2 catalytic domain variants. **A.M. Banach**, **D.E. Wilkinson**, E.M. Kolonko
- 126.** Exploring dynamic disulfide chemistry on supramolecular fibers. **E. Ferraro**, **R. Haddad**, A. Halmans, J.E. Smith-Carpenter
- 127.** Rational design and characterization of *Taq* DNA polymerases with improved accuracy. **K. Lee**, S. Gottlieb, S. Barrett, A. Leconte
- 128.** Quenched-fluorophore design for carbonic anhydrase sensing. **D. Tan**, R. Mehta, E.L. Que
- 129.** Crystallization, enzymatic, and inhibitory studies of *M. tuberculosis* encoded methyltransferase importance in pathogenesis. **S.S. Koka**, G. Loarer, D.R. Ronning
- 130.** Characterization of manganese uptake in *Chlorella vulgaris*. **P. Wiwekwin**, A. Smythers, D. Kolling
- 131.** Synthesis of asymmetrical cobalt complexes: Redox mediators in biohybrid dye sensitized solar cells. **A. Acord**, N. Nesheiwat, A. Teodor, M. Vaughn, B. Bruce, J. Bergkamp
- 132.** Analyzing resveratrol effects on SIRT1 with varying peptide substrates using an enzyme-coupled assay. **Y. Lee**, **J. Huynh**, C. Cabrerros, N. Wang
- 133.** Preliminary studies on the biosynthesis of the chemotherapeutic bleomycin by *Streptomyces verticillus*. **H. Befekadu**, C.T. Calderone
- 134.** Study of antioxidant activity of extracts of agraz (*Vaccinium meridionale*). **S. Velásquez**, E.J. Diaz
- 135.** Synthesis of fluorogenic amino acids to monitor transpeptidation. **A. Yevsikov**, Z. Poulos, C. Kelley, E. Kuru, J. Rittichier, G. Church

SECTION D
San Diego Convention Center
TBD

Undergraduate Research Posters
Chemistry Education

N. Di Fabio, D. Hendricks, *Organizers*

2:00 - 4:00

- 136.** Investigation of PdNi/MWCNT and Pd/MWCNT nanocomposites towards supercapacitor applications. **F. Beissel**, T.F. McFarland
- 137.** Synthesis and electrochemical characterization of PdCo/MWCNT towards formic acid fuel cells. **J. Morataya**, T.F. McFarland
- 138.** Synthesis and electrochemical characterization of Co/GO and Co/MWCNT supercapacitors. **M. Evenson**, T.F. McFarland
- 139.** Inference generation by liberal studies students in chemistry courses: Latent transition analysis of explanatory behavior over time. **S. Perez**, A. Villalta-Cerdas
- 140.** Synthesis and characterization of bipyridine cobalt complexes for photosystem-I biophotovoltaic application. **E. Ooi**, A. Teodor, M. Vaughn, B. Bruce, J. Bergkamp
- 141.** Advanced undergraduate lab: Kinetics and thermodynamics of formation of hypervalent iodine compounds. R. Kumar, **L. Camdzic**, N.V. Tsarevsky
- 142.** Design of chemical engineering experiences of liquid-liquid extraction into project-based experimentation for introductory chemistry laboratories. **J. Jimenez**, A. Villalta-Cerdas
- 143.** Developing student process skills in a freshman chemistry laboratory. **E. Suh**, G.J. Reynders, R. Sansom
- 144.** Observation of the amyloid beta 1–40 peptide's coverage shell on the nano-gold surface. **A. Ichiki**, **S. Hamazaki**, K. Yokoyama
- 145.** Cloning and characterizing D-luciferin and 4-bromoluciferin selective mutant luciferases for *in vivo* bioluminescence imaging. **J. Gewing-Mullins**, E. Reid-McLaughlin, M. Ornelas, W. Lieberman, J.A. Prescher, A. Leconte
- 146.** Infrared transmission and reflection of Titan aerosol analogues under vacuum. **A.L. Walker**, S.M. Horst, B. Hadnott, C. He, M. Yant
- 147.** Isolation of anti-inflammatory compounds in mastic gum. **L. Ciminera**, J.R. Pruitt
- 148.** Faculty perspectives of facilitating an online collaborative learning experience. **C. Pinder**, D. Skagen, L.A. Morsch, B. McCollum, M.T. Wentzel

149. Student authored metaphors of online collaborative learning: Is it a platypus or rivers merging?. **H. Hollinshead**, L.A. Morsch, B. McCollum, M.T. Wentzel, C. Meredith

150. Synthesizing macrocycles through Asao-Yamamoto benzannulation. **A.T. Champlin**, H. Arslan

151. Hands-on molecular models in color: 3D printing multi-part molecular models for teaching sterics and reactivity in organic chemistry. **H. Martin**, S. McAvoy, J.K. Klosterman

152. Creating a supercritical carbon dioxide chamber for classroom applications. **M. West**, B. Veldman

153. Agro-plastics in Mexico: Why not incinerate or leave them?. **G. Lopez-Reyes**, I. Gavilán-Cruz

154. Student perceptions of science practices in the general chemistry laboratory course. **J. Lampert**, C. Schnoebelen, S. Brydges, T.J. Bussey

155. First year of graduate school: Case study of teacher identity development for a chemistry teaching assistant. **D. Callahan**, C. Schnoebelen, S. Brydges, T.J. Bussey

156. Developing a method for investigating molecular structure that uses low-cost materials with no or limited toxicity in an undergraduate chemistry laboratory. **J. Milburn**, C.C. Langley

SECTION D
San Diego Convention Center
TBD

Undergraduate Research Posters
Computational Chemistry

N. Di Fabio, D. Hendricks, *Organizers*

2:00 - 4:00

- 157.** Preparation and use of an organoclay for the removal of triclosan in water. **L. Amézquita**, F. Arévalo, F. Cifuentes, D. Cujcuj, D. Díaz, C. Escobar, M. Hernández, A. Hernández, C. Hernández, J. Marroquín, J. Medina, G. Quevedo, R. Rivera, F. Tzunux, **C.E. Torres**, S. Echeverría
- 158.** Analyzing anion concentrations in San Antonio topwaters with ion chromatography. **P. Smith**, **N. Genthon**, C.A. Smith
- 159.** Size consistent real space geminal power. **I. Craig**, B. Van Der Goetz, E. Neuscamman
- 160.** Methanol, dimethylsulfide, and methylamine concentrations in peatland porewaters. **D. Chang**, C. Pierson, K. Ishimine, S. Schwager, J. David, E.L. Hanna, J. Keller, C. Zalman, W.J. De Bruyn
- 161.** Organic field effect transistors: Analytic

- simulation. **Z. Porche**, B. Veldman
- 162.** Simulations of serine vs. sulfoserine: Mass spectra and fragmentation pathways during CID. **K. Lucas**, G.L. Barnes
- 163.** Accumulation of particulate matter on local leaf samples. **M.K. Dustin**, **M. Kondel**, G. Chilom
- 164.** Encapsulation of fertilizer in starch-chitosan spheres: Synthesis, characterization, and application. **A.N. Quintana-Martinez**, A.M. Gonzalez-Mederos
- 165.** Partitioning, diffusion, and self-assembly dynamics of protein and fatty acid mixtures in marine aerosols. **A.R. Mitchell**, A. Dommer, R.E. Amaro
- 166.** Automated machine learning of accurate many-body potentials for molecular simulations. **E. Bull-Vulpe**, **K.R. Ganapathy**, M. Riera, Y. Zhai, F. Paesani, A.W. Goetz, S.E. Brown
- 167.** Insights into proton uptake in cytochrome c oxidase from DFT calculations. **T. Goh**, W.H. Du, Y. Chen, K.A. Hartfield, D.E. McRee, A.W. Goetz
- 168.** Theoretical studies of CO₂ adsorption and separation in two isostructural scandium-based metal-organic frameworks. **A. Varghese**, T. Pham

SECTION D

San Diego Convention Center
TBD

Undergraduate Research Posters

Green Chemistry & Sustainability

N. Di Fabio, D. Hendricks, *Organizers*

2:00 - 4:00

- 169.** Zeolite gas separation from methane in anaerobic digestion. **V.P. Bustamante**, J. Hansen, J. Richards
- 170.** Analysis of common anions in a small lake with a twenty-year old plus bird roost. **E. Nuno Gutierrez**, C.A. Smith
- 171.** Novel catalyst synthesis technique using atomic beam deposition. **B. Thompson**, R. Fushimi, R. Rodriguez
- 172.** Orange vs. green: Evaluating and modifying laboratory experiments for inclusion in an organic chemistry curriculum that focuses on sustainability and stewardship. **A. Rodriguez**, **K.G. Otto**, D. Gamarro, S. Battaglia, W. Kohman, D.A. Laviska

SECTION D

San Diego Convention Center
TBD

Undergraduate Research Posters

Inorganic Chemistry

N. Di Fabio, D. Hendricks, *Organizers*

2:00 - 4:00

- 173.** Syntheses, characterization, and reactivity of cobalt(II) model complexes for liver alcohol dehydrogenase. J.R. Miecznikowski, **S. Zygmunt**, **E.E. Mircovich**, J.P. Jasinski, E. Reinheimer, B.Q. Mercado
- 174.** Single-source vs multi-source approaches to chalcopyrite nanomaterials. **L.J. Maxton-Renner**, **M.J. Jenkins**, A.W. Holland
- 175.** Oxidative hydroarylation of styrenes with a Rh(I) catalyst: Single-step synthesis and isolation of stilbenes. **L.I. Frye**, W. Zhu, X. Jia, T.B. Gunnoe
- 176.** Determining metal contaminants in turtle scutes through X-ray fluorescence. **C. Laxdal**, R.L. Burke, S.G. Sobel
- 177.** Investigation of dimethyl methylphosphonate adsorption and decomposition activity with isotope-labeled materials. **C. Zweifel**, K. Huynh, M. Zachariah
- 178.** Analysis of thermite reaction behavior for ¹⁸O-labeled metal oxides. **K. Ehrhardt**, K. Huynh, M. Rehwoldt, M. Zachariah
- 179.** Mechanistic study of the chemical components in the solid electrolyte interphase. **D. Peterson**, K. Huynh, L. Wang, B.W. Eichhorn
- 180.** Magnetism and crystal structure of new Ti Co B structure-type quaternary borides: Zr MnRu B and Hf FeRu B. **N. Bakshi**, B. Fokwa, P. Shankhari

SECTION D

San Diego Convention Center
TBD

Undergraduate Research Posters

Medicinal Chemistry

N. Di Fabio, D. Hendricks, *Organizers*

2:00 - 4:00

- 181.** Examining methods for the synthesis of azo-indole compounds. **Z.T. Plummer**, C. Streu
- 182.** Photoactive nanoparticles for melanoma treatment. **D.M. Soddors**, N.H. Abd Ellah, M.R. Warmin, M.J. Baldwin, G.M. Pauletti, C.E. Larrabee
- 183.** Design, synthesis, and evaluation of 5-hydroxy-2-(3-phenylpropyl)chromone derivatives

as 5-HT_{2B} receptor ligands. M. Kim, M. Truss, V. Plascencia, H. Wang, S. Zaidi, Y. Zhang, D.A. Williams

184. Optimization and characterization of everolimus-releasing liposomes as a potential application for coronary stents coating to prevent restenosis. G. Torres Flores, A. Rodriguez-Garcia, Y. Vega, A. Gonzalez-Horta

SECTION D

San Diego Convention Center

TBD

Undergraduate Research Posters

Nanochemistry

N. Di Fabio, D. Hendricks, *Organizers*

2:00 - 4:00

185. Direct co-delivery of supramolecular nanoparticle-protein assemblies for genetic knock-in. V. Clark, D. Luther, V.M. Rotello

186. Synthesis and characterization of luminescent dual-ligand gold nanoparticles. C.R. Scholtz, B. Yoo, A. Mori-Kreiner, J.D. Steinkruger, C. Zhou

187. Synthesis and characterization of gold nanoparticles as electrochemical catalysts. V. Segui Barragan, M.G. Weir

188. Effect of hydrophobic counterions on undecylenic acid-based micelle formation. R.D. Burns, D.J. DuPonty, M.R. Warmin, C.E. Larrabee

189. Influence of synthesis method on the morphology and piezoelectric properties of Y_{0.07}Sr_{0.93}Ti_{0.8}F_{0.2}O_{3-δ} perovskite material. D.A. Sandoval Salaiza, S. Garza-Castillo, M.A. Velasco-Soto

190. Effects of pH on the oxidation of ethanol and methanol on Pt-decorated Ni electrodes. C. Guijon, E. Gillette

SECTION D

San Diego Convention Center

TBD

Undergraduate Research Posters

Organic Chemistry

N. Di Fabio, D. Hendricks, *Organizers*

2:00 - 4:00

191. Synthesis of enantiomerically pure orthogonally protected monosubstituted piperazines as intermediates for library production. M. Shah, S. Chamakuri, D. Young

192. Investigations into the biosynthesis of roseophilin. M.C. Guo, M.M. Vega, R.J. Thomson

193. Investigation of the synthesis of oxazolines through amide bond formation. C. Stobart, R. Grote

194. Synthesis of styryl-BODIPY with iodine substitution at 2,6 positions. I. Dickenson, P. Hewavitharanage

195. Evaluating the role of polarization in halogen bonding. O. Grounds, K. Auker, S.V. Rosokha

196. Spectral, structural, and thermodynamic characteristics of π-bonded dimers between cation-radicals of tetrathiafulvalene derivatives. J. Brown, S.V. Rosokha

197. Kinetic NMR investigation of the Steglich esterification. L.M. Williams, L.J. Rasmussen, E.M. Kolonko

198. Functionalizing a quinone chromophore for immobilization on electrode surfaces. G. Lindsay, H. Arslan

199. Coordination of phosphate diester ligands to bismuth(III). E. McKnight, Z. Ali, G. Bailey, N. Kretkos, C. Milander-Mashlan, J. Stromberg, R. LaLonde

200. Synthesis, screening, and polymerization of non-estrogenic BPA mimics. A. Basile, I. Parish, C. Anderson, J. Hankey, J. Lin, S. Grow, A.L. Hammock, P. Harrison, S.T. Hobson

201. 9-BBN catalyzed hydroboration of phenylacetylene with pinacolborane. G. Ruesch, S. Rowley, M. Mifflin, N.S. Werner

202. Syntheses of novel solvent molecules for use in solvate ionic liquids. J. Allred, A. Bennett, K. Roberts, S.C. Pilcher

203. Investigation of microwave energy in the synthesis of heterocycles related to medicinal chemistry. V. Brown, L. Maez, E.A. Nalley

204. Green synthesis of azolines and imidazoles using microwave and ultrasonic energy and their use in drug design. R. Paris, S.T. Myers, E.A. Nalley

205. Summer REU research in Bordeaux, France. T. Hinkle, E.A. Nalley

206. Green chemistry synthesis of imidazoles and other heterocyclic nitrogen compounds. R. Paris, S.T. Myers, E.A. Nalley

207. Photocatalytic degradation of acesulfame potassium using TiO₂/UVA, S₂O₈²⁻/Fe²⁺/UVA, and H₂O₂/Fe²⁺/UVA processes. S. McBride, C. Bryan

208. Characterization by 1D and 2D NMR of substituent effects on chalcone-like derivatives. P. Bowry, M. Young, P. Gordon, D. Nguyen, A. Zeng

209. Palladium-catalyzed cycloisomerization of allenes to access densely functionalized cyclopentenes. E.M. Landwehr, R.D. Reeves, J.M. Schomaker

SECTION D
San Diego Convention Center
TBD

Undergraduate Research Posters

Physical Chemistry

N. Di Fabio, D. Hendricks, *Organizers*

2:00 - 4:00

210. Identification of the pyrolysis products of gamma-butyrolactone. **T. Martin**, G.J. Brown, M.J. Ellis, H.N. Legg, K.M. Narkin, L.R. McCunn

211. Evaluation of surface treatment. **T. Tsareva**, M. Groth, M. Soriano, R. Ellis, B. Veldman

212. Spinel nanocrystals for insights into planet formation. **E.M. Valencia**, R.C. Fortenberry

SECTION D
San Diego Convention Center
TBD

Undergraduate Research Posters

Polymer Chemistry

N. Di Fabio, D. Hendricks, *Organizers*

2:00 - 4:00

213. Synthesizing and measuring the properties of an azobenzene-based photo-responsive liquid crystal elastomer. **T. Shea**, **A. Woodyard**, Z. Kurji

MONDAY EVENING – CHED

SECTION A
San Diego Convention Center
TBD

Successful Student Chapters

8:00 - 10:00

214. Essex County College discovery and innovating. **A. Gonzales**, N.H. Marashi

215. Withdrawn

216. San Diego Miramar College chemistry affiliate: ACS student chapter emphasizing diversity, discovery and community service. **G.L. Smith**, **A. Uribe**, **M.P. Troester**, **A. Peshina**, **K. Nagan**, **S. Chang**

217. From the chemistry to the community: ACS Uniandes international student chapter. **D. Garzon**, **C. Granados**, C. Lizarazo

218. Science and chemistry for everyone at Tecnológico de Monterrey. **N. Baeza**, P. Uribe, G. Torres, M. Medina, I. Palestino, M. Medina, A. Medrano, J. Arriaga, J. Matzui

219. Mexico's first ACS international student chapter "Catalyst". **C. Minutti Zanella**, **P. Crespo**, M.A. Mendez-Rojas

SECTION B
San Diego Convention Center
TBD

Sci-Mix

I. Black, P. L. Daubenmire, L. Wang, *Organizers*

8:00 - 10:00

7, 18, 37, 38, 39, 40, 41, 42, 43, 49, 50, 53, 54, 56, 71, 74, 78, 79, 105, 106, 107. See Previous Listings.

227, 237, 241, 277, 278, 304, 307, 308, 309, 310.

See Subsequent Listings.

TUESDAY MORNING – CHED

SECTION A
Marriott Marquis San Diego Marina
Carlsbad

GSSPC: From Oceans to Clouds: The Environmental Chemistry of Water

Cosponsored by PRES

K. J. Mayer, *Organizer*

M. Alves, *Organizer, Presiding*

K. Mayer, *Presiding*

8:30 Introductory Remarks.

8:40 **220.** Per- and polyfluoroalkyl substances (PFAS) in the environment: Lessons learned from studying adsorption to porous solids. **P. Edmiston**

9:20 **221.** Polymer-clay composite geomedia for trace contaminant removal in urban stormwater treatment systems. **J. Ray**, I. Shabtai, M. Teixeira, Y. Mishaal, D.L. Sedlak

10:00 Intermission.

10:10 **222.** Reactivity of iron in aerosols and cloud droplets: Adsorbed versus bulk water. **H.A. Al-Abadleh**

10:50 **223.** Influences of temperature, humidity, composition, volatility, and time on the amorphous phase transitions of organic aerosols. **M. Petters**, S. Petters, N. Rothfuss, A. Tandon, S. Kasparoglu, W. Champion, A. Grieshop, P. Ziemann, S. Kreidenweis, P.J. DeMott, A. Marsh, G. Rovelli, J. Reid

11:30 **224.** Thirty years with my head in the clouds: Laboratory studies of atmospheric water. **M. Tolbert**

SECTION B

Marriott Marquis San Diego Marina
Mission Hills

State of the Art: Diversity & Inclusion in Chemistry Education

Cosponsored by CEI and PROF

C. H. Middlecamp, *Organizer*

P. L. Daubenmire, *Organizer, Presiding*

- 8:30** Introductory Remarks.
- 8:35** **225.** Diversity and inclusion: Power of questions. **C.H. Middlecamp**
- 8:55** **226.** Where to start? A toolkit for broadening participation in STEM. **R.M. Burks**
- 9:15** **227.** Curricular reform in light of inclusive pedagogy: Faculty development and student support. **S.A. Kennedy**
- 9:35** **228.** Developing and implementing a plan for inclusive excellence within the POGIL Project. **G.H. Webster**
- 9:55** Intermission.
- 10:05** **229.** How active learning practices may impact students differently: Exploring the experiences of students with concealable identities. **S. Brownell, K. Cooper**
- 10:25** **230.** Where are the women? Diversity and inclusion in nuclear chemistry education in Tennessee. **J.M. Iriarte-Gross**
- 10:45** **231.** Learning about science ethics and diversity through movies: Case study approach. **D.J. Nelson**
- 11:05** **232.** DEIA in informal learning: Case study from the Museum of Science and Industry Chicago. **S. Raposo, L. Makdisi, N. Joseph**
- 11:25** Intermission.
- 11:35** **233.** UN sustainable development goals as a framework to introduce discussions of diversity and inclusion in chemistry education. **E.J. Brush**
- 11:55** **234.** Sharing cycle of science learning: Method to connect college STEM courses with tribal community topics that enhance sovereignty. **M.A. Griep, B. DeVore-Wedding, J. Woodard, H. Miller**
- 12:15** **235.** Chemistry at the margins: Joining the offerings of higher education to refugees in the Jesuit Worldwide Learning (JWL) network. **P.L. Daubenmire**

SECTION C

Marriott Marquis San Diego Marina
Balboa

Research in Chemistry Education

R. Komperda, *Organizer*

T. J. Bussey, *Organizer, Presiding*

- 8:30** Introductory Remarks.
- 8:35** **236.** Investigation of the impact of a zoo-context chemistry laboratory on undergraduate learning and conservation perspectives. **T.E. Hernandez, D. Donnelly, E.C. Person**
- 8:55** **237.** Chemistry communication practice through online collaborative learning. **L.A. Morsch, B. McCollum, M.T. Wentzel**
- 9:15** **238.** Student and faculty perceptions of science practices in undergraduate chemistry laboratory courses. **C. Schnoebelen, T.J. Bussey, S. Brydges**
- 9:35** Intermission.
- 9:50** **239.** Easy as one, two, three: Adapting CER for the college chemistry classroom. **R. Sansom**
- 10:10** **240.** Leveling the playing field: Flipped instruction as a tool for promoting equity in general chemistry. **S.F. Bancroft, S. Fowler, M. Jalaieian, K. Patterson**
- 10:30** **241.** Dissecting the flipped classroom: Research on which aspect of the flipped classroom most impacts student learning and implications for practitioners. **J.F. Eichler, M.D. Casselman**
- 11:10** Concluding Remarks.

Gerry Meyer: The First 100 Years

Sponsored by SCHB, Cosponsored by BMGT, CHED, ENFL, HIST and SCC

Henkel Outstanding Graduate Research in Polymer Chemistry in Honor of Jovan Kamcev

Sponsored by POLY, Cosponsored by CHED and PMSE

TUESDAY AFTERNOON – CHED

SECTION A

Marriott Marquis San Diego Marina
Carlsbad

GSSPC: From Oceans to Clouds: The Environmental Chemistry of Water

Cosponsored by PRES

K. J. Mayer, *Organizer*

M. Alves, *Organizer, Presiding*

K. Mayer, *Presiding*

- 1:30** Introductory Remarks.
- 1:40** **242.** Arctic chlorine chemistry influenced by snowpack photochemistry and NO_x pollution. **S. McNamara, A. Raso, S. Wang, K. Custard, P.B. Shepson, K.A. Pratt**
- 2:20** **243.** Can variability in the western North Atlantic plankton bloom be detected in the properties of

- ambient marine aerosol?. **P. Quinn**, T. Bates, D. Coffman, L. Upchurch
- 3:00** Intermission.
- 3:10** **244.** Atmospheric organic nitrates, secondary organic aerosol, and aqueous phase chemistry. **P.B. Shepson**, J. Slade, T. Jayarathne, A. Morales, J. Rindelaub
- 3:50** **245.** Water-air interfaces: Natural reaction environments. **V. Vaida**
- 4:30** **246.** Water as the “Great Enhancer” in gas phase and heterogeneous atmospheric reactions. **B.J. Finlayson Pitts**, V. Perraud, J. Xu, W. Wang, R.B. Gerber
- 5:10** Concluding Remarks.

SECTION B

Marriott Marquis San Diego Marina
Mission Hills

Hands-on Chemistry Beyond the Classroom: Chemical Education in Informal Settings

S. Raposo, *Organizer, Presiding*

- 1:30** Introductory Remarks.
- 1:35** **247.** Let’s do chemistry: Applying a framework for the design and facilitation of hands-on chemistry activities to promote interest, relevance, and self-efficacy. **D.F. Sittenfeld**
- 1:55** **248.** Theoretical framework of the *Let’s Do Chemistry* project: Overview of research findings that informed the evolution of the framework. **H. Velazquez**, E. Kunz Kollman, M. Bequette, M. Beyer, A. Anderson, G. Haupt, O. Weitzman, C. Heikel, G. Svarovsky, N. Lewis
- 2:15** **249.** Looking at space through Lake Michigan: Hands-on, learning-by-doing, and citizen science perspectives in informal settings. **S. Raposo**, L. Makdisi, C. Bresky
- 2:35** **250.** Chemistry education at the Grand Rapids Public Museum: Engaging students in water quality monitoring. **E.N. Koren**
- 2:55** Discussion.
- 3:05** Intermission.
- 3:20** **251.** Structural chemistry in an unstructured way: Teaching crystallography in informal settings. **A. Sarjeant**, S. Ward, M.P. Lightfoot, I. Bruno
- 3:40** **252.** Community engagement for healthy oceans: Green chemistry & bioplastics. **K. Anderson**, J. Butler
- 4:00** **253.** Instrument maintenance and use outside of the traditional classroom: Training the next generation of undergraduate students. **M.L. Agan**
- 4:20** Discussion.
- 4:30** Concluding Remarks.

SECTION C

Marriott Marquis San Diego Marina
Balboa

Research in Chemistry Education

T. J. Bussey, *Organizer*

R. Komperda, *Organizer, Presiding*

- 1:30** Introductory Remarks.
- 1:35** **254.** Impact of guided-inquiry approaches in physical science laboratory curriculum for K-8 teachers. **A. Sangha**, D. Donnelly
- 1:55** **255.** Using what students know: Learning how secondary chemistry teachers apply informal analysis techniques to assessment results. **A.G. Schafer**, E.J. Yezierski
- 2:15** **256.** PDConnect: Scalable community approach to improving instruction in AP Chemistry nationwide. **G.T. Rushton**, D. Yaron, L. Shah, C. Kulkarni
- 2:35** Concluding Remarks.

Gerry Meyer: The First 100 Years

Sponsored by SCHB, Cosponsored by BMGT, CHED, ENFL, HIST and SCC

WEDNESDAY MORNING – CHED

SECTION A

Marriott Marquis San Diego Marina
Balboa

3D Printing in Chemistry Education: Where, Wherefore & Whereto

A. Leontyev, *Organizer*

J. K. Klosterman, *Organizer, Presiding*

- 8:30** Introductory Remarks.
- 8:35** **257.** Applying 3D printing technology to K-12 STEM and high school internship education. **T. Zhang**, R.A. Bubeck
- 8:55** **258.** Skeletides: Modular, simplified physical model of protein secondary structure. P. Asachi, J. Dang, R.K. Spencer, H. Martin, **R.N. Zuckermann**
- 9:15** **259.** Multi-color space-filling molecular models: Simple method for single filament FDM 3D printing of multi-part molecular models. **J.K. Klosterman**, H. Martin, E. Eisner, S. McAvoy
- 9:35** **260.** Modeling polymers for tactile learning with 3D printing. **M.M. Nolan**, T. Davidson, S. Russell Gonzalez, E. Williams
- 9:55** **261.** Best practices for student-guided 3D printing activity in large lecture courses. **D. Fourches**, J.A. Feducia

- 10:15** Intermission.
- 10:30** **262.** Visualization of potential energy function using an isoenergy approach and 3D prototyping. **A. Teplukhin**, D. Babikov, B.K. Kendrick
- 10:50** **263.** 3D printing new models to teach potential energy concepts in organic chemistry. **F.A. Carroll**, D.N. Blauch, M.T. Bovino
- 11:10** **264.** Increasing accessibility and analytical accuracy in 3D-printable smartphone spectrophotometers. **A.W. Smith**
- 11:30** **265.** 3D-printed, low-cost direct-ink write auger extruder for expanding printable materials. **J. Misiaszek**, Y.J. Wang
- 11:50** **266.** Next generation 3D printed tools for active-learning in the chemistry laboratory: Advances in producing “multifunctional” and “smart” analytical instrumentation. **L.A. Porter**

SECTION B

Marriott Marquis San Diego Marina
Mission Hills

General Papers

S. A. Fleming, *Organizer*
R. Quinones, *Presiding*

- 8:30** Introductory Remarks.
- 8:35** **267.** Making the most of the first lab period of organic chemistry. **J.N. Nalbandian**
- 8:55** **268.** Development of a diboron(4)-mediated transition metal-catalyzed alkene transfer hydrogenation reaction for undergraduate instructional organic chemistry laboratories. **J. Alvarenga**, J. Ochoa, D. Jaramillo-Fellin, J.M. Leslie, B.J. Stokes
- 9:15** **269.** Comparing and contrasting undergraduate organic chemistry textbooks. **D.J. Nelson**
- 9:35** **270.** “Real-world” approach to qualitative organic analysis. **S.W. Bigger**, D. Caridi, A. Smallridge
- 9:55** Intermission.
- 10:10** **271.** Teaching chemistry and art through engaging case studies and hands-on activities. **L. Wang**
- 10:30** **272.** Lessons in stereochemistry: Resolution, synthesis, and characterization of biologically relevant amino acids. **A. Marciniak**, K.A. Scott, W.G. Benson, R. Polt
- 10:50** **273.** Comparing free radicals in sunscreen-treated pig skin as revealed by electron paramagnetic resonance spectroscopy. **R. Quinones**, D. Kolling, D.N. Shoup, A. Smythers, S.A. Nickel, T.D. Westfall, C. Epperly
- 11:10** **274.** Chemistry of water and wastewater: Undergraduate course in water chemistry. **E.A. Nalley**

- 11:30** **275.** Simultaneous determination of 6-gingerol and 6-shogaol in dried ginger by high-performance liquid chromatography in undergraduate research. K. Johnson, **G.R. Khalsa**

WEDNESDAY AFTERNOON – CHED

SECTION A

Marriott Marquis San Diego Marina
Balboa

Leveraging Collaborative Research for Collaborative Outreach

M. Krause, D. Watt, *Organizers, Presiding*

- 1:30** Introductory Remarks.
- 1:40** **276.** Leveraging resources to create lasting infrastructure to support STEM diversity. **M. Napoli**, A. Lubin, O. Aguirre, W. Ibsen, S. Davis
- 2:10** **277.** Workforce learning through a university-community college-government partnership for STEM professional success for underrepresented populations. **M. Napoli**, N. Balos, J. Green
- 2:40** **278.** Building pathways: Evolution of research and outreach alliance with HBCUs. **U. Okafor**, D. Watt
- 3:10** Intermission.
- 3:30** **279.** CCHF science outreach: Taking complex topics in chemistry to the community. **D. Bale**, **D. Morton**
- 4:00** **280.** Blogging as collaborative outreach. **M. Krause**
- 4:30** **281.** It’s all fun and games when the bond breaks: Collaborative research in science education games. **D. Watt**
- 5:00** **282.** Big friendly science: How scalability, modularity, and personability have allowed a chemistry research center to reach millions. **C. Parsons**, C. Conwell, J. Perry

SECTION B

Marriott Marquis San Diego Marina
Mission Hills

General Papers

S. A. Fleming, *Organizer*
D. Brock, *Presiding*

- 1:30** Introductory Remarks.
- 1:35** **283.** Continuing education in chemistry: My educational adventures. **A. Rahman**
- 1:55** **284.** Doing what we want our students to do: Video project to build connections across disciplines. **S. Seethaler**, A. Burgasser, T.J. Bussey, J. Eggers, S.M. Lo, J. Rabin, L. Stevens, H. Weizman

- 2:15** **285.** Computational notebooks for cheminformatics. **P.J. Kowalczyk**
- 2:35** Intermission.
- 2:50** **286.** Success starts in the summer before college begins: Workshop program for preparatory level college chemistry students with potential for revised placement. **R. Hatfield**, T. Moss, E. Houlihan, D.J. Wink, G.A. Papadantonakis
- 3:10** **287.** Assessment of chemistry competency in a first-year integrated science course. **D. Brock, F. Lee**
- 3:30** **288.** Withdrawn
- 3:50** Intermission.
- 4:05** **289.** Transformative education drive at the American University of Beirut. **B.R. Kaafarani**, D.A. El-Achi
- 4:25** **290.** Block-mode delivery of undergraduate chemistry: Eighteen months on. **D. Caridi**, S.W. Bigger, A. Smallridge
- 4:45** **291.** Engaging San Jose State University freshman students in authentic research experience. **L.E. Cheruzel**
- 5:05** **292.** Incorporation of benchtop NMR spectroscopy into undergraduate laboratories. **J. Araneda**, S. Riegel, T. Chu

THURSDAY MORNING – CHED

SECTION A

Marriott Marquis San Diego Marina
Mission Hills

Get the Facts Out: Faculty & Student Perceptions of K - 12 Teaching Careers

T. M. Chambers, K. Thompson, *Organizers, Presiding*

- 8:30** Introductory Remarks.
- 8:45** **293.** University of Northern Colorado Department of Chemistry and Biochemistry's secondary science teaching program. **R.W. Schwenz**
- 9:05** **294.** Informal science teaching as a gateway to careers in science education. **R. Sansom**
- 9:25** **295.** Newberry College Noyce program REMAST, recruit and engage math and science teachers, phase I (2009-2015) and phase II (2015-2020). **C.P. McCartha**, C. Horn, R. Stubbs, N. Simmons, S. Peters, C. Aulbach, K. Simmons, G. Rushton
- 9:45** Intermission.
- 9:55** **296.** Access to inquiry: Recruiting students for 6-12 STEM education. **C. Slown**
- 10:15** **297.** Understanding factors that influence students' choices to pursue a career in teaching. **M.L. Head**, A. Deason, G. Rushton, D. Rosengrant

- 10:35** **298.** Building support at the university, college, and department level for recruiting and retaining secondary education majors in chemistry, physics, and math. **J.B. Nielson**
- 10:55** Discussion.
- 11:15** Concluding Remarks.

SECTION B

Marriott Marquis San Diego Marina
Balboa

Technology in Chemical Education

C. Rezsnyak, *Organizer, Presiding*

- 8:30** Introductory Remarks.
- 8:35** **299.** Withdrawn
- 8:55** **300.** Modernization of a first-year chemistry course through a supported course redesign program. **D. Brock**, P. Kyriacou, **F. Lee**
- 9:15** **301.** Practical reflections and suggestions on creating video materials for flipping a class. **E.P. Stevens**
- 9:35** **302.** Supplementing physical solid state models with virtual reality models. **S.D. Wiediger**, T. Kiraz, M. Robinson, K. Tammen, R.M. Towne
- 9:55** **303.** Membrane proteins can be exciting too. **S. Austin**
- 10:15** **304.** Effective use of multi-media learning objects in teaching chemistry. **J. Selco**
- 10:35** Intermission.
- 10:50** **305.** Applying maker education to chemistry education. **S. Kang**
- 11:10** **306.** Raspberry Pi enabled OERs (open education resources). **R.E. Belford**, A. Holt, E.C. Bucholtz, D.S. Larsen, E. Dourlain, E. Choate, H. Agnew, P. Hudson
- 11:30** **307.** Active learning in organic chemistry integrating LibreTexts: OER multimedia digital resource. **L.A. Morsch**
- 11:50** **308.** Technology enhanced learning for organic chemistry. **K. Huynh**
- 12:10** **309.** Using Mathematica to bring computational chemistry into the classroom. **J.D. Biggs**
- 12:30** **310.** Integrating chemistry Wikipedia projects to foster scientific communication skills. **T. Qin**

CINF

DIVISION OF CHEMICAL INFORMATION

S. Cardinal, *Program Chair*

SUNDAY MORNING – CINF

SECTION A

Omni San Diego Hotel
Grand Ballroom A

Text-Mining & Natural Language Processing for Chemical Information: From Documents to Knowledge

R. J. Bienstock, *Organizer*
J. L. Nauss, *Organizer, Presiding*

- 9:00** Introductory Remarks.
- 9:05** 1. Enhancing data-driven summarization of relations between chemicals, genes, proteins, and diseases based on text mining of biomedical literature. **L. Zaslavsky**, A. Gindulyte, P. Thiessen, E. Bolton
- 9:25** 2. Introducing automated polymer data extractor tool. **C. Dai**, K. Schmidt, D.Y. Zubarev, V.A. Piunova, K. Surugucchi, D.P. Sanders
- 9:45** 3. Extraction of polymer-related information in the cheminformatics tool CIRCA. **K. Schmidt**, C. Dai, T.D. Griffin, K. Surugucchi, D.Y. Zubarev, V.A. Piunova, N. Park, J. Hedrick, L.C. Anderson, D.P. Sanders
- 10:05** Intermission.
- 10:20** 4. Abstract recommendation system: beyond word-level representations. V. Korolev, **A. Mitrofanov**, B. Sattarov, V. Tkachenko
- 10:40** 5. Current challenges in text-mining for chemical information. **R.A. Sayle**, J.W. Mayfield, N. O'Boyle
- 11:20** 6. MOLVEC: Open source library for chemical structure recognition. T. Peryea, D. Katzel, T. Zhao, N. Southall, **D. Nguyen**
- 11:40** Concluding Remarks.

SECTION B

Omni San Diego Hotel
Grand Ballroom D

Nothing New Under the Sun: The Practical Challenges of Patent Novelty Searching

Cosponsored by CHAL and CPRM
Financially supported by Patent Information Users Group (PIUG)
S. R. Adams, E. S. Simmons, *Organizers, Presiding*

- 8:10** Introductory Remarks.
- 8:20** 7. Patent novelty searching: Scope of prior art. **E.S. Simmons**
- 8:50** 8. Quality of indexing for non-patent literature and its implications for retrieval of relevant prior art. **S.R. Adams**
- 9:20** 9. Finding what others miss: Comprehensive prior-art resources for chemical substance searching. **J. Zabilski**
- 9:50** Intermission.
- 10:00** 10. Practical pointers for conducting prior art searches for small molecules, a patent practitioner's point of view. F.J. Koszyk, **X. Pillai**
- 10:30** 11. What's new with scientific content in Google patents. **I. Wetherbee**, **S. Boyer**, J. Frommer, V. Mehta, B. Arneson
- 11:00** 12. Non-patent literature citations in EPO opposition and limitation proceedings. **S.R. Adams**
- 11:30** 13. Inventions for sale? Navigating the on-sale bar under the America Invents Act. **J.L. Krieger**

SECTION C

Omni San Diego Hotel
Grand Ballroom E

Importance of Collaboration to Create Student Success in the Laboratory & Beyond

Financially supported by CAS
S. P. Kuhn, *Organizer*
M. Pozenel, *Presiding*

- 8:30** Introductory Remarks.

- 8:35** 14. Science librarian, a chemical educator, and an EHS professional walk into a lab: Laboratory safety as a collaborative teaching tool. **L.R. McEwen, S.B. Sigmann, R. Stuart**
- 9:00** 15. Innovative teaching collaboration provides students with practical drug discovery experience. **T.E. Mansley, R.L. Broadrup, B. Perry, H. Ahamed, T. Aramburu**
- 9:25** 16. Driving student success through undergraduate internships in biopharma. **N. Hawryluk**
- 9:50** 17. Evolving data needs in chemistry and biosciences: What role can a librarian play in creating student success?. **S. Ramachandran, K. Howell**
- 10:15** 18. Training the biomedical workforce for long-term career success. **A. Bankston**
- 10:40** 19. Business of student success. **J. Rosenberg**
- 11:05** Panel Discussion.
- 11:55** Concluding Remarks.

Bibliography of Chemistry

Chemical Bibliography

Sponsored by HIST, Cosponsored by CINF

Immersive Virtual Reality for Molecular Design

Sponsored by COMP, Cosponsored by CHED, CINF and COMSCI

Nanoinformatics: Information & Data Sciences Applied to Nanomaterials Synthesis, Properties & Biological Effects

Nanoinformatics for Nanomedicines

Sponsored by COLL, Cosponsored by CINF

SUNDAY AFTERNOON – CINF

SECTION A Omni San Diego Hotel Grand Ballroom A

Text-Mining & Natural Language Processing for Chemical Information: From Documents to Knowledge

R. J. Bienstock, *Organizer*
J. L. Nauss, *Organizer, Presiding*

- 1:30** Introductory Remarks.
- 1:35** 20. Automatic identification of relevant chemical compounds from patents. S.A. Akhondi, H. Rey, M. Schwörer, **M. Maier**, J. Toomey, H. Nau, G. Ilchmann, M. Sheehan, M. Irmer, C. Bobach, M. Doornenbal, M. Gregory, J. Kors
- 1:55** 21. Augmenting manual curation of chemical

- patent information in the Derwent World Patents Index. **A. Klein, S. McGhee, J. Hookes**
- 2:15** 22. Journey continues: Addition of French, Russian, Chinese, Korean, and Japanese patents to PATENTSCOPE ChemSearch. **J. Eiblmaier, C. Mazenc, D. Geppert, L. Isenko, H. Saller**
- 2:35** Intermission.
- 2:50** 23. Automating chemical structure and inhibition data extraction from patents: Text-mining approach. F. Costa, I. Haldoupis, **J.L. Nauss, A. Hinton**
- 3:10** 24. BioAssay express: Creating and exploiting assay metadata. **P. Cheung, A. Clark, J. Darlington**
- 3:30** 25. Building fast, robust, and reliable prediction models using very large biological data sets. **L. Weber, H. Boehm**
- 3:50** Concluding Remarks.

SECTION B Omni San Diego Hotel Grand Ballroom D

Chemical Nomenclature & Representation: Past, Present & Future

Cosponsored by HIST and NTS
Financially supported by International Union of Pure and Applied Chemistry (IUPAC); Chemical Structure Association Trust (CSA Trust); InChI Trust
G. Grethe, H. A. Lawlor, L. R. McEwen, *Organizers*
M. M. Rogers, *Organizer, Presiding*

- 1:15** Introductory Remarks.
- 1:20** 26. IUPAC and its role in the development of chemical nomenclature and structure representation. **R. Hartshorn**
- 1:45** 27. IUPAC brief guides on nomenclature: Summary of the key nomenclature principles addressed in IUPAC colored books. **M.M. Rogers**
- 2:10** 28. Evolution of CAS nomenclature: Past, present, and future. **M.A. Strausbaugh**
- 2:35** 29. Updating the Braille Code of Chemical Notation 1997. **P. Verhalen**
- 3:00** Intermission.
- 3:15** 30. Carbon nanotube nomenclature: Challenges of naming emerging materials. **E. Mansfield**
- 3:40** 31. Chemical nomenclature from books to computers: ACD/Name and IUPAC Division VIII. **A. Yerin**
- 4:05** 32. IUPAC, nomenclature, and chemical representation: From the perspective of a worldwide structural database. **M.P. Lightfoot, I. Bruno, C. Tovee, S. Ward, S. Wiggin**
- 4:30** 33. Chemical representation: Toolbox for human and machine collaboration. **L.R. McEwen, E. Hepler-Smith**

SECTION C
Omni San Diego Hotel
Grand Ballroom E

Importance of Collaboration to Create Student Success in the Laboratory & Beyond

Financially supported by CAS

S. P. Kuhn, *Organizer*

M. Pozenel, *Presiding*

- 1:30** Introductory Remarks.
- 1:35** **34.** Helping students stand out in the academic job market. **R.J. Gilliard**
- 2:00** **35.** Connecting the dots across academia and industry to ensure skill alignment. **M. Grandbois**
- 2:25** **36.** Creating digital learning objects for chemistry. **Y. Sevryugina**
- 2:50** **37.** RA21: Secure, seamless access for research. **R. Youngen**
- 3:15** **38.** Experiences in scientific information literacy education. **J. Ji**
- 3:40** **39.** Identifying the different definitions of student success between young scientists, faculty and administration in academia and hiring managers in industry. **M. Pozenel**
- 4:05** Concluding Remarks.

150 Years of the Periodic Table

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Nanoinformatics: Information & Data Sciences Applied to Nanomaterials Synthesis, Properties & Biological Effects

Nanoinformatics for Nanomaterials

Sponsored by COLL, Cosponsored by CINF

SUNDAY EVENING – CINF

SECTION A
San Diego Convention Center
TBD

CINF Scholarships for Scientific Excellence: Student Poster Competition

Financially supported by ACS Publications

E. Alvaro, M. Qiu, *Organizers*

6:30 - 8:30

- 40.** Withdrawn
- 41.** Crystal-structure prediction via basin-hopping global optimisation employing tiny periodic simulation cells and multipole expansion. C. Burnham, P. Samanta, **M. Ghaani**, N. English

42. CDD vault: Complexity simplified. **J. Darlington**, W.W. Smith, B.A. Bunin

43. Withdrawn

44. Medicinal chemistry based measure of R group similarity. **N. O'Boyle**, R.A. Sayle

45. Systematic pipeline for automated structure-based molecular design: Beyond the static picture of hepatic organic anion transporting polypeptides. **A. Tuerkova**, B. Zdrzil

46. Public database supporting evidence-based exposomics. **R.R. Sayre**, J. Wambaugh, K. Phillips, A.J. Williams, C. Grulke

MONDAY MORNING – CINF

SECTION A
Omni San Diego Hotel
Grand Ballroom A

Driving Drug Discovery via Innovative Data Visualization

D. F. Ortwine, *Organizer*

P. Beroza, *Organizer, Presiding*

- 8:30** Introductory Remarks.
- 8:35** **47.** Coupling the 1D, 2D, and 3D data worlds to facilitate drug discovery. **D.F. Ortwine**
- 9:05** **48.** Using knowledge graphs for prediction and visual hypothesis generation in drug discovery. **D.J. Wild**
- 9:35** **49.** Visualizing relationships between protein targets, GO annotations and diseases via dynamic network representations. **B. Zdrzil**, L. Richter, N. Brown
- 10:05** Intermission.
- 10:20** **50.** How a visual vocabulary defines what you see in your data. **R. Guha**
- 10:50** **51.** Molecular viz: I feel the need...the need for speed...and usability. **J. Boström**
- 11:20** **52.** Is virtual reality useful for visualizing and analyzing molecular structures?. **T.E. Ferrin**

SECTION B
Omni San Diego Hotel
Grand Ballroom D

Chemical Nomenclature & Representation: Past, Present & Future

Challenges & Opportunities in Chemical Representation

Cosponsored by HIST and NTS

Financially supported by International Union of Pure and Applied Chemistry (IUPAC); Chemical Structure

Association Trust (CSA Trust); InChi Trust
L. R. McEwen, M. M. Rogers, *Organizers*
G. Grethe, H. A. Lawlor, *Organizers, Presiding*

- 8:15** Introductory Remarks.
8:20 **53.** Chemical structure standardization and synonym filtering in PubChem. **S. Kim**, P. Thiessen, Q. Li, B. Yu, E. Bolton
8:45 **54.** Challenges in chemical registration system migrations, and how to deal with them. **G. Blanke**
9:10 **55.** Making a hash of it: Advantage of selectively leaving out structural information. **N. O'Boyle**, R.A. Sayle
9:35 **56.** Crafting persistent identifiers and structure-based representations in DSSTox as surrogates for chemical names to better support interoperability in computational environments. **C. Grulke**, A. Richard, A.J. Williams
10:00 Intermission.
10:15 **57.** Classification of reactions by type or name. **G. Grethe**, J. Eiblmaier, H. Kraut, D. Kunzman, P. Loew
10:40 **58.** UDM: Enabling exchange of comprehensive reaction information. **F. van den Broek**, G. Blanke
11:05 **59.** Reimagining IUPAC recommendations as a chemical ontology for semantic chemistry. **S.J. Chalk**
11:30 **60.** Publishing FAIR spectral data and chemical structures: Report from the NSF workshop in Orlando. **L.R. McEwen**, **V.F. Scalfani**

SECTION C

Omni San Diego Hotel
Grand Ballroom E

Successful Projects Fueled by Open-Source Tools

R. J. Bienstock, *Organizer, Presiding*

- 8:30** Introductory Remarks.
8:35 **61.** SciWalker: Comprehensive ontology-based chemical search. **L. Weber**, C. Bobach, F. Berthelmann, T. Boehme, S. Boyer, M. Irmer, K. Kruse, U. Laube, J. Ludwig, A. Pueschel, C. Ruttkies, I. Wetherbee
9:00 **62.** RDKit: Open-source cheminformatics from machine learning to chemical registration. **G. Landrum**
9:25 **63.** How the RCDK enables open source cheminformatics in R: From fingerprints to mass spectra. **R. Guha**, E.L. Schymanski, T. Schulze, M.A. Stravs
9:50 Intermission.
10:00 **64.** Applying commonly overlooked corrections to DFT frequency calculations with GoodVibes. **G. Luchini**, R.S. Paton
10:25 **65.** Analysis of the acid/base profile of natural

products as starting points of epigenetic drug discovery. **M.G. Santibanez-Moran**, J. Naveja, B. Pilón-Jiménez, M. Rico-Hidalgo, D. Manallack, J.L. Medina-Franco

- 10:50** **66.** Pharos: Open-source target illumination platform. **T. Sheils**, D. Nguyen, V. Siramshetty, N. Southall, T.I. Oprea
11:15 Intermission.
11:25 **67.** Using open data, services, and source software to deliver the EPA CompTox Chemicals Dashboard. **A.J. Williams**, C. Grulke, K. Mansouri, J. Dunne, J. Edwards
11:50 **68.** Facilitating community-based chemical curation by providing an open source version of the DSSTox chemical and list registration software that supports the EPA CompTox Chemicals Dashboard. **C. Grulke**, A.J. Williams, A. Singh, J. Dunne, J. Edwards, A. Richard

Connecting Professionalism, Safety & Ethics: Opportunities & Challenges

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150 Years of the Periodic Table

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MONDAY AFTERNOON – CINF

SECTION A

Omni San Diego Hotel
Grand Ballroom A

Driving Drug Discovery via Innovative Data Visualization

D. F. Ortwine, *Organizer*

P. Beroza, *Organizer, Presiding*

- 1:30** Introductory Remarks.
1:35 **69.** Matched molecular pair (MMP) and matched molecular series (MMS) visualizations for drug discovery. **C. Keefer**
2:05 **70.** Using DOCK and ZINC to visualize ultra-large chemical libraries. **J.J. Irwin**, B. Shoichet, L. Jiankun, T.E. Balias, R.A. Sayle, I. Singh, A. Levit, Y. Moroz, M. O'Meara, C. Dandarchuluun, B. Wong, J. Young, K. Tang
2:35 **71.** Emerging AI and machine learning approaches for designing novel chemicals and materials with the desired properties. **M. Popova**, O. Isayev, **A. Tropsha**
3:05 Intermission.

- 3:20 **72.** Visualizing structure-based deep learning scoring functions for protein-ligand interactions. **D. Koes**
- 3:50 **73.** Cheminformatics-powered visualization methods of complex multidimensional SAR data. **D. Fourches**
- 4:20 **74.** Data visualization for compound library enhancement: Application of artificial intelligence algorithms from computer chess. **R.A. Sayle, N. O'Boyle, N. Zorn, R. Affentranger**

SECTION B

Omni San Diego Hotel
Grand Ballroom D

Chemical Nomenclature & Representation: Past, Present & Future

InChI'ng Forward

Cosponsored by HIST and NTS

Financially supported by International Union of Pure and Applied Chemistry (IUPAC); Chemical Structure Association Trust (CSA Trust); InChi Trust

G. Grethe, H. A. Lawlor, M. M. Rogers, *Organizers*

L. R. McEwen, *Organizer, Presiding*

M. G. Hicks, *Presiding*

- 1:15 Introductory Remarks.
- 1:20 **75.** Reaction InChI (RInChI): Present and future. **G. Blanke, J.M. Goodman, G. Grethe, H. Kraut**
- 1:45 **76.** Chemical mixtures: File format, open source tools, example data, and mixtures InChI derivative. **A. Clark, P. Cheung, J. Darlington, L.R. McEwen**
- 2:10 **77.** Organometallics: InChI'ng forwards to better representations and happier chemists. **I. Bruno, C. Batchelor, J.M. Goodman, G. Blanke**
- 2:35 **78.** Names for structural variability: Alkanes from maximum efficiency to the limits of existence. **J.M. Goodman**
- 3:00 Intermission.
- 3:15 **79.** IUPAC SMILES+ specification: Proposed community effort to advance interoperability of the SMILES chemical structure representation. **V.F. Scalfani, L.R. McEwen, C. Grulke, E. Bolton, G. Landrum, H. Cooke, I. Yamada, J.J. Irwin, J.L. Medina-Franco, M.Q. Olozabal, O. Koepler, S. Richardson**
- 3:40 **80.** InChI open education resource (OER). **R.E. Belford, E.C. Bucholtz, S.P. Wathen, M.A. Walker, J. Cuadros, T. Gupta, N. Brown, V.F. Scalfani**
- 4:05 **81.** Keeping up the momentum: Brief report from the InChI San Diego workshop. **R.J. Boucher, R. Kidd, I. Bruno, S.R. Heller, L.R. McEwen**
- 4:20 Discussion.

SECTION C

Omni San Diego Hotel
Grand Ballroom E

Materials Informatics

H. Senderowitz, A. Tropsha, *Organizers, Presiding*

- 1:00 Introductory Remarks.
- 1:05 **82.** Fast and accurate interatomic potential models by genetic programming. **A. Hernandez, A. Balasubramanian, F. Yuan, S. Mason, T. Mueller**
- 1:30 **83.** Accelerating design of inorganic materials with machine learning and AI. **O. Isayev**
- 1:55 **84.** Deep learning from crystallographic representations of periodic systems. **P.M. Maffettone, A.I. Cooper**
- 2:20 **85.** Application of machine learning tools for the analysis of combinatorial libraries of all metal-oxides photovoltaic cells. **H. Senderowitz, A. Yosipof, O. Kaspi**
- 2:45 Intermission.
- 3:00 **86.** Database of low-energy cluster structures for atomically precise nanoclusters across the periodic table calculated using density functional theory. **P. Lile, T. Mueller**
- 3:25 **87.** Self-assembly of metal-organic frameworks. **Y.J. Colon, A. Guo, L.W. Antony, K. Hoffmann, J.J. De Pablo**
- 3:50 **88.** Accelerated discovery of high-refractive-index polyimides via *First-Principles* materials modeling and informatics. **J. Hachmann**
- 4:15 **89.** Experiment specification, capture and laboratory automation technology (ESCALATE): Software pipeline for automated chemical experimentation and data management, with application to metal halide perovskite discovery. **J. Schrier**
- 4:40 **90.** Standardization of structural representation of polymers used in medicinal products. **Y. Borodina, I. Filippov, T. Peryea, Y. Pevzner**

Connecting Professionalism, Safety & Ethics: Opportunities & Challenges

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MONDAY EVENING – CINF

SECTION A

San Diego Convention Center
TBD

Sci-Mix

S. K. Cardinal, *Organizer*

8:00 - 10:00

18, 40, 41, 42, 44, 45, 46, 80, 84, 86. See Previous Listings.

100, 114, 133, 135, 155, 158, 172. See Subsequent Listings.

TUESDAY MORNING – CINF

SECTION A

Omni San Diego Hotel
Grand Ballroom A

Herman Skolnik Award Symposium Honoring Dr. Kimito Funatsu

Cosponsored by PROF

Financially supported by Schrödinger

S. K. Cardinal, K. Funatsu, *Organizers*

M. Sugimoto, *Presiding*

- 8:30 91.** Monitoring progress in lead optimization. **J. Bajorath**
- 8:55 92.** Electronic-structure informatics using 3D descriptors of molecules. **M. Sugimoto**
- 9:20 93.** Fast evaluation of potential synthesis routes using DFT calculations on the basis of Transition State Data base (TSDB). **K. Hori**
- 9:45 94.** Development using materials informatics in Japanese companies. **Y. Uchi**
- 10:10 95.** Prediction and control of vacuum deposition process by data-driven method. **Y. Takeda, Y. Zushi, T. Ogushi, E. Kuribe**
- 10:35** Intermission.
- 10:40 96.** Designing synthesizable bioactive compounds with chemistry-savvy machine intelligence. **G. Schneider, D. Merk, F. Grisoni, A. Button, L. Friedrich, J.A. Hiss, P. Schneider**
- 11:05 97.** Activity landscape and its application to molecular design. **K. Hasegawa**
- 11:30 98.** Data-driven drug discovery and medical treatment by machine learning. **Y. Yamanishi**
- 11:55 99.** Development of data driven chemistry in chemistry and chemical engineering. **K. Funatsu**
- 12:20** Award Presentation.

SECTION B

Omni San Diego Hotel
Grand Ballroom D

Extended Reality (XR) in Libraries & Beyond

S. K. Cardinal, *Organizer*

M. Qiu, N. Ruhs, *Organizers, Presiding*

- 8:15** Introductory Remarks.
- 8:25 100.** Application of extended reality (XR) technologies in the academic library to support innovative research and instruction in the physical sciences and engineering disciplines. **E. Cabada, M.C. Schlembach**
- 8:55 101.** Deploying a VR workstation and molecular visualization at Caltech library. **T.E. Morrell, D. Wrublewski**
- 9:25 102.** Librarians and extended reality: Enhancing teaching and learning in the chemical sciences. **S. Putnam, M.M. Nolan, E. Williams**
- 9:55** Intermission.
- 10:10 103.** Using XR to teach about chemical lab safety. **S. Ramachandran, R. Broyer, S. Cutchin, S. Fu**
- 10:40 104.** Digital collections at Cal Poly Pomona and the California State University campuses. **J. Selco**
- 11:10** Panel Discussion.
- 11:40** Concluding Remarks.

SECTION C

Omni San Diego Hotel
Grand Ballroom E

Drug Discovery: Informatics Approaches

E. Davis, *Organizer, Presiding*

- 8:15 105.** Discovery of novel inhibitors of human galactokinase by virtual screening. **M. Shen, X. Hu**
- 8:40 106.** Measuring R group similarity using medicinal chemistry data. **N. O'Boyle, R.A. Sayle**
- 9:05 107.** Mechanism and prediction of UGT metabolism. **M. Öeren, P. Hunt, D.J. Ponting, M. Segall**
- 9:30** Intermission.
- 9:45 108.** Signals lead discovery as the Corteva Cheminformatics Workbench. **D. Tomandl, S. Smith, J. Wilmot**
- 10:10 109.** Probing allosteric modulators of AMP-activated protein kinase. **X. Hu, J.J. Marugan, W. Zheng**
- 10:35 110.** Underlying scientific evidence discovery for FDA orphan drug designations from the GARD integrative knowledge graph: Towards drug discovery for rare diseases. **Q. Zhu, D. Nguyen, N. Southall**

Connecting Safety, Education, Training & Productivity in Analytical Laboratories

Sponsored by ANYL, Cosponsored by CCS, CHAS, CINF and PRES

TUESDAY AFTERNOON – CINF

SECTION A

Omni San Diego Hotel
Grand Ballroom A

Machine Learning & Artificial Intelligence in Computational Chemistry

Drug Discovery

T. Robertson, *Organizer, Presiding*

- 1:30** Introductory Remarks.
- 1:35** **111.** Explore, exploit, and extrapolate: How AI-driven SAR navigation facilitates lead optimisation in drug discovery. **D. Marcus**, C. Luscombe, S. Pickett, S. Senger, D. Green
- 2:05** **112.** AI-driven drug design across the discovery spectrum: Case studies. **J.H. Griffin**
- 2:35** **113.** What compound to synthesize next? How machine learning and artificial intelligence impact compound optimization. **D. Kuhn**, K. Preuer, M. Krug, G. Klambauer, S. Hochreiter, F. Rippmann
- 3:05** Intermission.
- 3:25** **114.** Pretraining deep learning molecular representations for property prediction. **B. Liu**, W. Hu, J. Leskovec, P. Liang, V.S. Pande
- 3:55** **115.** Modeling protein flexibility with conformational sampling improves ligand pose and bioactivity prediction. **K.A. Stafford**, J. Sorenson, I. Wallach
- 4:25** **116.** Machine learning for the discovery of v_6 integrin antagonists. **J.D. Hirst**, S. Oatley, E. Guest, T. Gaertner, S.J. MacDonald
- 4:55** Concluding Remarks.

SECTION B

Omni San Diego Hotel
Grand Ballroom D

One Million Crystal Structures: A Wealth of Structural Chemistry Knowledge

M. Stahl, *Organizer*

H. Abourahma, I. Bruno, *Organizers, Presiding*

- 1:30** Introductory Remarks.
- 1:40** **117.** One million crystal structures in the CSD: Cause for celebration, cause for consideration. **R. Taylor**, I. Bruno

- 2:10** **118.** Leveraging the CSD's one million structures in course-based undergraduate research experience. **H. Abourahma**, A. Sarjeant
- 2:35** **119.** Use of the Cambridge Structural Database in the undergraduate chemistry curriculum. **A.T. Royappa**
- 3:00** **120.** Examining research data through a crystal lens: Teaching students about primary data, data representation, and data management using crystal structure databases. **J.N. Currano**
- 3:25** Intermission.
- 3:40** **121.** Materials genome approach to functional materials discover using the CSD. **K.R. Cousins**, **S.B. Rodriguez**
- 4:05** **122.** Building a collection of metal-organic frameworks in the Cambridge Structural Database for materials discovery. **D. Fairen-Jimenez**
- 4:30** **123.** Improved crystal structure determination from powder diffraction data using the Cambridge Structural Database system. **K. Shankland**, E. Kabova, J. Cole
- 4:55** **124.** Million opportunities: Using the CSD to design color changing molecular switches. **P.R. Raithby**

SECTION C

Omni San Diego Hotel
Grand Ballroom E

Biologic Informatics

R. J. Bienstock, *Organizer, Presiding*

- 1:30** Introductory Remarks.
- 1:35** **125.** Biologics information in PubChem. **J. Zhang**, P. Thiessen, T. Cheng, B. Shoemaker, E. Bolton, N. O'Boyle, R.A. Sayle
- 2:00** **126.** Current progress in HELM representation, integration, and data migration. **D. Deng**, T. Yuan, J. Lee, R. Hotchandani
- 2:25** **127.** Representational and algorithmic challenges in biologic informatics 2019. **R.A. Sayle**, N. O'Boyle
- 2:50** Intermission.
- 3:00** **128.** Notation for identification of glycans contained in glycoproteins, glycolipids, and other biomolecular structure data. **I. Yamada**, N. Miura, S. Tsuchiya, K.F. Aoki-Kinoshita
- 3:25** **129.** Trends in biologics research and development: Analytic studies based on CAS-curated data. **C.Y. Liu**, Y. Li, Y. Deng
- 3:50** **130.** Biosequence searching: How CAS is expanding workflow solutions for IP searchers and beyond. **R.J. Walczak**

SECTION A

Omni San Diego Hotel
Grand Ballroom A

Machine Learning & Artificial Intelligence in Computational Chemistry

Materials Science

T. Robertson, *Organizer*
Y. An, *Presiding*

- 8:30 Introductory Remarks.
- 8:35 **131.** Pesticide quantitative structure-greenhouse-activity relationship models. **D. Tomandl**, C. Klittich, J. Herbert, N.M. Satchivi, D. Demeter
- 9:05 **132.** Pore volumes and surface areas of metal-organic frameworks as descriptors for materials discovery. **A. Mroz**, C.H. Hendon
- 9:35 **133.** Artificial neural network-based approach to thermodynamic property estimation. **R. Van de Vijver**, P. Plehiers, P. Verberckmoes, G.B. Marin, C.V. Stevens, K. Van Geem
- 10:05 Intermission.
- 10:25 **134.** Persistent homology for chemical applications: Story of birth and death. **K.D. Vogiatzis**, A. Cherne, J.K. Kirkland, V. Maroulas, C. Putman Micucci, J. Townsend
- 10:55 **135.** ML models that both learn and teach chemistry via partitioning reactive trajectories by reaction product in phase space using support vector machines. **G. Grazioli**, S. Roy, C.T. Butts
- 11:25 **136.** Deep neural network model for MD-level packing density predictions and its application in the study of 1.5 million organic molecules. **J. Hachmann**
- 11:55 Concluding Remarks.

SECTION B

Omni San Diego Hotel
Grand Ballroom D

One Million Crystal Structures: A Wealth of Structural Chemistry Knowledge

I. Bruno, M. Stahl, *Organizers*
H. Abourahma, *Organizer, Presiding*

- 9:00 Introductory Remarks.
- 9:05 **137.** Pervasive approximate symmetry in *P1* and high-*Z'* organic crystals: Implications for crystal nucleation. **C.P. Brock**
- 9:30 **138.** One million crystal structures: One million disappearing polymorphs waiting to happen?. **J. Helfferich**, J. van de Streek, M. Neumann

- 9:55 **139.** What the Cambridge Structural Database tells us about hydrates. **J. Werner**, J.A. Swift
- 10:20 **140.** Energetics of co-crystal formation: Informing prediction through combining the database with large scale simulations and machine learning. **G.M. Day**, C.R. Taylor, D. McDonagh, W. Fyffe, C. Skylaris
- 10:45 Intermission.
- 11:00 **141.** Using knowledge-based tools to evaluate solid-form design and risk assessment. **B. Sandhu**, C.B. Aakeroy, S.M. Reutzel Edens, A. Sarjeant, S. Vyas
- 11:25 **142.** What did the CSD ever do for drug discovery?. **J. Liebeschuetz**
- 11:50 **143.** Improved structure-based drug design with one million small molecule crystal structures. **B. Kuhn**

SECTION C

Omni San Diego Hotel
Grand Ballroom E

Web-Based Chemistry Databases

A. J. Williams, *Organizer*
C. Grulke, A. Williams, *Presiding*

- 8:00 Introductory Remarks.
- 8:05 **144.** Computational database for first-row transition metals. **K. Basemann**, A. Leffel, A.D. Sadow, T.L. Windus
- 8:25 **145.** Open chemistry: Democratizing web-based chemistry databases. **M.D. Hanwell**, C. Harris, A. Genova, M. El Khatib, M. Haghghatlari, J. Hachmann, W. Dejong
- 8:45 **146.** KinaMetrix: Web resource to investigate kinase conformations and inhibitor space. **R. Rahman**, P.M. Ung, A. Schlessinger
- 9:05 **147.** Structure-based search of chemical libraries with Pharmit. **D. Koes**
- 9:25 **148.** Molecular malthusianism? Next three logs of the growth of purchasable chemical space. **J.J. Irwin**
- 9:45 Intermission.
- 10:00 **149.** Searching for similar reactions and molecules using the power of graph databases and the graph edit distance metric. **V. Delannee**, M.C. Nicklaus
- 10:20 **150.** Helping chemists identify new opportunities during chemistry research: Building and turning high-quality data into actionable insights. **J. Swienty Busch**
- 10:40 **151.** Challenges and opportunities of delivering structural data on the web. **M.P. Lightfoot**, I. Bruno, S. Ward
- 11:00 **152.** Withdrawn
- 11:20 **153.** PubChem: Improving access to chemical information on the web. **A. Gindulyte**

SECTION A
Omni San Diego Hotel
Grand Ballroom A

Machine Learning & Artificial Intelligence in Computational Chemistry

New Methods

T. Robertson, *Organizer*
K. Marshall, *Presiding*

- 1:30** Introductory Remarks.
- 1:35** **154.** Neural network potential for modeling radical reactions. **R. Messerly**, P. St. John, A.E. Roitberg, S. Kim
- 2:05** **155.** Predicting NMR in real-time through message-passing neural network. **Y. Guan**, R.S. Paton
- 2:35** **156.** Practical applications of deep learning to imputation of drug discovery data. T. Whitehead, B. Irwin, P. Hunt, **M.D. Segall**, G. Conduit
- 3:05** Intermission.
- 3:25** **157.** Protein binding site fingerprinting for activity screening in machine learning. **B. Bergman**, K.A. Stafford, D. Bernard, S. Schroedl
- 3:55** **158.** Multiagent consensus equilibrium (MACE) for addressing the scaling challenges of computational chemistry. **J.R. Ulcickas**, G.J. Simpson
- 4:25** **159.** New approach to regression uncertainty analysis and applications to drug design. **M. Waldman**, R. Clark
- 4:55** Concluding Remarks.

SECTION B
Omni San Diego Hotel
Grand Ballroom D

One Million Crystal Structures: A Wealth of Structural Chemistry Knowledge

H. Abourahma, M. Stahl, *Organizers*
I. Bruno, *Organizer, Presiding*

- 1:30** Introductory Remarks.
- 1:35** **160.** Insights from CSD crystallographic data applied to drug discovery. **N. Nevins**
- 2:00** **161.** What fragment hit to follow and how? Using hotspots to prioritise chemistry resources. M. Smilova, P. Curran, C. Radoux, W. Pitt, J. Cole, A. Bradley, **B. Marsden**
- 2:25** **162.** Traversing interoperability: Drug development harnessing the CSD and PDB. **A. Brink**
- 2:50** Intermission.

- 3:05** **163.** Semantic representation of CIF files: Mining crystal structures in the CSD. **S.J. Chalk**
- 3:30** **164.** Learning from a database of a million crystalline materials. **R.I. Cooper**
- 3:55** **165.** From structure to crystallisation and manufacturing: Journey in applications of the CSD. **C.C. Wilson**
- 4:20** **166.** New frontiers beyond one million: New horizons for structural chemistry. **J. Harter**, I. Bruno

SECTION C
Omni San Diego Hotel
Grand Ballroom E

Web-Based Chemistry Databases

A. J. Williams, *Organizer*
C. Grulke, A. Williams, *Presiding*

- 1:30** **167.** US EPA CompTox Chemicals Dashboard: Integrating chemistry and biology data to serve computational toxicology and environmental science. **A.J. Williams**, C. Grulke, A. Richard, R. Judson, G. Patlewicz, I. Shah, J. Wambaugh, K. Paul-Friedman, J. Dunne, J. Edwards
- 1:50** **168.** Lessons learned in building the CompTox Chemicals Dashboard: Engineering a more sustainable web-based chemical database. **C. Grulke**, A.J. Williams, A. Singh, J. Dunne, A. Richard, J. Edwards
- 2:10** **169.** In the world of free, is there room for subscription solutions?. **J.W. Taylor**, M.A. Pozenel
- 2:30** **170.** Google BigQuery for analysis of scientific datasets. **S. Boyer**, **I. Wetherbee**, L. Weber, J. Frommer
- 2:50** **171.** Google BigQuery for analysis of scientific datasets: Interactive exploration and analysis of the data using KNIME analytics platform. **G. Landrum**, M. Pawletta, J. Prinz
- 3:10** Intermission.
- 3:25** **172.** ChEMBL, SureChEMBL and UniChem: Web-based chemistry databases for drug discovery and chemical research. **R. Arcila**
- 3:45** **173.** CIRCA: Your cheminformatics assistant. **T.D. Griffin**, E.W. Louie, S. Boyer, L. Anderson, K. Schmidt, D.P. Sanders
- 4:05** **174.** Transforming quality chemical data handbooks into web-based chemistry databases. **J. Rumble**, F. Macdonald
- 4:25** **175.** Does bigger mean better in the world of chemistry databases?. **A.J. Williams**, C. Southan
- 4:45** **176.** Evolution of the public chemistry databases: Past and the future. **V. Tkachenko**, R. Zakharov
- 5:05** Concluding Remarks.

CMA

COMMITTEE ON MINORITY AFFAIRS

R. Joseph, *Program Chair*

SUNDAY MORNING – CMA

Water, Health, & Environmental Justice in Marginalized Communities

(A) Toxic Chemicals in Water; & (B) Sanitation & Wastewater Resource Recovery Technologies

Sponsored by ENVR, Cosponsored by CMA and PRES

SUNDAY AFTERNOON – CMA

Water, Health, & Environmental Justice in Marginalized Communities

Socio-Cultural & Economic Dimensions of Water & Health

Sponsored by ENVR, Cosponsored by CMA and PRES

TUESDAY AFTERNOON – CMA

SECTION A

Hilton San Diego Bayfront
Aqua Salon C

Elucidating Reaction Mechanisms with Computational & Experimental Chemistry

Cosponsored by COMP and PROF

D. Afzal, M. L. Agan, R. Joseph, *Organizers*

- 1:00 Introductory Remarks.
- 1:05 1. Computational studies of formyl CH-O hydrogen bonds in asymmetric catalysis. **M. Grayson**
- 1:30 2. Theoretical and experimental developments of catalytic partial oxidation of lignin to simple phenols. **S. Kim**

- 1:55 3. Mechanism, selectivity and orbital symmetry of contractive C–C coupling at pentacoordinate phosphorous. **R.S. Paton**
- 2:20 4. Computational study of mechanisms in catalysis using metal organic frameworks. **C. Gaggioli**, T. Scott, L. Gagliardi
- 2:45 Intermission.
- 3:00 5. Mechanistic studies of asymmetric Fe-catalyzed cross-coupling reactions as a platform for reaction discovery. **O. Gutierrez**
- 3:25 6. Application of computational reaction modeling to the development of pharmaceuticals. **C.Y. Lam**
- 3:50 7. Multireference computations to understand the origins of substituent effects in photochemical 4π -disrotatory ring closing reactions of halogenated arenes. **S.A. Lopez**, J. Cox
- 4:15 8. High-throughput first-principles and machine learning discovery of open-shell transition metal catalyst design rules. **H.J. Kulik**, A. Nandy
- 4:40 Concluding Remarks.

TUESDAY EVENING – CMA

Water, Health, & Environmental Justice in Marginalized Communities

Sponsored by ENVR, Cosponsored by CMA and PRES

COLL DIVISION OF COLLOID AND SURFACE CHEMISTRY

R. Nagarajan, *Program Chair*

SUNDAY MORNING – COLL

SECTION A

San Diego Convention Center
Room 6E

Adsorption & Reaction at Surfaces: Symposium in Honor of Charles T. Campbell

Catalysis

Cosponsored by CATL

J. Rodriguez, S. L. Tait, *Organizers*

D. Starr, *Organizer, Presiding*

L. Grabow, *Presiding*

- 8:30** 1. Surface science of molecular catalysis and integration of the three fields of catalysis: Heterogeneous, homogeneous, and enzyme. **G.A. Somorjai**
- 9:00** 2. Identifying single-atom catalysts for CO oxidation from density functional theory. T. Kropp, M. Rebarchik, **M. Mavrikakis**
- 9:30** 3. Single-site catalysts by metal-ligand complexation at surfaces: From model systems in vacuum to high-pressure catalysis on oxide supports. **S.L. Tait**
- 10:00** 4. Interactions of methane on and near high-temperature liquid surfaces. **E. McFarland**, H. Metiu
- 10:30** Intermission.
- 10:50** 5. 2-Propanol dehydration on single-facet-dominant TiO₂ (101) and (001) nanopowder catalysts. **F. Gao**, F. Lin, Y. Wu, B. Sudduth, H. Wang, D. Mei, Y. Wang
- 11:20** 6. Applying low temperature titration for determination of metallic sites on active oxide supported catalysts. **Y. Yang**, Z. Liu, J. Li, Y. Dai
- 11:40** 7. Catalysis with metal phosphides: Synthesis, properties, and reactivity. **M.E. Bussell**, J.D. Springer, R.P. Lynch, R.H. Hagmann

SECTION B

San Diego Convention Center
Room 6F

Colloidal Quantum Dots for Emerging Technologies

F. Rosei, A. Vomiero, *Organizers*

O. K. Varghese, *Presiding*

- 9:00** 8. Failure modes in quantum dot bioimaging agents: It's all about the coating. K. Lee, T. Porter, C. Mcpherson, L. Brillson, **J.O. Winter**
- 9:30** 9. Measuring the absolute photoluminescence quantum yield of colloidal nanoparticles with multipoint method. **Y. Li**, X. Lu, Y. Xue, Z. Ye, H. Qin, X. Peng
- 9:50** 10. Colloidal perovskite quantum dots as scalable emitters of coherent single photons. **H. Utzat**, W. Sun, A. Kaplan, F. Krieg, M. Ginterseder, B. Spokoyny, N. Klein, K. Shulenberger, C. Perkinson, M. Kovalenko, M.G. Bawendi
- 10:10** 11. Colloidal quantum dots-based nano-heterostructures for solar fuel generation. **O.K. Varghese**
- 10:40** 12. Impact of spacers on controlling the optical properties of silicon quantum dots: Fluorescein dyad. **M. Abdelhameed**, D. Machin, P. Charpentier
- 11:00** 13. Noble- and heavy-metal-free colloidal semiconductor branched frame photocatalyst. **D. Chen**
- 11:20** 14. Colloidal carbon dots for solar technologies. **D. Benetti**, H. Zhao, A. Vomiero, F. Rosei
- 11:40** 15. Investigating nucleation and growth kinetics of indium phosphide quantum dots in a continuous flow reactor. **A. Vikram**, A. Zahid, A. Khare, T. SinghRachford, D. Shenai, P. Trefonas, M. Shim, P.J. Kenis
- 12:00** 16. HgCdSe/HgS/CdZnS colloidal quantum wells with bright short-wave infrared light emission. **S. Lim**

SECTION C
San Diego Convention Center
Room 31B

Confined Dynamics of Molecules & Particles at Interfaces, in Pores & under Crowded Conditions

Molecular Scale Confinement

J. Conrad, D. K. Schwartz, *Organizers, Presiding*

- 9:00 Introductory Remarks.
- 9:05 **17.** On the confined orientational motions of dyes diffusing in surfactant templated cylindrical silica mesopores. **D.A. Higgins**, R. Kumarasinghe, T. Ito
- 9:40 **18.** Multicomponent diffusion in mesoporous materials evaluated via diffusion NMR: Guest/host interfacial transport. **A. Erfani**, N. Pickering, C. Aichele, J.L. White
- 10:00 **19.** View of confinement from the perspective of water molecules, as observed by Overhauser dynamic nuclear polarization. **J. Franck**
- 10:25 Intermission.
- 10:35 **20.** Infiltration of polymers into disordered nanoparticle packings: Polymers under extreme nanoconfinement. **D. Lee**
- 11:10 **21.** Quantitative measurement of nanoconfinement effects on molecular transport and chemical reaction with a core-shell mesoporous particle. **N. Fang**, B. Dong, Y. Pei, W. Huang
- 11:35 **22.** Water permeation behavior thorough vertically-aligned carbon nanotube array/polymer composite membranes: Effect of temperature. **H. Matsumoto**, S. Shirahama, S. Zhang, A. Saeki, M. Ashizawa, H. Inoue, Y. Hayashi, S. Tsuruoka
- 12:00 **23.** Dielectric constant of interfacial water over charged interfaces. **F. Geiger**, M. Boamah

SECTION D
San Diego Convention Center
Room 31A

Nanoinformatics: Information & Data Sciences Applied to Nanomaterials Synthesis, Properties & Biological Effects

Nanoinformatics for Nanomedicines

Cosponsored by CINP

S. Jiang, A. Schroeder, *Organizers*

J. Dahlman, D. A. Heller, *Organizers, Presiding*

- 9:00 **24.** Exploration of the nanomedicine-design space with high-throughput screening and machine learning. **C.A. Mirkin**

- 9:40 **25.** Machine learning-driven design of nanomaterials: Ingredients for success. **B. Meredig**
- 10:10 **26.** Nanoinformatics in drug delivery: Matching drugs to carriers. **Y. Shamay**
- 10:40 Intermission.
- 10:50 **27.** caNanoLab: Enhancing retrieval and sharing of cancer nanotechnology data. **L. Russell**, M. Heiskanen, M. Lijowski, C. Liu, P. Grodzinski
- 11:20 **28.** Synthetic closed-loop smart insulin patch. **Z. Gu**
- 11:50 **29.** Nanoinformatics as a driver for nanoparticle synthesis and biomedical imaging paradigms in MRI and CT. **E. Shapiro**

SECTION E
San Diego Convention Center
Room 30E

Nanomaterials

Self-Assembly of Soft Nanomaterials

J. A. Hollingsworth, R. Nagarajan, *Organizers*

J. R. McBride, *Organizer, Presiding*

- 9:00 **30.** Controlled assembly of block copolymer coated nanoparticles in 2D-arrays. **V. Leffler**, L. Mayr, M. Dulle, P. Paciok, H. Du, R. Dunin-Borkowski, **S. Förster**
- 9:20 **31.** Molecular design strategies for creating liquid crystals forming gyroid nanostructures and their advanced functions. **T. Ichikawa**, H. Takeuchi, T. Kobayashi, N. Uemura, X. Zeng
- 9:40 **32.** Controlling orientational orders in self assembly of quantum dot gold heterostructural nanocrystals. **H. Zhu**, Z. Fan, Y. Yuan, M.A. Wilson, D. Eggert, Y. Nagaoka, Y. Liu, Z. Wei, X. Wang, J. He, J. Zhao, R. Li, Z. Wang, M. Gruenwald, O. Chen
- 10:00 **33.** Controlled self-assembly of conjugated block copolymers driven by π - π interactions. **F. He**
- 10:20 **34.** Exerting control over random media by directed self-assembly for optical applications. **J.R. Miller**, C. Wang, Z. Liu, C.D. Keating
- 10:40 **35.** Synthesis and self-assembly of Janus dumbbell nanocrystals. **S. Jiang**, F. Liu, S. Goyal, M. Forrester, K. Miller, T. Ma, L. Zhou
- 11:00 **36.** Surface-directed, DNA-programmed crystallization of nanoparticles. **R. Macfarlane**
- 11:20 **37.** Activity-enhanced self-assembly of a colloidal kagome lattice. **S. Mallory**, A. Cacciuto
- 11:40 **38.** Multi-stimuli responsive nanocomposite tectons. **Y. Wang**, R. Macfarlane
- 12:00 **39.** Thin carbon nanostructure mat with high electromagnetic interference shielding performance. **H. Younes**, A. Al Ghaferi, A. Bani Younes

SECTION F

San Diego Convention Center
Room 30D

Formulation Strategies to Control the Physicochemical Parameters of Drug & Nucleic Acid Delivery Systems

M. A. Ilies, *Organizer*

K. Sakurai, *Organizer, Presiding*

- 9:00** 40. Novel self-assembling drugs for amino-acid delivery system. **Y. Nagasaki**
- 10:00** 41. Hyperloaded poly(2-oxazoline) micelles as personalized drug carriers for brain tumors. D. Hwang, T. Dismuke, E.P. Rosen, J.R. Kagel, C. Lim, W. Zamboni, A.V. Kabanov, T.R. Gershon, **M. Sokolsky-Papkov**
- 10:30** Intermission.
- 10:45** 42. Effects of the polymer corona on the drug loading in ultra-high drug loaded poly(2-oxazoline)/poly(2-oxazine) micelles. H.S. Malik, M. Lübtow, **R. Luxenhofer**
- 11:15** 43. Drug-loaded polymer scaffold parameters on treatment of postsurgical glioblastoma. E. Graham-Gurysh, **K. Moore**, E.M. Bachelder, C.R. Miller, S.D. Hingtgen, K.M. Ainslie

SECTION G

San Diego Convention Center
Room 30C

Frontiers & Challenges in Nanoparticle-Mediated Chemical Transformations

Metallic Nanomaterials

H. Fan, Y. Sun, *Organizers*

O. Chen, J. He, *Organizers, Presiding*

- 8:30** Introductory Remarks.
- 8:35** 44. Chemical transformations of nanostructures. **Y. Yin**
- 9:05** 45. Immobilized metal nanoparticle catalysts for energy applications. **Q. Xu**
- 9:35** 46. Phase engineering of novel nanomaterials. **H. Zhang**
- 10:05** Intermission.
- 10:15** 47. Designing highly durable core@shell electrocatalysts. **S.E. Skrabalak**
- 10:45** 48. Selective chemical transformations on ordered surfaces of intermetallic nanoparticles. **W. Huang**
- 11:15** 49. Tailoring cooperative metal-support interfaces for catalysis. **S. Dai**
- 11:45** 50. Phase-controlled synthesis of colloidal metal nanocrystals. **Y. Xia**

SECTION H

San Diego Convention Center
Room 29B

Water & Tribological Interfaces From Nature to Biomimicking Systems

F. Mangolini, M. Ruths, *Organizers, Presiding*

- 9:00** Introductory Remarks.
- 9:05** 51. Why is ice slippery? Simulations of solid-liquid friction and the shear viscosity of the quasi-liquid layer on ice. **J.D. Gezelter**
- 9:35** 52. Ice-rubber friction mechanisms. D. Mazuyer, S. Hemette, **J. Cayer-barrioz**
- 10:05** 53. Partial slip takes time. **D. Johannsmann**, F. Meyer
- 10:25** Intermission.
- 10:35** 54. Relating dermal friction to water and skin moisture content. **M. Masen**, E. de Vries
- 11:05** 55. Psychotribology: How friction, materials properties, and age influence tactile perception. **M.W. Rutland**
- 11:35** 56. Structure of water inside thin polysaccharide films. H. Ro, O. Zavgorodnya, G. Yuan, M. Chawathe, L. Granado, C.M. Stafford, **D. Bendejacq**
- 11:55** 57. Macroscale water-based superlubricity achieved by PDMS under boundary lubrication regime. **Y. Li**, S. Li, Y. Tian

SECTION I

San Diego Convention Center
Room 33C

Hierarchical Assembly of Peptide & Protein: From Interaction & Structure to Application

M. Dong, *Organizer*

S. Zhang, *Organizer, Presiding*

C. Chen, *Presiding*

- 8:30** 58. Withdrawn
- 9:00** 59. Hierarchical folding and assembly of protein-mimetic nanomaterials. S. Xuan, A.I. Nguyen, **R.N. Zuckermann**
- 9:30** 60. Peptide assembly at interfaces templated by striped phases of amphiphiles. **S.A. Claridge**
- 9:50** 61. Multicomponent coordination self-assembly toward hierarchical supramolecular nanocolloids for efficient photodynamic therapy. **Q. Zou**, X. Yan
- 10:10** 62. Predictive modeling of bionanomaterials from picometers to micrometers. **H. Heinz**
- 10:40** 63. Synthesis and applications of peptoid-based crystalline nanomaterials. **C. Chen**
- 11:10** 64. Peptide-modulated self-assembly of photosensitive nanocolloids for antitumor phototherapy. **X. Yan**, S. Li, R. Chang

- 11:40 65.** Hierarchically assembled three-dimensional array materials composed of virus-like particles (VLPs). **M. Uchida**, N. Brunk, K. McCoy, B. Lee, V. Jadhao, T. Douglas
- 12:00 66.** Two-step model for liquid-liquid phase separation in therapeutic antibody solutions. **B.A. Rogers**, K.B. Rembert, E.A. Graff, M. Poyton, H. Okur, A.R. Kale, T. Yang, J. Zhang, P.S. Cremer

Nanotechnology & Single Cell Analysis in Biology & Medicine

Nanoscience, Biology & Medicine

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

Ambient Pressure Spectroscopy in Complex Environments

Sponsored by CATL, Cosponsored by COLL

SUNDAY AFTERNOON – COLL

SECTION A

San Diego Convention Center
Room 6E

Adsorption & Reaction at Surfaces: Symposium in Honor of Charles T. Campbell

Reactions at Surfaces

Cosponsored by CATL

J. Rodriguez, D. Starr, S. L. Tait, *Organizers*
L. Arnadottir, F. Gao, *Presiding*

- 1:30 67.** Reactions in confined space: Can surface science contribute?. **H. Freund**
- 2:00 68.** Computational approach to determine entropy of adsorbates in catalytic reactions. **L. Arnadottir**, C.T. Campbell, L.H. Sprowl
- 2:30 69.** How water improves the selectivity of preferential oxidation of CO in the presence of excess H₂ over Au/TiO₂. **L. Grabow**, K. Sravan Kumar, T.N. Whittaker, B.D. Chandler
- 3:00 70.** Heterolytic H₂ cleavage and water-assisted hydrogen spillover on single palladium atoms supported on Fe₃O₄(001). N. Doudin, S. Yuk, M. Marcinkowski, M. Nguyen, J. Liu, Y. Wang, B. Kay, J. Li, V. Glezakou, G. Parkinson, R. Rousseau, **Z. Dohnalek**
- 3:30** Intermission.

- 3:50 71.** Control the reactions on surfaces. **J. Zhu**
- 4:20 72.** Parahydrogen-induced hyperpolarization on ordered surface of intermetallic nanoparticles. E. Zhao, R. Maligal Ganesh, C.R. Bowers, **W. Huang**
- 4:40 73.** Selective oxidation of acetaldehyde to acetic acid on Pd–Au(111) bimetallic surfaces. **S. Han**, K. Shin, G.A. Henkelman, C.B. Mullins
- 5:00 74.** Surface reactions of complex molecular systems: From supported graphene to hydrogen storage molecules. **H. Steinrueck**

SECTION B

San Diego Convention Center
Room 6F

Colloidal Quantum Dots for Emerging Technologies

F. Rosei, A. Vomiero, *Organizers*

D. Kilin, P. V. Radovanovic, *Presiding*

- 2:00 75.** Impact of shell imperfections in colloidal quantum dots. **J.R. McBride**, S. Click, K.R. Reid, M.F. Chisholm, J.A. Hollingsworth, S.J. Rosenthal
- 2:20 76.** Linker-free deposition of Au nanoparticles from a Au colloid. **N.J. Quitarano**
- 2:40 77.** Modulating ferroelectric response in colloidal semiconductor nanocrystals through cation exchange. **C. Bradsher**, J.R. McBride, S.J. Rosenthal
- 3:00 78.** First-principles modeling of photoluminescence of colloidal nanostructures. Y. Han, A. Forde, D.J. Vogel, F. Fatima, T.M. Inerbaev, E. Hobbie, **D. Kilin**
- 3:30 79.** Shortwave infrared highly emissive nanostructures derived from Cd/Hg chalcogenide platelets. S. Tenney, V. Vilchez, **J.R. Caram**
- 3:50 80.** Influence of quantum dot and nanomaterial composition on aqueous and non-aqueous digital microfluidics. **U.N. Tohgha**, N.P. Godman
- 4:10 81.** Controlling carrier polarization in plasmonic semiconductor nanocrystals. **P.V. Radovanovic**
- 4:40 82.** High temperature digestive ripening and size focusing of semiconductor nanocrystals in ligand-saturated solutions. **D. Porotnikov**, M. Zamkov
- 5:00 83.** Synergistic approach towards understanding the mechanistic behavior for eradication of superbugs using multifunctionalized nanoplatforms. **A. Pramanik**, K. Gates, Y. Gao, S. Begum, P.C. Ray

SECTION C
San Diego Convention Center
Room 31B

Confined Dynamics of Molecules & Particles at Interfaces, in Pores & under Crowded Conditions

Confined Biomacromolecules

J. Conrad, D. K. Schwartz, *Organizers, Presiding*

- 2:00** 84. Linking interfacial protein dynamics to macroscale elutions. **C.F. Landes**
- 2:35** 85. Single-molecule spectroscopy study of crowding-induced protein spontaneous denature and crowding-perturbed unfolding-folding conformational fluctuation dynamics. **H. Lu**
- 3:00** 86. Superresolution (fcsSOFI) imaging of porous polymer support and active control of protein dynamics. **C. Dutta**, S. Chatterjee, C.F. Landes
- 3:20** 87. Cadherin cluster formation in two dimensional confinement. **C. Thompson**, V. Vu, D.E. Leckband, D.K. Schwartz
- 3:40** 88. Reversible nanobubble surface modifications form protective surface layers at solid/liquid interfaces. **D. Bull**, D. Kienle, A. Chaparro Sosa, N. Nelson, D. Konetski, S. Roy, C. Bowman, J. Cha, D.K. Schwartz, J. Kaar, A.P. Goodwin
- 4:00** Intermission.
- 4:10** 89. Impact of confinement and crowding on the kinetics of enzyme encapsulated in virus-like particles. **J. Sharma**
- 4:30** 90. Manipulating biological systems with polymer chemistry: Encapsulating enzymes. **J.A. Martin**, E. Pinkhassik

SECTION D
San Diego Convention Center
Room 31A

Nanoinformatics: Information & Data Sciences Applied to Nanomaterials Synthesis, Properties & Biological Effects

Nanoinformatics for Nanomaterials

Cosponsored by CINP

J. Dahlman, D. A. Heller, *Organizers*

S. Jiang, A. Schroeder, *Organizers, Presiding*

- 2:00** 91. Experimental and computational search strategies for function in the peptide sequence space. **R. Ulijn**, T. Tuttle
- 2:30** 92. Combinatorial targeting for phenotypic targeting. **G. Battaglia**
- 3:00** 93. Transitioning to predictive analysis for nanoparticle biocorona studies. **K. Wheeler**, A.J. Chetwynd, M. Findlay, I. Lynch

- 3:30** 94. Rapidly identifying nanoparticles for *in vivo* RNA and gene editing using DNA barcoding. **J. Dahlman**
- 4:00** Intermission.
- 4:10** 95. Learning to predict single-wall carbon nanotube-recognition DNA sequences. **A. Jagota**, Y. Yang, M. Zheng
- 4:40** 96. Chemometric analysis of nanosensor libraries for developing short-wavelength infrared optical probes for anthracyclines. **J.T. Del Bonis-O'Donnell**, R. Pinals, S. Jeong, A. Thakrar, R. Wolfinger, M. Landry
- 5:10** 97. Development of targeted nanomedicines facilitated by nanoinformatics. **D.A. Heller**, Y. Shamay, J.D. Chodera, M. Isik

SECTION E
San Diego Convention Center
Room 30E

Nanomaterials

Synthesis & Functional Design of Colloidal Nanocrystals

J. A. Hollingsworth, J. R. McBride, R. Nagarajan, *Organizers*
G. Strouse, *Presiding*

- 2:00** 98. Seeded growth and cation exchange strategies for the synthesis of complex multi-component nanoparticles. **R.E. Schaak**
- 2:30** 99. Molecular programming the phase determination of colloidal nanocrystals with dichalcogenide precursors. **R.L. Brutchey**
- 3:00** 100. Quantum dot design strategies for accurate molecular imaging in cells and tissues. **A. Smith**
- 3:30** 101. Metal-tipped CdSe@CdS tetrapods: Enhanced solar energy conversion and fuel generation enabled by precision nanoscale syntheses and Interface engineering. **N.G. Pavlopoulos**, J. Pyun
- 3:50** 102. Soft-release of captured cells via plasmonic gold nanostars. **G. Vinnacombe**, N. Chiang, L. Heidenreich, Y. Hu, I. Frost, Y. Gong, D. Inouye, T. Fisher, L. Scarabelli, P.S. Weiss, S.J. Jonas
- 4:10** 103. Colloidal ReO₃ nanocrystals: Extra rhenium d-electron instigating a plasmonic response. **S. Ghosh**
- 4:30** 104. Dielectric environment effects on doping efficiency in PbSe nanostructures. **Q. Zhao**, T. Zhao, C.R. Kagan
- 4:50** 105. Gelation of plasmonic metal oxide nanocrystals by polymer-induced depletion attractions. **C. Saez Cabezas**, G. Ong, R. Jadrach, B. Lindquist, A. Agrawal, T. Truskett, D.J. Milliron

SECTION F

San Diego Convention Center
Room 30D

Formulation Strategies to Control the Physicochemical Parameters of Drug & Nucleic Acid Delivery Systems

K. Sakurai, *Organizer*

M. A. Ilies, *Organizer, Presiding*

- 2:00 106. *In vivo* nucleic acid delivery systems for therapeutic targeting of multiple myeloma-microenvironment interactions. **M. Mitchell**
- 2:30 107. Functionalized cationic lipid systems for the delivery of nucleic acid and small molecule therapeutics. **K.K. Ewert**, V. Steffes, E.A. Wonder, C.R. Safinya
- 3:00 108. Machine-learning approach for *in silico* prediction of lipid-based nanoparticles self-assembly. E. Selwa, **B.I. Iorga**
- 3:30 Intermission.
- 3:45 109. Development of gene therapies with novel tropisms by high-throughput *in vivo* screening of lipid nanoparticles. **C. Sago**
- 4:15 110. Tailoring HDL mimetics for *in vivo* delivery of mRNA. **N. Fischer**, W. He, A. Rasley, M.A. Coleman
- 4:45 111. RNAi therapeutics delivered. **M. Manoharan**

SECTION G

San Diego Convention Center
Room 30C

Frontiers & Challenges in Nanoparticle-Mediated Chemical Transformations

Phase & Surface Chemistry of Nanomaterials

H. Fan, Y. Sun, *Organizers*

O. Chen, J. He, *Organizers, Presiding*

- 1:30 Introductory Remarks.
- 1:35 112. Low temperature selective oxidation of methane using unsupported gold-palladium colloidal catalysts. N. Agarwal, S.J. Freakley, R.D. Armstrong, N. Dimitratos, Q. He, **M. Douthwaite**, D.J. Morgan, R.L. Jenkins, D.J. Willock, S.H. Taylor, C. Kiely, G. Hutchings
- 2:05 113. Probing surface sites on metal/alloy nanocatalysts in gas-phase catalytic oxidation reactions. **C. Zhong**
- 2:35 114. Designing oxide-based nanomaterials for energy applications. **T. Hyeon**
- 3:05 115. Structure-function properties of electrocatalysts at nanoscale. D. Strmcnik, P. Papa Lopes, D. Jung, N. Becknell, N. Markovic, **V. Stamenkovic**

- 3:35 Intermission.
- 3:45 116. Nanoparticles for oxygen in heterogeneous catalysis and electrocatalysis. **H. Yang**
- 4:15 117. Plasmonic circular dichroism of Janus nanoparticle emulsions. **S. Chen**
- 4:45 118. To pNP or not to pNP? Broader scope study of nitrophenol reduction with noble metal nanoparticles. **T. Jurca**
- 5:10 119. Controlling acid diffusion rate into gold nanoparticle doped silica-based sol-gel material. **K. Yokoyama**

SECTION H

San Diego Convention Center
Room 29B

Water & Tribological Interfaces

Water & Solid Lubricants: Friends or Foe?

F. Mangolini, M. Ruths, *Organizers*

A. C. Dunn, J. M. Helt, *Presiding*

- 2:00 120. Friction on graphite in the presence of adsorbates: Physical and chemical effects on the basal plane and at step edge defects. **A. Martini**
- 2:30 121. Experiments and simulations of the humidity dependence of friction: Role of interfacial contact quality. **R. Carpick**, K. Hasz, Z. Ye, A. Martini
- 3:00 122. Friction and mechanochemical reactivity of 2D nanomaterials. **J.D. Batteas**
- 3:20 123. Lubricated friction at surface nano-defects. **C. Cafolla**, J.W. Foster, K. Voitchovsky
- 3:40 Intermission.
- 3:50 124. Mechanisms underlying lubrication of faults. Y. Diao, **R.M. Espinosa-Marzal**
- 4:20 125. Energy barriers and the temperature-dependent friction of MoS₂. **A.R. Hinkle**, M. Chandross, J. Curry, T. Babuska, M. Wilson, M. Dugger, N. Argibay
- 4:40 126. Probing and understanding elementary steps in tribochemical reactions. **W.T. Tysoe**
- 5:00 127. Ambient-pressure friction force microscopy studies on ultrananocrystalline diamond films: Effect of environment on nanoscale friction. **J. Kim**, J. Choi, J. Kim, J. Park

SECTION I

San Diego Convention Center
Room 33C

Hierarchical Assembly of Peptide & Protein: From Interaction & Structure to Application

M. Dong, *Organizer*

S. Zhang, *Organizer, Presiding*

R. Alberstein, *Presiding*

- 1:30** **128.** Heterodimer assembly from *de novo* repeat protein structures. **p. huang**
- 2:00** **129.** Functional protein assemblies by chemical design. **F.A. Tezcan**, R. Alberstein, R. Subramanian, Z. Zhang
- 2:30** **130.** Reconfigurable hybrid colloids: Using solid-binding proteins to control nanoparticle assembly and disassembly. **F. Baneyx**
- 3:00** **131.** Nucleation pathway selection yields morphologically diverse two-dimensional protein crystals at solid-liquid interfaces. **R. Alberstein**, S. Zhang, J.J. De Yoreo, F.A. Tezcan
- 3:20** **132.** Nanomaterials for nervous regeneration. **F. Gelain**
- 3:50** **133.** Polymer particles for bio-nano interactions and cancer therapy. **J. Cui**
- 4:20** **134.** Phospholipid self-assembly-based artificial cells. **x. han**
- 4:50** **135.** Self-assembling endogenous biliverdin as a versatile near-infrared photothermal nanoagent. **R. Xing**, K. Chen, X. Yan
- 5:10** **136.** Water-induced β -sheet crosslinking of α -helix rich spider prey-wrapping silk. **B. Addison**, D. Stengel, D. Onofrei, G.P. Holland

Nanotechnology & Single Cell Analysis in Biology & Medicine

Nanoscience

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Ambient Pressure Spectroscopy in Complex Environments

Sponsored by CATL, Cosponsored by COLL

SUNDAY EVENING – COLL

SECTION A

San Diego Convention Center
TBD

Adsorption & Reaction at Surfaces: Symposium in Honor of Charles T. Campbell

Posters

J. Rodriguez, D. Starr, S. L. Tait, *Organizers*

5:30 - 7:30

- 137.** Tuning metal (hydr)oxide composites via functionalized polymers. **R.B. Balow**, J. Lundin
- 138.** Interactions of ascorbic acid on copper for fuel cell applications. **J. Cruz**, M. Groves

- 139.** Quantifying sorption and diffusion in polymeric materials: Experimental results and high fidelity modeling. **S. Matt**, H.N. Sharma, J. Knipe, P. Roy, S. Castonguay, Y. Sun, E. Glascoe

SECTION A

San Diego Convention Center
TBD

Basic Research in Colloids, Surfactants & Interfaces

Posters

R. Nagarajan, *Organizer*

5:30 - 7:30

- 140.** Withdrawn
- 141.** New finds about the mechanism of wormlike micelle formation involving a cationic surfactant and salicylate. **R.N. Nunes de Souza**, M.Z. Jora, L.T. Duarte, T.D. Atvars, E. Sabadini
- 142.** Functional superhydrophobic and icephobic coatings made of new biomimetic “gecko leg” soft dendritic colloids. **A. Williams**, S. Roh, O.D. Velev
- 143.** Removing fine solids suspended in oil media through wettability modification and water-assisted agglomeration. **J. Liu**
- 144.** Structure-dependent properties of nanoporous hydrogels: Rheology and swelling. **Z. Abbasian Chaleshtari**, J. Banuelos, R. Foudazi
- 145.** Dynamics and mechanism of polyelectrolyte-neutral block copolymer micellization in aqueous solution by atomistic MD simulations. **U. Natarajan**
- 146.** Multiresponsive microspheres crosslinked by rotaxane networks. **S. Hiroshige**, T. Kureha, D. Aoki, J. Sawada, D. Aoki, T. Takata, D. Suzuki
- 147.** Thioether–polyglycidol as multivalent and multifunctional coating system for metal nanoparticles. **K. Albrecht**, S. Feineis, J. Lutz, J. Groll, E. Endl
- 148.** Enzyme triggered rapid disassembly of polymeric nanoassemblies. **V. Kumar**, Y. Bae, O. Munkhbat, M. Franc, S. Thayumanavan
- 149.** Hydrothermal synthesis of monodisperse tin oxide nanoparticles and doped tin oxide nanoparticles. **R. Medhi**, T. Lee, T. Lee
- 150.** Interfacial rheology with sub-phase exchange used to investigate dynamics of cyclopentane hydrate film formation and dissociation. **J. Samaniuk**, D. Goggin
- 151.** Olefin-linked dithiol adsorbates for the generation of self-assembled monolayers on gold. **S. Sakunkaewkasem**, T. Lee, M.D. Marquez, M.A. Gonzalez

- 152.** Seedless, one-pot synthesis and simulations of infrared-absorbing silver nanoparticles. **N. Yamamoto, M.P. Zepeda Torres, D. Harris, D.P. Pullman**
- 153.** Bidentate phosphonic acid-based self-assembled monolayers on silver oxide. **J. Lee, T. Lee**
- 154.** New water-free method for the synthesis of chiral QDs and fine tuning of their optical activity. **K. Varga, Y. Joh, S. Tannir, J. Kubelka, M. Balaz**
- 155.** Monitoring the temperature-responsive behavior of cholesteric liquid crystal films and emulsions using QCM-D. **K. Swana, P. D'Angelo, C. Tang**
- 156.** Synthetic methods for preparing partially fluorinated and selectively deuterated adsorbates for self-assembled monolayers. **M. Valverde, H. TranVu, T. Yu, M.D. Marquez, H. Lee, O. Zenasni, T. Lee**

SECTION A

San Diego Convention Center
TBD

Biomaterials & Biointerfaces

Posters

S. Romero-Vargas Castrillon, *Organizer*

5:30 - 7:30

- 157.** Coacervate droplets formation of methylated -cyclodextrin-threaded polyrotaxanes in aqueous media and their applications as an injectable protein carrier. **A. Tamura, K. Nishida, N. Yui**
- 158.** Palladium nanoparticles as ROS scavengers. **M. Moglianetti**
- 159.** Synergistic O₂ generation by manganese ferrite/ceria co-decorated nanoparticles induce M2 polarization of macrophages for rheumatoid arthritis treatment. **J. Kim, T. Hyeon**
- 160.** Application of hemoglobin-capped fluorescent gold nanoclusters for cancer cell targeting and inhibition of cancer cell proliferation. **S. Tan, T. Kuo**
- 161.** Evaluation of cancer progression and inhibition of cancer cell proliferation by using target-specific 2A3 antibody-conjugated gold nanoclusters. **J. Kuo, T. Kuo**
- 162.** Metabolic mechanism of cysteine conjugated fluorescent gold nanoclusters in *Escherichia coli*. **T. Chang, T. Kuo**
- 163.** Synthesis of cysteine-conjugated silver-gold alloy nanoclusters and their application in antimicrobial. **C. Su, T. Kuo**
- 164.** Cysteine conjugated silver nanoclusters for the detection and inhibition of *Escherichia coli*. **P. Hsu, T. Kuo**
- 165.** General model for the permeation of nanoparticles through cellular membranes. **C. Liu, P. Elvati, Y. Wang, A. Violi**
- 166.** Thermal responses of multi-L-arginyl-poly-L-aspartate conjugated with polyethylene glycol. **W. Tseng, Y. Lin**
- 167.** Supported lipid bilayer stripping by buffer flow. **M.J. Ornstead, R. Hunter, C. Cooper, M.L. Valentine, S.K. Smith, C.F. Monson**
- 168.** Surface modification of nanofibrous mats with polymeric micelles for enhanced tissue regeneration. **V. Albright, Y. Wang, C. Mao, M. Stack, H. Hlushko, S. Hernandez, H. Wang, S.A. Sukhishvili**
- 169.** Synthetic charge-invertible polymer for rapid and complete implantation of layer-by-layer microneedle drug films for enhanced transdermal vaccination. **Y. He, C. Hong, J. Li, M. Howard, Y. Li, M. Turvey, D.S. Uppu, J.R. Martin, K. Zhang, D.J. Irvine, P.T. Hammond**
- 170.** Size-matching hierarchical micropillar arrays for detecting circulating tumor cells. **Z. Wang, D. Xu, N. Lyu**
- 171.** Directed cell positioning and photothermally enhanced drug delivery on patterned gold nanorods. **K. TaeHo, H. An, J. Song, I. Choi**
- 172.** Supported lipid bilayer coated microfluidic device for capturing circulating tumor cells. **L. Kawakami, S. Zhang, J. Belling, J. Jackman, N. Wattanatorn, L. Scarabelli, N. Cho, S.J. Jonas, P.S. Weiss**
- 173.** Using scanning force microscopy to unveil the main factors responsible for microorganism adhesion. **E.M. Hudzik, J. Blakeman, J. Clarke, P. McGeechan, J. Petkov, M. Geoghegan**
- 174.** Design of adaptive magnetic carbon nanotubes to mimic stimuli-responsive cell culture substrates. **G. Spiaggia, D. Septiadi, B. Rothen-Rutishauser, A. Fink**
- 175.** Acoustofluidic gene delivery for cancer immunotherapies. **Y. Gong, J. Belling, J. Park, T. Chiou, N. Chiang, S. De Oliveira, P. Weiss, S.J. Jonas**
- 176.** NaCl induced changes in unilamellar DOPC liposomes. **J. De Mel, S. Gupta, R. Perera, L. Ngo, P. Zolnierczuk, A. Farone, M. Bleuel, G. Schneider**
- 177.** Experimental study on the self-assembly of polyesters. **E. Liatsi-Douvitsa, M. Sipin, G. Battaglia**
- 178.** Characterization of the bioaccessibility of nanoparticles in consumer products advertised to contain colloidal silver. **K.R. Rogers**

SECTION A

San Diego Convention Center

TBD

Colloid & Surface Chemistry in Industry: Applications & Career Opportunities

Posters

N. A. Falk, R. I. Maccuspie, *Organizers*

5:30 - 7:30

179. Low-field NMR relaxometry for characterizing wetted surface area in colloids and polymer particle dispersions. **R. Ma**

180. Building and testing a budget-friendly tensiometer. **M. West**, B. Veldman

181. Biopolymer functionalized liposomes for enhanced dispersion stability of nano vesicles. **L. Hyppolite**

182. Effects of humidity on the formation of indoor organic thin films. **S. Schwab**, M. Belsuzarri, V.W. Or, M. Alves, V.H. Grassian

183. Treated diatomaceous earth particles on polymers. **H.J. Perera**, F.D. Blum

184. Impact of gold nanostar morphology on bioassay sensitivity. **P. Ansari**, R.C. Willson, T. Lee

185. Cyclodextrin functionalized 3D-graphene for the removal of Cr(VI) with the easy and rapid separation strategy. **Z. Wang**, F. Lin, L. Huang, Y. Lu, J. Chen

SECTION A

San Diego Convention Center

TBD

Colloidal Quantum Dots for Emerging Technologies

Posters

F. Rosei, A. Vomiero, *Organizers*

5:30 - 7:30

186. Effects of alloying on exciton recombination in InP-ZnSe quantum dots. **S. Click**, K.R. Reid, J.R. McBride, S.J. Rosenthal

187. Second harmonic generation in mesoscale semiconductor helices. **D. Law Hine**, J. Kim, N. Kotov

188. CdHgSe/HgS/CdZnS colloidal quantum wells: Bright short-wave infrared nanoemitter. **G. Lee**, W. Jeong, J. Seo, D. Chung, H. Choi, H. Lyu, S. Lim

189. Doping metal ions into CsPbCl₃ perovskite nanocrystals with improved optical properties for potential optoelectronic applications. **T. Cai**, H. Yang, K. Hills-Kimball, J. Song, H. Zhu, E. Hofman, W. Zheng, B.M. Rubenstein, O. Chen

190. Investigation of the effects of quantum confinement and grain size on the photoconductivity of CdSe nanocrystal thin films. **J. Cassidy**, M. Zamkov

191. Role of spacers towards directing the interactions in silicon quantum dots: Fluorescein dyads. **M. Abdelhameed**, s. Aly, D.D. Machin, P. Charpentier

SECTION A

San Diego Convention Center

TBD

Colloids & Nanomaterials for Water Purification

Posters

C. Drew, *Organizer*

5:30 - 7:30

192. Synthesis and photocatalytic performance of recyclable core-shell mesoporous Fe₃O₄@Bi₂WO₆ nanoparticles. Q. Zhang, Y. Wu, **M. Wang**, S. Zhuo, H. Wang, X. Ge

193. Fibrous N-doped hierarchical porous carbon microspheres: Synthesis and adsorption performance. Y. Xie, W. Yang, M. Wang, **X. Ge**

194. Prussian blue immobilized filter materials for the selective removal of aqueous cesium. **Y. Hwang**, Y. Seo, H. Kim, D. Oh, S. Kang

195. Withdrawn

196. Synthesis of hollow structured CuO-rutile phase TiO₂ hybrid nanoparticles and applications for water purification under visible light condition. **H. Lee**, J. Joo, G. Lee, J. Kim

197. Novel graphene oxide based thin film composite nanofiltration membranes assisted by rapid codeposition of metal-phenolic network/piperzaine. **Y. Yang**, Y. Li, Y. Wang, R. Wang

198. Gold-decorated barium titanate nanoparticles for enhanced photocatalysis. **P. Srinoi**, T. Lee, T. Lee

199. Which aminosilane molecules are the most suitable for surface functionalization of GO toward hexavalent chromium adsorption?. **J. Lee**, H. Kim, J. Lee, J. Choi, S. Lee

SECTION A

San Diego Convention Center

TBD

Confined Dynamics of Molecules & Particles at Interfaces, in Pores & under Crowded Conditions

Posters

J. Conrad, D. K. Schwartz, *Organizers*

5:30 - 7:30

200. Effect of dielectric saturation on the ion activities in membranes. **A. Paspureddi**, M.M. Sharma, L.E. Katz

SECTION A
San Diego Convention Center
TBD

SECTION A
San Diego Convention Center
TBD

Formulation Strategies to Control the Physicochemical Parameters of Drug & Nucleic Acid Delivery Systems

Posters

M. A. Ilies, K. Sakurai, *Organizers*

5:30 - 7:30

201. PLGA fiber containing AuNRs for on-off controlled anticancer drug release system. **Y. Park**, H. Seo, E. Jeong, D. Hyun, **G. Moon**

202. Delivery of the SN50 peptide via PLGA particles for increased immunological control and delayed boosting. **B. Ross**, B. Moser, A. Esser-Kahn

SECTION A
San Diego Convention Center
TBD

Frontiers & Challenges in Nanoparticle-Mediated Chemical Transformations

Posters

O. Chen, H. Fan, J. He, Y. Sun, *Organizers*

5:30 - 7:30

203. Piezoelectrically-mediated mechanochemical reactions for adaptive materials. **J.L. Ayarza**

204. Piezocatalytic activity of piezoelectric nanoparticles induced by audible frequency vibrations. **J. Wang**, Z. Wang, A. Esser-Kahn

205. Pd nanoparticle-quantum dot nanodisc hybrids for photo-enhanced colloidal catalysis. **B. Wang**, Y. Shon

206. Liposome-embedded hydrophobic palladium nanoparticles for biphasic catalysis in water. **D. Ortega**, Q. Tufono, N. Pavlakovich, Y. Shon

207. Pressure induced transformation of formamidinium lead halide perovskite and quantum dot gold heterostructural nanocrystals. **H. Zhu**, Y. Nagaoka, T. Cai, M. Que, J. Song, K. Hills-Kimball, R. Tan, R. Li, B.M. Rubenstein, Z. Wang, O. Chen

Fundamental Research in Colloids, Surfaces & Nanomaterials

Posters

R. Nagarajan, *Organizer*

5:30 - 7:30

208. Using spin coating to fabricate polydopamine thin films. **W. Chen**

209. Photophysics of fluorescent probe molecules in confined environments. **M. Opolz**, **N. Meaux**, R.K. Nayak

210. Interactions of nanomaterials with model lipid bilayer. **M. Skinner**, **R. Warmoth**, S. Lee

211. Anti-inflammatory drugs and the lipid bilayer. **A. Liles**, M. Wood, M.J. Morales, E. Miller, A. Jagarnath, B. O'Sullivan, S. Lee

212. Interactions of PAMAM dendrimers with lipid bilayers. **L. Chong**, E. Perez, S. Zurbriggen, S. Lee

213. Confocal Raman microspectroscopy for biomembrane characterization. **J. Giancaspro**, M. Krmic, E. Miller, P. Scollan, S. Lee

214. Insights into biomembrane structure by water permeability and raman spectroscopy. **P. Scollan**, J. Rosario, E. Miller, S. Foley, S. Lee

215. Computational studies of the effect of caffeine on water permeability in DOPC/cholesterol model membrane. **T.A. Johnson**, S. Lee, R. Versace

216. Role of cis and trans double bond on water permeability of model membrane in the presence and absence of cholesterol: Computational studies. **J. Rosario**, S. Lee, R. Versace

217. Computational studies on water permeability across a DOPC biological membrane: Effect of cation. **J. Villa**, S. Lee, R. Versace

218. Ultrasound-stimulated cargo release at low temperature for spatiotemporally and quantitatively controllable contrast enhancement by magnetic resonance guided high intensity focused ultrasound. **C. Cheng**, W. Chen, J.I. Zink, L. Zhang, H. Wu

219. Amoebae assemble synthetic spherical particles to form reproducible constructs. **T.J. McCarthy**, P. Bian

220. Enzyme immobilization in mesoporous silica shells of magnetic nanoparticle cluster supports: Does pore size matter?. **M. Carbonell**, B.P. Lawson, A.M. Sulman, B.D. Stein, V.G. Matveeva, L. Bronstein

221. Magnetically recoverable Pd and Ru nanoparticulate catalysts based on

polyethyleneimine or chitosan: Major factors in nitroarene reduction. **T.A. Dickstein**, L. Gregor, Y. Losovyj, B.D. Stein, L. Bronstein

222. Evaluation of stability of concentrated hydrosol with the droplets of unsaturated lipid. **Y. Watanabe**, M. Shinada

223. High-efficiency electrocatalyst for the oxygen reduction reaction: Atomic Fe-dispersed on N-doped carbon hollow nanospheres. **Y. Chen**, S.E. Skrabalak, L. Xu, Y. Tang

224. Self-assemblies of truncated tetrahedral quantum dots with anisotropic patchiness. **Y. Nagaoka**, O. Chen, H. Zhu

225. Amplifying hot electrons with Schottky barrier lowering by application of an external bias on a metal–semiconductor nanodiode. **B. Jeon**, C. Lee, J. Park

226. Generation of hot electrons at metal-oxide interfaces during the decomposition of hydrogen peroxide on Pt nanowire/Si nanodiodes. **H. Kim**, **Y. Kim**, **Y. Jung**, **J. Park**

227. Effect of functionalization of porous silica as nanoreactor for preparation of fluorescent carbon dots. **A. Mikhralieva**, H. Motta, V. Zaitsev

228. Study of collective magnetic behavior of iron oxide at nanoscale interparticle distances through DNA-assisted self-assembly. **P. Rahmani**, T. Ye

229. High-spatial single cell histone mapping using optically tunable nanoparticles. **H. An**, K. TaeHo, I. Choi

230. Novel nanohybrids of chemically active boron based nanosheets with gold nanoparticles and graphene: Assembling mixed dimensional heterostructures in solution. **A. James**, S. Khandelwal, A. Dutta, **K. Jasuja**

231. Cu-catalyzed synthesis of CdZnSe-CdZnS alloy quantum dots with highly tunable emission. **Y. Yuan**, H. Zhu, X. Wang, D. Su, J. Zhao, O. Chen

232. Quantum-well CdS/CdSe/CdS nanoshells exhibiting long-lived biexciton populations. **D. Harankahage**, N.N. Kholmicheva, D. Budkina, D. Porotnikov, A.N. Tarnovsky, M. Zamkov

233. Magnetic chaining of PDMS beads in new gels and anchor sites for the improvement of wall slip conditions. **N.I. Morales Castellanos**, B. Bharti, O.D. Velez

Hierarchical Assembly of Peptide & Protein: From Interaction & Structure to Application

Posters

M. Dong, S. Zhang, *Organizers*

5:30 - 7:30

234. Formation of 2D liquid crystal phases by *de novo* designed proteins at crystal-solution interfaces. **J. Chen**, S. Zhang, J. Edison, Z. Preisler, S. Whitelam, J.J. De Yoreo

235. Development of virus-like hierarchical silica nanoparticles using an engineered capsid protein for biomedical applications. **C. Kim**

Nanomaterials

Posters

J. A. Hollingsworth, J. R. McBride, R. Nagarajan, *Organizers*

5:30 - 7:30

236. Interlayer structure control and self-assembly of two-dimensional MXene thin films for gas sensors. **S. Kim**, H. Koh, H. Jung, C. Ahn, Y. Gogotsi

237. 2D Pd-based multimetallic nanosheets. **C. Si**, W. Lu

238. On solid lipid nanoparticles. **D. Pink**, J. Lawrence, C. Lorenz

239. Creation of gyroid nanostructured polymer films having 3D continuous aqua-sheet for fast proton conduction. **T. Kobayashi**, X. Zeng, T. Ichikawa

240. Formation of double gyroid nanostructures by self-organization of atropisomeric ionic amphiphiles. **N. Uemura**, T. Kobayashi, K. Goossens, X. Zeng, G. Watanabe, T. Ichikawa

241. Polymerization of vinylimidazolium-based amino acid ionic liquids in bicontinuous cubic liquid-crystalline assemblies. **H. Takeuchi**, T. Ichikawa

242. Assembly of anisotropic nanomaterials for flexible resistive switching device. **Y. Park**, E. Jeong, G. Moon

243. Growth and control of 2D rhombus supramolecular structures of fluorescent block copolymers. **L. Han**

244. Well-controlled rectangular and square platelet micelles self-assembled by poly(3-

hexylthiophene)-b-polyethylene glycol. **R. Qi**

245. Self-assembled nanochamber arrays for liquid cell transmission electron microscopy. **Y. BAE**, B. Kim, J. Park

246. Colloidal gold nanostars as a SERS substrate for the detection of methimazole in urine using a handheld Raman spectrometer. **C. Rusin**, A. Mahmoud, M.T. McDermott

247. Seed-mediated co-reduction as a route to shape-controlled PdCu-PtCu core-shell nanoparticles. **S. Atehortua Bueno**, S.E. Skrabalak

248. *In situ* monitoring of the heterogeneous nucleation of a second metal on silver nanocubes using an isocyanide molecular probe. **J. Ahn**, Y. Zhang, Y. Wu, D. Qin

249. Glycation of human serum albumin alters nanoparticle-protein interactions. **K. Fahy**, **K. Leung**, M. Eiken, K. Baumgartner, H. Park, K.R. Riley, K. Wheeler

250. Tuneable emission in mercury chalcogenide nanoplatelets. **S. Tenney**, J. Caram

251. Aqueous stability and SERS activity of polydopamine functionalized aluminum nanocrystals. **D. Renard**, S. Tian, B.D. Clark, A. Ahmadivand, C.J. Desantis, P.J. Nordlander, N.J. Halas

252. Aluminum nanocubes have sharp corners. **B.D. Clark**, C. Jacobson, M. Lou, A. Ali, G. Wu, L. Bursi, D. Renard, A. Tsai, P.J. Nordlander, N.J. Halas

253. Synthetic control of nanowire structure for high resolution electron microscopy. **A. Bruefach**, **X. Song**, M. Scott

254. Visible-transparent and UV-reflective supraballs of hollow silica nanospheres in solution. **S. Lee**, G. Yi

255. Quantum-size effect of the bond dissociation enthalpies and formation enthalpies in single walled carbon nanotubes. **C.D. Zeinalipour-Yazdi**, E. Loizidou, A. Chutia

256. Ultrathin hydroxide nanosheets for old paper deacidification. **S. Wang**, S. Lei, X. Zeng

257. Tuning the nitrogen species content in N-doped CNTs for catalytic applications. **J.M. Ruiz Marizcal**, D. Morales G., E. Contreras, H. Borbón Núñez, D. Dominguez, H. Tiznado, O.E. Contreras, J.M. Romo-Herrera

258. Inclusion of plasmonic nanoparticles into low density materials. **I. Becerril Castro**, A. Castro-Ceseña, F. Muñoz-Muñoz, J. Romo-Herrera

259. Nanoscale interactions between liposomes and magnetic/plasmonic nanoparticles investigated by means of (surface - enhanced) Raman spectroscopy. **G.F. Stiufluic**, S. Nitica, V. Toma, C.M. Lucaciu, R.I. Stiufluic

260. AgAu alloy nanoshell: Decorated BaTiO₃/TiO₂ and SrTiO₃/TiO₂ for photoelectrochemical catalysis. **Y. Chang**, T. Lee, Y. Hsu, R. Medhi, P. Srinoi, T. Liu, M.D. Marquez

261. Tunable 3D DNA origami-gold nanoparticle hybrid: Self-assembled ultrasensitive SERS substrate. **Y. Zhang**, H. Cao, T. Ye

262. Computational study on the binding affinities of aliphatic α -amino acids with graphene. **J. Lazare**, T. Dinadayalane

263. Effects of template and molecular nanostructure on the performance of organic-inorganic photomechanical actuator membranes based on aligned nanocrystals. **X. Dong**, C. Bardeen

264. Relationship between surface topography and ice adhesion on superhydrophobic surfaces. **Y. Wang**

265. Withdrawn

266. Potential of click nucleic acids in widening nanoparticle functionality. **A. Harguindey Sanchez**

267. Functionalized nanodiamonds in the investigation of the aggregation phenomenon. **L. Lott**, C. Winstead

268. Chemically modified titanium boride nanosheets: High yield synthesis and hierarchical assembly into paper-like macrostructures. **A. James**, N. Pandey, M. Lenka, K. Jasuja

SECTION A

San Diego Convention Center
TBD

Surface Chemistry

Posters

S. L. Tait, *Organizer*

5:30 - 7:30

269. Enhancing electrochemical efficiency of hydroxyl radical formation on diamond electrodes by functionalization with hydrophobic monolayers. **A.H. Henke**, T. Saunders, J.A. Pedersen, R.J. Hamers

270. Intramolecular insights into adsorbate-substrate interactions by tip-enhanced Raman spectroscopy at the angstrom-scale. **J.F. Schultz**, S. Mahapatra, L. Li, N. Jiang

271. Evaluating the binding of ligands on silver nanocubes by *in situ* surface-enhanced Raman spectroscopy. **J. Ahn**, B. Vannatter, D. Qin

272. Breathable moisture responsive fibrous materials. **L. Lao**, J. Fan

273. Identifying the barriers to sub-nanometer resolution non-contact atomic force microscopy of hydrophobic surfaces in liquid. **W.A. Nanney**, Q. Yang, X. Hu, A. Martini, T. Ye

- 274.** Domain structures in mechanically exfoliated single-layer MoS₂ on Au(111). **F. Wu**, Z. Liu, N. Hawthorne, M. Chandross, N. Argibay, J. Curry, J.D. Batteas
- 275.** Surface immobilized thermos- and light-responsive hybrid microgels for modulation of surface properties. **C. Ou**, S. Giasson
- 276.** Antioxidant hydrogen-bonded coatings of linear synthetic polyphenol polymers. **R. Hlushko**, H. Hlushko, S.A. Sukhishvili
- 277.** Noncovalent microcontact printing for hierarchically patterned striped phases of polymerized lipids. **T.C. Davis**, J.O. Bechtold, T.R. Hayes, T.A. Villarreal, S.A. Claridge
- 278.** Intermolecular π -interactions lead to homogeneously mixed phenyl-terminated self-assembled monolayers. **T. Yu**, M.D. Marquez, T. Lee
- 279.** Recovering rare earth elements (REEs) from coal fly ash and power plant wastewater sludge leachates with an engineered sorbent. **M. Dardona**, T.M. Dittrich, J. Hovey, M.J. Allen, S.K. Mohanty
- 280.** Reactivity of 4-NBD with single and multilayer MoS₂ on Au(111). **Z. Liu**, F. Wu, J.D. Batteas
- 281.** Copper-based oligomerization/functionalization of patterned, ligand presenting, self-assembling monolayers (SAMs) at the liquid-HOPG interface. **L. Wilczek**, M. Zimmt
- 282.** Highly efficient, biofriendly exfoliation of α -zirconium phosphate nanosheets in water using proteins. **M. Malhotra**, C.L. Baveghems, J. Gascon, C.V. Kumar

SECTION A

San Diego Convention Center

TBD

Surfaces & Interfaces in the Environment: Symposium in Honor of Vicki Grassian

Posters

Cosponsored by ENVR

A. P. Ault, J. Baltrusaitis, *Organizers*

5:30 - 7:30

- 283.** Experimental and theoretical study of the optical properties of benzoic acid and benzoate, for understanding complex macromolecular photosensitizers. **N. Karimova**, M. Luo, R. Gerber, V.H. Grassian
- 284.** Using easy ambient sonic-spray ionization mass spectrometry (EASI-MS) for depth profiling organic particles. **L.M. Wingen**, B.J. Finlayson Pitts
- 285.** Stability of lipid monolayers at the air/sea water interface. **M. Luo**

- 286.** Atmospheric organic aerosol acidity sensing via polymer degradation. **Z. Lei**, S.E. Bliesner, C. Mattson, K.A. Pratt, J.N. Albert, A.P. Ault
- 287.** Surface potential of aqueous fatty acid and alcohol surfaces: Understanding temperature effects and ice nucleation. **M.G. Vazquez de Vazquez**, H.C. Allen
- 288.** Synergistic performance of antimicrobial coatings deposited on air particulate filters. **O.V. Ezeh**, Y. Li, W. Han, K. Yeung
- 289.** Effects in cellular physicochemical properties by copper oxide nanoparticulate matter. **S. Hsieh**, M. Kung, J. Wang, A.K. Dwivedi, C. Tang, S. Huang, M. Tai, S. Hsieh
- 290.** Nanoscale morphology and spectroscopic analyses of glass surfaces in indoor environments. **V.W. Or**, **M. Alves**, M. Wade, S. Schwab, M. Belsuzarri, R. Corsi, A. Novoselac, V.H. Grassian
- 291.** Investigation of monoethanolamine adsorption on oxide surfaces. **A. Rose**, I. Sit, V.H. Grassian
- 292.** Impact of concentration and the presence of salt on the surface pKa of fatty acids at the air-water interface. **M. Song**
- 293.** AFM-IR and SFG analysis on various geochemical interfaces with adsorbed BSA. **D. Kim**, H. Chen, W. Xiong, V.H. Grassian
- 294.** α -Amino acid adsorption onto metal oxide nanoparticles: A spectroscopic study to understand the effects of pH and particle type. **I.B. Ustunol**, N.I. Gonzalez-Pech, V.H. Grassian
- 295.** DNA adsorption on iron (III) oxide: Effects of pH and ionic strength on surface interactions. **I. Sit**, V.H. Grassian

SECTION A

San Diego Convention Center

TBD

Targeted Delivery of Nanomedicines In Vivo

Posters

P. del Pino, N. Feliu Torres, W. J. Parak, *Organizers*

5:30 - 7:30

- 296.** Design of multi-functionalized liposomes for adsorbing and neutralizing target molecules *in vivo*. **S. Hirano**, H. Koide, T. Ide, Y. Hamashima, N. Oku, T. Asai
- 297.** Golden age revisited: Developing a resource sparing gold nanoparticle platform to rapidly triage immune cell targeting ligands in discovery. **L. Austin**, N.L. Sullivan, W.A. Rose II, P. Huo, L. Yan, J.S. Smith, G. Swaminathan, S.T. Spagnol, I.T. Raheem, A.J. Bett, M. Gindy

298. Facile preparation of Au/Silk nanoparticles as a multifunctional drug delivery system. **A.T. Dao**, H. Kasai

SECTION A

San Diego Convention Center

TBD

Theoretical & Experimental Investigations of Water Interactions with Materials

Posters

Cosponsored by ANYL

D. Donadio, T. Guo, *Organizers*

5:30 - 7:30

299. Counterintuitive droplet motion mediated by printed charges. **Q. Sun**, X. Deng

300. Designing the armor for ultra-robust superhydrophobic surfaces. **D. Wang**, X. Deng

301. Identification of natural evaporation-induced ionovoltaic electrical energy conversion system. **S. Yoon**, H. Jin, W. Lee, Y. Kim

302. Omni-liquid droplet manipulation platform. **J. Guo**, X. Deng

303. Quantitatively revealing the distribution of water within hydrophobic polymers via differential scanning calorimetry and theoretical prediction of hydrated polymer thermal profiles. **C. Liu**, A. Tripathi, J. Tsavalas

304. Ionovoltaic device for monitoring ion dynamics in aqueous-phase. **W. Lee**, S. Yoon, H. Jin, J. Han, Y. Cho, Y. Kim

305. Electrical energy generation from water droplets infiltration in porous copper oxide nanowires film. **H. Jin**, S. Yoon, W. Lee, J. Han, Y. Cho, Y. Kim

SECTION A

San Diego Convention Center

TBD

Water & Tribological Interfaces

Posters

F. Mangolini, M. Ruths, *Organizers*

5:30 - 7:30

306. Potential-induced nonlinear friction behavior between silica microsphere and gold surfaces in aqueous solution. **S. Li**, P. Bai, Y. Li, Y. Meng, L. Ma, Y. Tian

307. Intrinsically lubricating hydrogel coatings for HIV prevention. **M.B. Elinski**, A.I. Bennett, H. Wang, W. Chen, W.Y. Lin, J.A. Bauermeister, S. Yang, R. Carpick

308. Non destructive method to calibrate the torsional spring constant of atomic force microscope cantilevers in viscous environments. **C. Cafolla**, A.F. Payam, K. Voitchovsky

309. Static friction phase diagram for hydrogel-like materials. **T. Shoaib**, R.M. Espinosa-Marzal

310. Understanding the IL-solid interface using water as molecular probes. **M. Han**, R.M. Espinosa-Marzal

311. Investigating pressure-solution and frictional behavior of calcite with an extended surface forces apparatus. **Y. Diao**, R.M. Espinosa-Marzal

Structure at Solid-Liquid Interfaces: Effects of Confinement & Chemical Patterning

Sponsored by ANYL, Cosponsored by COLL

MONDAY MORNING – COLL

SECTION A

San Diego Convention Center

Room 5B

Adsorption & Reaction at Surfaces: Symposium in Honor of Charles T. Campbell

Mechanisms & Kinetics

Cosponsored by CATL

J. Rodriguez, D. Starr, S. L. Tait, *Organizers*

Z. Dohnalek, J. Zhu, *Presiding*

8:00 312. Interactions between arsenic and ferric iron during ferric coprecipitation treatment: Effect of arsenic on ferric oxides formation, and possible formation of ferric arsenate complexes. **Q. Shi**, S. Zhang, C. Christodoulatos, X. Meng

8:20 313. Vibrationally energy-driven reactions of CO₂ on Cu surfaces. **J. Nakamura**

8:50 314. Oxygen reduction reaction on Pt electrodes: From kinetics and spectroscopy to new materials. **S. Lincic**

9:20 315. Kinetics of 1,4-bis (phenylethynyl) benzene (DEB) in Pd/C catalyzed hydrogenation. **H.N. Sharma**, E. Sangalang, C. Saw, G. Cairns, W. McLean, R.S. Maxwell, L. Dinh

9:40 316. Mechanistic studies for the water-gas shift reaction on Cu-ceria catalysts. **J. Rodriguez**
Intermission.

10:10 317. Recent advances in methods for finding the mechanism and rate of surface processes. **H. Jonsson**

11:00 318. Ion imaging measurements of velocity resolved reaction rates: New insights into CO

oxidation on Pt. J. Neugeboren, D. Borodin, H.W. Hahn, J. Altschäffel, A. Kandratsenka, **D. Auerbach**, C.T. Campbell, D. Schwarzer, D.J. Harding, A.M. Wodtke, T. Kitsopoulos

- 11:30 319.** Kinetics studies of the direct conversion of methane to methanol by Cu/mordenite zeolites: What can they tell us about fundamental and process related aspects of the “Holy Grail” of catalysis?. **M. Newton**, A.J. Knorpp, D. Stoian, H. Emerich, J.A. van Bokhoven

SECTION B

San Diego Convention Center
Room 6F

Surfaces & Interfaces in the Environment: Symposium in Honor of Vicki Grassian

Catalysis, Surfaces & Minerals

Cosponsored by ENVR and WCC

A. P. Ault, J. Baltrusaitis, *Organizers, Presiding*

- 8:30** Introductory Remarks.
- 8:35 320.** Surface chemistry of transition metal doped MgO nanoparticles and their reaction products *in situ*. **J. Baltrusaitis**, M. Silva, D. Kiani
- 9:00 321.** Metal nodes in metal-organic frameworks as active sites for gas-phase catalytic hydrogenation. D.M. Shakya, O.A. Ejegbavwo, R. Thayalan, S. Farzandh, A.J. Brandt, S.D. Senanayake, A. Ebrahim, A. Frenkel, J.R. Monnier, K.D. Vogiatzis, N.B. Shustova, **D.A. Chen**
- 9:30 322.** Nanostructured adsorbents and catalysts for environmental applications. **W. Song**
- 9:50 323.** Kinetics study of heterogeneous reactions of n-butylamine with succinic acid using an ATR-IR flow reactor. **Y. Liu**, X. Gao
- 10:10 324.** Coupling molecular catalysts with light-harvesting surfaces for solar CO₂ reduction. P. Huang, S. Pantovich, J. Rondeau, S. Xu, **G. Li**
- 10:30** Intermission.
- 10:40 325.** SFG spectro-microscopy for self-assembled materials. **W. Xiong**
- 11:00 326.** Heterogeneous molecular interactions at the silica/water interface. D. Lesnicki, Y. Fang, K. Wall, S. Parashar, M. Gaigneot, V. Vaida, V.H. Grassian, **M. Sulpizi**
- 11:20 327.** From calcite to nanospheres: Closing the surface gap between cloud condensation nuclei activity and water adsorption. **C.D. Hatch**, P.R. Tumminello, M. Cassingham, R. Parham, K. Morris, H. Hayes, H. Dana, C. Botner, O. Eddings
- 11:40 328.** Surface chemistry of airborne mineral dust aerosols: Environmental and health implications. **G. Rubasinghege**

SECTION C

San Diego Convention Center
Room 31B

Confined Dynamics of Molecules & Particles at Interfaces, in Pores & under Crowded Conditions

Dynamics in Crowded Conditions

J. Conrad, D. K. Schwartz, *Organizers, Presiding*

- 8:30** Introductory Remarks.
- 8:35 329.** Colloidal glass transition in confined spaces. **E.R. Weeks**, C. Cao, X. Huang, C.B. Roth
- 9:10 330.** Appearance of a slow mode of polymer surface diffusion on polymer brush-patterned surfaces in aqueous solution. C.G. Clarkson, A. Johnson, G.J. Leggett, **M. Geoghegan**
- 9:35 331.** Advancements in fluorescence correlation spectroscopy super resolution optical fluctuation imaging (fcsSOFI) to quantify anomalous diffusion in crowded environments. **L. Kisley**
- 10:00 332.** Complex salt dependence of polymer diffusion in polyelectrolyte multilayers. **D.F. Kienle**, D.K. Schwartz
- 10:20** Intermission.
- 10:30 333.** Modeling the Brownian hydrodynamics of intracellular motion. **R. Zia**, A. Maheshwari, D. Endy, E. Gonzalez, A.M. Sunol
- 11:05 334.** Brownian motion within lipid bilayers is correlated over large distances. **R.L. Schoch**, I. Barel, F.L. Brown, G. Haran
- 11:25 335.** Controlling the location of membrane components in planar supported bilayers. S. Sun, C. Liu, **P.S. Cremer**

SECTION D

San Diego Convention Center
Room 31A

Colloid & Surface Chemistry in Industry: Applications & Career Opportunities

Financially supported by Natural Immunogenics Corporation

N. A. Falk, R. I. Maccuspie, *Organizers, Presiding*

- 8:30** Introductory Remarks.
- 8:35 336.** Career using colloidal and surface science in government, academia, and industry. **R.I. Maccuspie**
- 9:05 337.** R&D careers at the Clorox Company: Making a difference every day. **N.A. Falk**
- 9:35 338.** My experience from grad school to an industrial career at P&G. **D. Hosseinpour**
- 10:05 339.** Careers at the industry-academia interface: Insights from sustainable nanotechnology and

- entrepreneurship. **M. Hull**
- 10:35** Intermission.
- 10:50** **340.** Not what I had thought: Surprising commercial applications of colloidal nanoparticles. **S. Oldenburg**
- 11:20** **341.** Contact lenses, insulation, memory foam, and composite lumber: Surface science is in everything!. **S. Diamanti**
- 11:50** **342.** One research chemist's career path in the public sector. **J.M. Gorham**

SECTION E

San Diego Convention Center
Room 30E

Nanomaterials

Metal Nanocrystals

J. A. Hollingsworth, J. R. McBride, R. Nagarajan, *Organizers*
E. Chan, *Presiding*

- 9:00** **343.** Assembly of anisotropic quantum dots from periodic superlattices to aperiodic quasicrystals. **O. Chen**
- 9:30** **344.** Growth mechanism of five-fold twinned nanowires from multi-scale theory and simulations. **K.A. Fichthorn**
- 10:00** **345.** Citrate-coated, size-tunable octahedral platinum nanocrystals: Novel route for advanced electrocatalysts. **M. Moglianetti**, J. Solla-Gullón, P. Pompa
- 10:20** **346.** Maneuvering the surface chemistry of plasmonic Mg nanoparticles. J. Asselin, C. Boukouvala, J.S. Biggins, **E. Ringe**
- 10:40** **347.** Integration of sequential reactions in a continuous flow droplet reactor: Route to architecturally defined bimetallic nanostructures. **J.S. Santana**, S.E. Skrabalak
- 11:00** **348.** General synthetic strategy toward metal stannides, materials for next generation batteries. A. McGrath, S. Ganapathi, F. Ronning, **S. Ivanov**
- 11:20** **349.** Liquid cell electron microscopy reveals origin of heterogeneity of individual nanocrystals and their 3D atomic structures. **B. Kim**, J. Heo, J. Kim, S. Kim, J. Park

SECTION F

San Diego Convention Center
Room 30D

Formulation Strategies to Control the Physicochemical Parameters of Drug & Nucleic Acid Delivery Systems

M. A. Ilies, *Organizer*
K. Sakurai, *Organizer, Presiding*

- 8:30** **350.** Tuning long-acting HIV drug release from a nanogel-based *in situ* forming implant. A.R. Town, J. Taylor, K. Dawson, E. Niezabitowska, N. Elbaz, A. Corker, E. Garcia-Tuñón, **T.O. McDonald**
- 9:00** **351.** Fabricating Janus particles using seeded emulsion polymerization: Loading and simultaneous release of two drugs. E. Dehghani, M. Salami-Kalajahi, H. Roghani-Mamaqani, **V. Karimkhani**
- 9:30** **352.** Solubilization of binary mixture of hydrophobic solutes in multicompartiment polymer nanoparticle. **R. Nagarajan**
- 10:00** Intermission.
- 10:30** **353.** Designed FN3 domains for extrahepatic delivery of oligonucleotides. **S. Goldberg**
- 11:00** **354.** Polypeptide-based polyplexes to boost effective gene silencing in CNS disorders. I. Conejos-Sánchez, E. Gallon, A. Niño-Pariente, J. Smith, A. Guzman, L. DiCanio, S. Pluchino, R. Franklin, **M.J. Vicent**

SECTION G

San Diego Convention Center
Room 30C

Frontiers & Challenges in Nanoparticle-Mediated Chemical Transformations

Nanocatalysts for Energy Applications

H. Fan, J. He, Y. Sun, *Organizers*
O. Chen, *Organizer, Presiding*
H. Wang, *Presiding*

- 8:30** Introductory Remarks.
- 8:35** **355.** Single-site catalysts on nanostructured semiconductor surfaces for solar CO₂ reduction. E. Shaaban, N. Okolie, P. Huang, **G. Li**
- 9:05** **356.** Single surface charges on aliovalently doped semiconductor nanocrystals determine their photoluminescence properties. A.R. Freyer, P. Sercel, Z. Hou, B. Savitzky, L. Kourkoutis, A.L. Efros, **T.D. Krauss**
- 9:35** **357.** Selective photochemistry with quantum dots. Y. Jiang, **E.A. Weiss**
- 10:05** **358.** Hot carriers in action: Plasmon-driven photocatalysis and photocorrosion. **H. Wang**
- 10:35** Intermission.
- 10:45** **359.** Plasmon-mediated charge transfer and energy transfer in photocatalysis. **N. Wu**
- 11:15** **360.** Photoinduced hot charge transfer at aluminum nanohole array/C₆₀ interfaces. x. Liu, Y. Qian, g. deng, M. Mirotznik, B. Debbrecht, B.G. DeLacy, **Y. Rao**

- 11:45 361.** Potential dependent plasmonic catalyzed cleavage of the C-Br bond of 8-bromo adenine on silver electrodes of nanostructures. **J. Liu, W. Sun, M. Zhang, J. Zhou, D. Wu, Z. Tian**

SECTION H

San Diego Convention Center
Room 29B

Water & Tribological Interfaces

Bioinspired Polymer Coatings

F. Mangolini, M. Ruths, *Organizers*

X. Banquy, A. Pitenis, *Presiding*

- 8:30 362.** Stimuli-responsive and nanostructured polymer films for modulating adhesion and friction between surfaces: Fabrications, applications and limitations. **S. Giasson, C. Drummond, L. Giraud, P. Vialar-Trarieux**
- 9:00 363.** Lubrication and wear protection of soft materials using bioinspired polymers. **X. Banquy, J. Faivre, L. David, S. Benayoun, B. Ratna Shrestha, K. Matyjaszewski, G. Xie**
- 9:30 364.** Interaction forces and nanotribology of surfaces modified with bioinspired polymer coatings. **M. Ruths**
- 9:50 365.** Tribological properties of polyelectrolyte brushes in water. **A. Takahara**
- 10:10** Intermission.
- 10:20 366.** Multi-responsive hierarchical coatings: Synthesis and characterization. **A. Guerron, S. Giasson**
- 10:40 367.** Soft and slippery: Microgel-coated surfaces under shear. **P. Vialar, S. Giasson, C. Drummond**
- 11:00 368.** Low-pressure contact experiments reveal multiple modes of relaxation in polyacrylamide hydrogels. **C.L. Johnson, J. Kim, A.C. Dunn**
- 11:20 369.** Water content and lubricity in aqueous gels. **G.D. Degen, A. Pitenis**
- 11:40 370.** Water content and adhesion in aqueous gels. **G. Degen, A. Pitenis**
- 12:00 371.** Humidity-dependent and aqueous-immersion AFM: Nanotribological analysis of biomedical coatings. **G.D. Haugstad, G. Yu, A. McCormick, K. Wormuth, M. Zeng**

SECTION I

San Diego Convention Center
Room 30A

Hierarchical Assembly of Peptide & Protein: From Interaction & Structure to Application

M. Dong, S. Zhang, *Organizers, Presiding*

- 8:30 372.** Nanostructured protein capsules. **T. Knowles**
- 9:00 373.** Transmission mechanism of pathological alpha-synuclein. **X. Mao**
- 9:30 374.** Phosphorylated amyloid protein forms different stains leading to neurodegenerative diseases. **Y. Li**
- 10:00 375.** Peptide networking of beta 2 microglobulin over nano-gold colloidal particles' surfaces. **K. Yokoyama**
- 10:20 376.** Peptide assembly nanostructures: Structure, modulation and clinical applications. **Y. Yang, L. Zhu, C. Wang**
- 10:50 377.** Determination of polypeptides conformation in water with infrared nano-spectroscopy. **A. Centrone**
- 11:20 378.** Characterizing the microscopic dynamics of biological macromolecules during folding reactions via direct observation of transition paths. **M. Woodside**
- 11:50 379.** Bioinspired siRNA delivery system based on higher order architecture of designer peptides. **K. Slowinska**
- 12:10 380.** NMR characterization of spider silk protein nanoparticle pre-assemblies. **D. Onofrei, D. Stengel, S.J. Trescott, R.Z. Alabdali, A.Y. Soni, I.A. Villalba, B. Addison, G.P. Holland**

Nanotechnology & Single Cell Analysis in Biology & Medicine

Nanoscience

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

Ambient Pressure Spectroscopy in Complex Environments

Sponsored by CATL, Cosponsored by COLL

Structure at Solid-Liquid Interfaces: Effects of Confinement & Chemical Patterning

Sponsored by ANYL, Cosponsored by COLL

Future of Biomacromolecules at a Crossroads of Polymer Science & Biology

Synthetic Cells

Sponsored by POLY, Cosponsored by BIOL, CARB, CELL, COLL, ENVR, MEDI, PHYS and PMSE

SECTION A

San Diego Convention Center
Room 5B

Adsorption & Reaction at Surfaces: Symposium
in Honor of Charles T. Campbell

Adsorption & Binding at Surfaces

Cosponsored by CATL
J. Rodriguez, D. Starr, *Organizers*
S. L. Tait, *Organizer, Presiding*
L. Gamble, *Presiding*

- 1:40 381. Interaction of atomic oxygen with the Ag(111) surface. S.B. Isbill, **S. Roy**
- 2:00 382. Oxygen dissociation on the Ag/Cu(111) near surface alloy. **L. Cramer**, E.H. Sykes
- 2:20 383. On-surface topochemistry of helicenenes. **K. Ernst**
- 2:50 Intermission.
- 3:10 384. Lithium-doped TiO₂(110): Electronic structure and reactivity. **R.S. Somaratne**, J.E. Whitten
- 3:30 385. Synthetic surface chemistry: Versatile route to low-dimensional nanostructures. **J. Gottfried**
- 4:00 386. Designing nanostructures for plasmon-enhanced spectroscopies to probe chemistry at surfaces. C. Coplan, W. Scholl, M.A. Ticknor, M.M. Swartz, C.A. Lancaster, **J.S. Shumaker-Parry**
- 4:30 387. Neutron scattering investigations of molecular interactions with surfaces of nanomaterials. **J.Z. Larese**

SECTION B

San Diego Convention Center
Room 6F

Surfaces & Interfaces in the Environment:
Symposium in Honor of Vicki Grassian

Aqueous Surfaces to Ocean & Organic-Surface
Interactions

Cosponsored by ENVR and WCC
A. P. Ault, J. Baltrusaitis, *Organizers, Presiding*

- 2:00 388. Heterogeneous reactions on atmospherically relevant sea spray aerosols. **K.A. Prather**
- 2:20 389. Environmental marine interfaces: Inherent electric fields from dipole and electrolyte organization. **H.C. Allen**
- 2:40 390. Catching the freshwater wave: Lakes, aerosols, and algal blooms. **A.P. Ault**, N.E. Olson, N. May, J. Axson, K.A. Pratt
- 3:00 391. Integrated computational and experimental

strategies to explore air-water interfaces in sea spray aerosols and related model systems. **R.E. Amaro**

- 3:20 Intermission.
- 3:30 392. Physical chemistry of environmentally relevant multicomponent interfaces. **H.A. Al-Abadleh**
- 3:50 393. Surface-mediated photochemical pathways for the formation of HONO and NO_x. **J.G. Navea**
- 4:10 394. Surface chemistry at a primarily undergraduate institution. **J.D. Schuttlefield Christus**
- 4:30 395. Thermodynamics and phase of sea spray aerosol droplets using microfluidics. L. Nandy, S. Liu, **C. Dutcher**

SECTION C

San Diego Convention Center
Room 31B

Confined Dynamics of Molecules & Particles at
Interfaces, in Pores & under Crowded Conditions
Interfaces & Pores

J. Conrad, D. K. Schwartz, *Organizers, Presiding*

- 2:00 396. Nanoparticle diffusion at liquid-solid interfaces and its implications on *in situ* liquid phase TEM studies. **U. Mirsaidov**
- 2:35 397. Dynamics of fluorescein embedded to amyloid beta peptide 1-40 at nano-scale gold surface. **K. Yokoyama**
- 3:00 398. Characterization of carfentanil and remifentanil in solution and on surfaces. **M.L. McEntee**, M. Winemiller, A. Walz, F. Hsu, A. Schenning, M.L. Sheahy, I. Iordanov, J. Landers, G.W. Peterson
- 3:25 Intermission.
- 3:35 399. Interfacial, confined, and concentrated colloidal diffusion. **M.A. Bevan**
- 4:10 400. Electrostatic barriers to nanoparticle escape from cavities in a porous matrix. **H. Wu**, R. Sarfati, D. Wang, D.K. Schwartz

SECTION D

San Diego Convention Center
Room 31A

Colloid & Surface Chemistry in Industry:
Applications & Career Opportunities

Financially supported by Natural Immunogenics Corporation
N. A. Falk, R. I. Maccuspie, *Organizers, Presiding*

- 2:00 **401.** From Ph.D. lab bench researcher to multi-national startup cofounder. **T.A. Dankovich**
- 2:30 **402.** How does your academia experience support successful industrial career in colloidal science and nanotechnology?. **N. Qin**
- 3:00 **403.** Colloidal science: Advancing human health. **D. Gorka**
- 3:30 Panel Discussion.

SECTION E

San Diego Convention Center
Room 30E

Nanomaterials

Modulating the Photophysics of Colloidal Nanocrystals

J. A. Hollingsworth, J. R. McBride, R. Nagarajan, *Organizers*
A. Smith, *Presiding*

- 1:30 **404.** Photophysical properties of mixed-dimensional heterojunctions. **S. Padgaonkar, S. Amsterdam, H. Bergeron, T.J. Marks, M. Hersam, E.A. Weiss**
- 2:00 **405.** Investigating the role of aliovalent doping of quantum dots: From magnetic frustration in Fe:ZnSe (CdSe) to plasmonic behavior in Sn:In₂O₃. **G.F. Strouse**
- 2:30 **406.** Discovery and controlled assembly of lanthanide-doped nanoparticles for ultra-low-threshold upconversion microlasers. **E. Chan**
- 3:00 **407.** *In situ* elucidation of oxidation pathways to high quality magnetic nanoparticles. **J. Watt, D. Huber, A. Begay**
- 3:20 **408.** Evaluating the effect of dopants on the oxygen storage behavior of bixbyite vanadium sesquioxide (V₂O₃) nanocrystals. **L. Reimnitz, D.J. Milliron**
- 3:40 **409.** One-pot construction of Au-FeO_x@SiO₂ core-shell nanostructure with both high catalytic activity and good thermal stability. **H. Yin, Z. Guo**
- 4:00 **410.** Stabilization and functionalization of iron oxide colloidal nanoparticles for applications at harsh environment. **W. Wang**
- 4:20 **411.** Microwave synthesis of tailored lanthanide oxide nanoparticles and their surface modification to generate homogeneous nanocomposites. **L.J. Treadwell, J.P. Lassa, C. Wheeler-Davis**
- 4:40 **412.** Ultrafast charge carrier dynamics of indium-alloyed thick-shell InP/ZnSe quantum dots. **N. Freymeyer, S. Click, K.R. Reid, J.R. McBride, S.J. Rosenthal**

SECTION F

San Diego Convention Center
Room 30D

Formulation Strategies to Control the Physicochemical Parameters of Drug & Nucleic Acid Delivery Systems

K. Sakurai, *Organizer*
M. A. Ilies, *Organizer, Presiding*

- 2:00 **413.** Re-engineering immuno-exosome as theranostics. **S. Aryal, S. Rayamajhi, T. Nguyen, R. Marasini**
- 2:30 **414.** Transglutaminase-mediated lipid bilayer decoration with proteins using lipid-fused peptide amphiphile substrates. **M. Takahara, R. Wakabayashi, K. Minamihata, M. Goto, N. Kamiya**
- 3:00 **415.** Vesicle-to-sheet morphological control of lipid bilayers using polycation-chaperoned peptide system. **T. Ochiai, T. Takenaka, W. Sakamoto, T. Masuda, N. Shimada, A. Maruyama**
- 3:30 **416.** Impact of thermal annealing on physicochemical properties, serum stability, and transfection efficiency of pyridinium based lipoplexes. **U. Satyal, H. Nguyen, V.D. Sharma, M.A. Ilies**
- 4:00 **417.** New synthetic lipid chains incorporated in the structure of cationic amphiphiles for nucleic acid delivery. **A. BOURAOUI, M. Berchel, R. Ghanem, V. Vie, L. Deschamps, O. Lozach, T.L. Gall, T. Montier, P. Jaffres**
- 4:30 **418.** Novel formulation strategies to overcome endosomal barriers for enhanced nucleic acid delivery. **S. Patel, G. Sahay**

SECTION G

San Diego Convention Center
Room 30C

Frontiers & Challenges in Nanoparticle-Mediated Chemical Transformations

O. Chen, H. Fan, J. He, Y. Sun, *Organizers*
G. Li, *Presiding*

- 1:15 Introductory Remarks.
- 1:20 **419.** Withdrawn
- 1:50 **420.** Effect of surfactant on nanosynthesis of noble metal nanocrystals: Case of dioctadecyldimethylammonium chloride (DODAC). **H. Lv, D. Xu, B. Liu**
- 2:20 **421.** Organochalcogenide reagents for the phase control of transition metal sulfides and selenides. **J. Macdonald, E.A. Hernandez-Pagan, E.H. Robinson, J.M. Rhodes, Y. Zhao, J. Veglak**

- 2:50 Intermission.
- 3:00 **422.** Polymer-guided synthesis of asymmetric multicomponent nanoparticles with enhanced catalytic activity. **Z. Nie**
- 3:30 **423.** Engineering metal-oxide interface at atomic scale in well-defined nanoparticles for catalytic conversion of small molecules. **H. Zhu**
- 4:00 **424.** Heterogeneous nanostructure integration for energy conversion and production. **P. Gao**
- 4:30 **425.** Metal-organic framework coated nanoparticles. **C. Tsung**

SECTION H

San Diego Convention Center

Room 29B

Water & Tribological Interfaces

Specialty Lubricants & Ionic Liquids

F. Mangolini, M. Ruths, *Organizers*

C. Drummond, W. T. Tysoe, *Presiding*

- 2:00 **426.** Biobased lubricant additives from vegetable oils and other renewable feedstocks. **G. Biresaw**, G. Bantchev, R.E. Harry-O'kuru
- 2:30 **427.** Influence of surface coverage on friction performance of stearic acid on iron oxide. **A.M. Schilowitz**, A. Jaishankar, A. Jusufi, J. Vreeland, S. Deighton, J. Pelletiere
- 2:50 **428.** Tricresyl phosphate reactions with ferrous surfaces: Effect of surface composition, molecular isomer, and atmospheric content. **J. Mogonye**, R. Pesce-Rodriguez, A. Kajeh, A. Martini, S. Berkebile
- 3:10 **429.** Using ionic liquids as lubricant additives together with friction modifiers. W. Li, C.K. Kumara, H.M. Meyer III, H. Luo, **J. Qu**
- 3:30 Intermission.
- 3:40 **430.** Laboratory studies of spacecraft fluid lubricants. **J.M. Helt**, P.P. Frantz, S.V. Didziulis
- 4:00 **431.** Ionic liquids as environmentally friendly additives for hydraulic fluids. **X. He**, H. Luo, T.J. Mathews, J. Qu
- 4:20 **432.** Synergistic interactions between thiolate-protected silver and palladium nanoparticles and their tribological properties. **C. Kumara**, H.M. Meyer III, J. Qu

SECTION I

San Diego Convention Center

Room 6E

Biomaterials & Biointerfaces

S. Romero-Vargas Castrillon, *Organizer*

J. Groll, *Presiding*

- 2:00 **433.** Sputtering-enabled intracellular X-ray photoelectron spectroscopy (SEI-XPS): New lab-based technique to investigate the biological fate of metal nanoparticles. **M. Moglianetti**, A. Turco, C. Malitesta, P. Pompa
- 2:20 **434.** Design near infrared absorbing triplet-triplet annihilation nanoparticles and application in tumor immunotherapy. **L. Huang**
- 2:40 **435.** Orchestrating cellular organization and phenotype in small diameter bi-layered vascular grafts by heterotypic scaffold design. T. Jüngst, I. Pennings, T. Rosenberg, D. Gawlitta, **J. Groll**
- 3:10 **436.** Silica nanofibers-based extracellular matrix scaffolds with tunable nanostructure. **Y. Nie**, N. Hao, J. Zhang
- 3:30 **437.** New synthesis methodology for making FITC labeled PMMA nanoparticles: Understanding effect of crosslinked vs. surfactant-stabilized nanoparticles on conjugation. **N. Mirza Nasiri**, B. Kamras, S.B. Marpu, D.P. Simmons, R.A. Petros, M.A. Omary
- 3:50 **438.** Role of core stiffness in regulating the intracellular fate of GM3-functionalized polymer nanoparticles. **B. Eshaghi**, N. Alsharif, K.A. Brown, S. Gummuluru, B.M. Reinhard
- 4:10 **439.** Reactive oxygen species sensitive dendrimers for chronic wound healing. **S. Wijetunge**, Y. Sun
- 4:30 **440.** Preparation and properties of POSS/HA composite film layer. **Y. Xiao**, W. Liu, **x. zhang**

Nanotechnology & Single Cell Analysis in Biology & Medicine

Nanoscience

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

Water, Ice, & Clathrate Hydrate Geochemistry: Molecular Structures, Microscopic Properties, & Energetics

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Ambient Pressure Spectroscopy in Complex Environments

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Structure at Solid-Liquid Interfaces: Effects of Confinement & Chemical Patterning

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Future of Biomacromolecules at a Crossroads of Polymer Science & Biology

Tissue Engineering

Sponsored by POLY, Cosponsored by BIOL, CARB, CELL, COLL, ENVR, MEDI, PHYS and PMSE

MONDAY EVENING – COLL

SECTION A

San Diego Convention Center
TBD

Sci-Mix

R. Nagarajan, *Organizer*

8:00 - 10:00

139, 143, 146, 148, 152, 168, 171, 172, 173, 174, 175, 176, 177, 181, 186, 187, 188, 197, 200, 204, 205, 206, 224, 228, 229, 230, 233, 234, 238, 239, 247, 248, 251, 252, 253, 254, 261, 262, 263, 269, 270, 273, 274, 277, 279, 280, 281, 285, 286, 287, 288, 290, 293, 294, 299, 300, 302, 307, 308, 309, 310, 311. See Previous Listings
594, 595, 626, 637, 673, 694, 695, 696, 698, 699, 714, 719. See Subsequent Listings.

TUESDAY MORNING – COLL

SECTION A

San Diego Convention Center
Room 5B

Adsorption & Reaction at Surfaces: Symposium in Honor of Charles T. Campbell

Electrocatalytic & Liquid Interfaces

Cosponsored by CATL

D. Starr, S. L. Tait, *Organizers*

J. Rodriguez, *Organizer, Presiding*

K. Ernst, *Presiding*

- 8:30 **441.** Can surface science help explain biology?. L. Gamble
- 9:00 **442.** Aqueous-phase adsorption energies of model bio-oil compounds on Pt and Rh: Comparison between experiment and theory. N. Singh, B.R. Goldsmith, J. Akinola, I. Barth
- 9:20 **443.** Active structures and species of modified transition metal oxide electrocatalysts for the oxygen evolution reaction. B.E. Koel
- 9:50 Intermision.
- 10:10 **444.** Role of open circuit and external potentials to control electrocatalytic reductions. J.A. Lercher, O.Y. Gutierrez Tinoco, Y. Liu
- 10:40 **445.** Electrocatalytic alcohol oxidation by size-selected Pt clusters. A.C. Cass, H.F. McKnight, S.L. Anderson

- 11:00 **446.** Ambient pressure X-ray photoelectron spectroscopy with application to solar water splitting materials. D.E. Starr
- 11:30 **447.** Greatest hits album: Campbell group. C.T. Campbell

SECTION B

San Diego Convention Center
Room 6F

Basic Research in Colloids, Surfactants & Interfaces

Colloidal Assembly

R. Nagarajan, *Organizer*

S. Fujii, *Presiding*

- 8:30 **448.** Self-assembly of soft colloids into quasicrystals. M. Dulle, T. Jurczyk, T. Gruhn, S. Förster
- 9:00 **449.** Switchable regioselective assemble of triblock microparticles based on surface material recognition. M. Liu, X. Zheng, D. Pine, M. Weck
- 9:20 **450.** Magnetic assembly of anisotropic nanostructures into responsive photonic crystals. Z. Li, Y. Yin
- 9:40 **451.** Investigation of the aggregates formation mechanism of Amyloid beta 1-40 coated nano-gold particles. K. Yokoyama
- 10:00 **452.** Polyhedral liquid marbles. S. Fujii, F. Geyer, Y. Asami, D. Vollmer, H. Butt, J. Fujiwara, Y. Nakamura
- 10:30 **453.** Block copolymer assembly of ligand stripped nanocrystals. G. Ong, D.J. Milliron
- 10:50 **454.** All-organic crystalline colloidal array for full color electrophoretic reflective display. W. Lee, H. Lee, E. Park
- 11:10 **455.** Templated capillary assembly of liquid colloidal particles. C. Shillingford, M. Weck

SECTION C

San Diego Convention Center
Room 31B

Confined Dynamics of Molecules & Particles at Interfaces, in Pores & under Crowded Conditions Reactions & Structure in Confinement

J. Conrad, D. K. Schwartz, *Organizers, Presiding*

- 8:30 **456.** Catalytic activity in nanoporous materials with inhibited transport: Pore diameter dependence of PNB conversion to aldol in MSN. J.W. Evans, A. Garcia, I.I. Slowing

SECTION E

San Diego Convention Center
Room 29B

Nanomaterials

2D Nanoparticles

J. A. Hollingsworth, J. R. McBride, R. Nagarajan, *Organizers*
B. Sadtler, *Presiding*

- 8:30 470.** Modulation of precursor reactivity in colloidal syntheses of WSe_2 -based nanostructures. **A.M. Schimpf**, J.Q. Geisenhoff
- 9:00 471.** Colloidal Pb-free halide perovskite and group IV nanomaterials. **M. Panthani**
- 9:30 472.** Tuning the band gap of semiconducting two-dimensional materials by changing the structure of polymer assembled on their surface. **M.A. Mahmoud**
- 9:50 473.** Effect of the heterostructure on charge transfer processes in Pbse/Cdse Janus quantum dots functionalized by Ru(II) dyes. **S. Kilina**, J. Mohammed
- 10:20 474.** Spanning the atomic to the agglomerate dimensions in colloidal dispersions of 2D lead halide perovskites. **C.J. Dahlman**, N.R. Venkatesan, P.B. Corona, R.M. Kennard, N. Smith, M.E. Helgeson, M.L. Chabiny
- 10:40 475.** Synthesis and characterization of modified hydroxyapatites. **S. Alexandratos**, H. Benhaim, A. Ashfaq, E. Amin
- 11:00 476.** Air-stable $CuInSe_2$ nanocrystal transistors and circuits *via* post-deposition cation exchange. **H. Wang**, D.J. Butler, D.B. Straus, N. Oh, F. Wu, J. Guo, K. Xue, J. Lee, C.B. Murray, C.R. Kagan
- 11:20 477.** Fundamental study of graphene oxide-metal nanoparticle material hybrids for electromagnetic energy interference mitigation: Systematic structure/function analysis. **J.R. Uzarski**, W. Gary, S. Karna

SECTION F

San Diego Convention Center
Room 30E

Formulation Strategies to Control the Physicochemical Parameters of Drug & Nucleic Acid Delivery Systems

M. A. Ilies, *Organizer*
K. Sakurai, *Organizer, Presiding*

- 8:30 478.** Understanding the excipient's effects on functionality of glass and polymer pre-filled syringes. **L. Fang**

- 8:55 457.** Enhanced selectivity in air separation by tumbling movement through a bilayer nanoporous graphene membrane. **S. Wang**, D. Jiang
- 9:15 458.** Transforming the potential energy landscape to suppress deactivation pathways in surface supported catalysts. **S.C. Hayden**, H. Li, A. France-Lanord, E. Converse, T. Pilyugina, B.S. Hanna, J.C. Grossman
- 9:40 459.** Self-assembly of deformable soft hydrogel microspheres at the air/water interface. **H. Minato**, Y. Sazuka, M. Takizawa, K. Honda, D. Suzuki
- 10:05 460.** Surface segregation of binary particles in photonic colloidal assemblies. **Z. Hu**, N.C. Gianneschi
- 10:25 461.** Structure and dynamics of a confined ionic liquid studied by an x-ray surface force apparatus. **M. Mezger**, M. Valtiner, V. Honkimäki
- 10:50 462.** Investigation of water adlayers confined between 2D interface. **Q. Li**
- 11:15 463.** Ionic liquid confined between metallic surfaces: What is the role of image charges?. S. Ntim, **M. Sulpizi**
- 11:40 464.** Effect of confinement on phase transitions of hydrocarbons in nanoporous materials. **H. Cho**, T. Jordan, M.D. Deo

SECTION D

San Diego Convention Center
Room 31A

Targeted Delivery of Nanomedicines In Vivo

P. del Pino, *Organizer*
N. Feliu Torres, W. J. Parak, *Organizers, Presiding*

- 8:30** Introductory Remarks.
- 8:35 465.** Design and synthesis of inorganic nanomaterials for medical applications. **T. Hyeon**
- 9:05 466.** Aqueous stable gold nanostar/ZIF-8 nanocomposites for light triggered release of active cargo inside living cells. **P. del Pino**
- 9:35 467.** Engineering metal-organic-framework nanoparticles for enhanced chemoradiation of breast cancer. M. Neufeld, A. DuRoss, M. Landry, **C.G. Sun**
- 10:05** Intermission.
- 10:35 468.** Fluorinated nanomaterials for efficient nucleic acids delivery with medium serum. T. Zhang, Y. Huang, X. Ma, W. Guo, **X. Liang**
- 11:05 469.** Design and implementation of gold-nanoparticle formulations as MUC1-directed cancer vaccines. **R. Fiammengo**, V. Mangini, I. Compañón, A. Guerreiro, G. Bernardes, F. Corzana

- 9:00 479.** Protein-excipient interactions via diffusion NMR: Case study of zwitterions. **A. Erfani**, N. Pickering, J.L. White, J.D. Ramsey, C. Aichele
- 9:30 480.** Furry nanoballs bearing D_4^H/D_4^V silicone: Synthesis, structural characterization, and their robust stability *in vivo*. **J. Matsuno**, S. Fujii, J. Lee, R. Takahashi, K. Sakurai
- 10:00 481.** Versatile single chain polymer nanoparticles in controlled drug delivery. J. Paats, N. Hamelmann, P. Kröger, **J.M. Paulusse**
- 10:30 482.** Chaperone effect of cationic comb-type copolymers for an amphiphilic peptide disturbing lipid membranes. **W. Sakamoto**, N. Shimada, A. Maruyama
- 11:00 483.** Macromolecular HPMA-based nanoparticles with cholesterol for solid tumor targeting: Synthesis, internal structure, and interaction with blood plasma proteins. **S. Filippov**
- 11:30 484.** Quantifying drug adsorption to lipid membranes using second harmonic generation. **G.Y. Stokes**

SECTION G

San Diego Convention Center
Room 30D

Frontiers & Challenges in Nanoparticle-Mediated Chemical Transformations Hybrid Nanomaterials & Applications

O. Chen, H. Fan, J. He, Y. Sun, *Organizers*
B. Liu, *Presiding*

- 8:30** Introductory Remarks.
- 8:35 485.** Modulation of surface states on bimetallic nanoicosahedra toward catalytic energy conversion. **C. Kuo**, M. Lu, Y. Chuang, D.A. Cullen
- 9:05 486.** Highly tunable platform for biomimetic catalysis from nanocrystal-polymer composites. **M. Cargnello**, A. Riscoe, C. Wrasman, A. Herzing, S. Bare
- 9:35 487.** Nanoscale metal-organic supercontainers as biomimetic catalysts. **Z. Wang**
- 10:05** Intermission.
- 10:15 488.** Hierarchical nanocrystal assembly driven by structural transformation of biomolecules. **E. Zhu**, S. Wang, Y. Huang, H. Heinz
- 10:35 489.** Mechanically initiated free radical polymerization. **Z. Wang**, J.L. Ayarza, A. Esser-Kahn
- 10:55 490.** Coupling magnetic and plasmonic anisotropy in hybrid nanorods for mechanochromic films. **Z. Li**, Y. Yin
- 11:15 491.** 3D-porous plate-like Ag nanostructures for efficient CO_2 electroreduction. **S.C. Abeyweera**, Y. Sun

- 11:35 492.** Remotely operable and highly functional plasmonic nanoreactors for NIR-light-induced bioorthogonal catalysis in living cells. **A. Kumar**, I. Lee

SECTION H

San Diego Convention Center
Room 5A

Colloids & Nanomaterials for Water Purification

C. Drew, *Organizer, Presiding*

- 8:30** Introductory Remarks.
- 8:35 493.** Enhanced virus removal in a practical sand filter. **L. Samineni**, B. Xiong, R. Chowdhury, T.H. Nguyen, C. Maranas, D. Velegol, M. Kumar, S.B. Velegol
- 8:55 494.** Use of rotifers as self-propelling biohybrid microcleaners. **F. Soto**, M.A. Lopez-Ramirez, I. Jeerapan, A. Nourhani, J. Wang
- 9:15 495.** Determining the properties of flocs made of aluminum oxide particles and lignin-acrylic acid polymers. **P. Fatehi**
- 9:35 496.** Bioinspired nanomaterials for water remediation. **S.V. Patwardhan**, E. Routoula, H. Patel
- 9:55 497.** Space-confined seeded growth of black silver nanostructures for solar steam generation. **J. Chen**, Y. Yin
- 10:15 498.** Remediating aqueous waste with supramolecular gels to create smart materials with high-tech applications. **D.K. Smith**
- 10:35 499.** Imprinted copolymer/SiO₂ hybrid for selective adsorption of bisphenol A. **K. Chin**, S. Chang
- 10:55 500.** Electrospun nanofibrous poly-cyclodextrin membrane for efficient removal of polycyclic aromatic hydrocarbons (PAHs) and heavy metals from water. **A. Celebioglu**, F. Topuz, Z.I. Yildiz, T. Uyar
- 11:15 501.** Core-shell Fe-SiO₂-polyamine magnetic nanoparticles for metal recovery using a continuous flow pipeline reactor. **E. Rosenberg**, R. Latterman, E. Deluca
- 11:35 502.** Hydrophobic-force-driven removal of organic compounds from water by reduced graphene oxides generated in agarose hydrogels. **C. Cheng**
- 11:55 503.** Surface modified magnetic nanoparticles as efficient adsorbents for heavy metals removal from wastewater: Progress and prospects. **M.O. Ojemaye**, O.O. Okoh, A. Okoh
- 12:15** Concluding Remarks.

SECTION I

San Diego Convention Center
Room 6E

Biomaterials & Biointerfaces

S. Romero-Vargas Castrillon, *Organizer*
K. Burke, *Presiding*

- 8:30** **504.** Visualizing the inner architecture of poly(ϵ -caprolactone)-based biomaterials and its impact on performance optimization. **B. Li**, Y. Wu, A.J. Bauer
- 8:50** **505.** Substrate-independent micropatterning of polymer brushes using chemical vapor deposition-based polymerization initiator films. **R. Kumar**, A. Welle, I. Kopyeva, F. Becker, J. Lahann
- 9:10** **506.** Is hydroxyl functionality a prerequisite for inducing stasis in human pluripotent stem cell colonies immersed within block copolymer worm gels?. **N.J. Penfold**, M. Sponchioni, I. Canton, S.P. Armes
- 9:30** **507.** Upper critical solution temperature (UCST) behavior of core cross-linked polymer micelle in water. **S. Yusa**, M. Ohshio, K. Ishihara, A. Maruyama, N. Shimada
- 9:50** **508.** Tailoring surfaces of silk fibroin films to control protein adhesion. D. Heichel, S.P. Ward, D.H. Adamson, **K. Burke**
- 10:20** **509.** Mechanochemical phenomena in free and constrained polyacrylamide hydrogels induced by osmotic swelling. **A. Parameswar**, K. Fitch, D. Bull, V. Duke, A.P. Goodwin
- 10:40** **510.** Catechol-modified poly(oxazoline)s with tunable degradability facilitate cell invasion and lateral cartilage integration. J. Blöhbaum, O. Berberich, J. Tessmar, T. Blunk, **J. Groll**
- 11:00** **511.** Scalable synthesis of on-demand degradable hydrogel particles. **P. Shieh**, J.A. Johnson
- 11:20** **512.** Effect of the shape on phagocytosis: Phagocyte type matters!. **H. Safari**, E. Saito, W. Kelley, L. Carethers, L. Shea, O. Eniola-Adefeso

Water, Ice, & Clathrate Hydrate Geochemistry: Molecular Structures, Microscopic Properties, & Energetics

Sponsored by GEOC, Cosponsored by COLL and PHYS

Surfactant & Colloid Science Applied to Formulations

Sponsored by AGRO, Cosponsored by COLL

TUESDAY AFTERNOON – COLL

SECTION A

San Diego Convention Center
Room 5B

Langmuir Lectures, NanoLetters Award Lecture, ACS Materials & Interfaces Award Lecture

R. Nagarajan, *Organizer*
L. Tribe, *Presiding*

- 2:00** Introduction of Langmuir Lecturer, **A. Sen**
- 2:10** **513.** Fantastic voyage: Designing self-powered nano/microbots. **A. Sen**
- 3:00** Introduction of of Langmuir Lecturer, **K. Ariga**
- 3:10** **514.** Langmuir science teaches everything: Molecular machine operation, nanocarbon synthesis, and life regulation at liquid interfaces. **K. Ariga**
- 4:00** Introduction of ACS AMI Lecturer, **J. Schiffman**
- 4:10** **515.** Interfacing polymer materials with microbiology. **J.D. Schiffman**

SECTION B

San Diego Convention Center
Room 6F

Basic Research in Colloids, Surfactants & Interfaces

Molecular Self-Assembly

R. Nagarajan, *Organizer*
Z. Niroobakhsh, *Presiding*

- 2:00** **516.** End-group ionisation enables the use of poly(N-(2-methacryloyloxy)ethyl pyrrolidone) as an electrosteric stabiliser block for polymerisation-induced self-assembly in aqueous media. **R. Gibson**, S.P. Armes
- 2:20** **517.** Hydrodynamic instabilities in fatty acid/surfactant self-assembling systems. **Z. Niroobakhsh**, J. LaNasa, A. Belmonte, R. Hickey
- 2:50** **518.** Rediscovering micelle-like behavior of resorcinarene capsules and their unique aggregation number corresponding to Platonic structures. **S. Fujii**, K. Sakurai, J. Lee, R. Takahashi
- 3:10** **519.** Dynamic self-assembly and rheological behaviour of light-responsive surfactants. E. Kelly, J. Houston, **R.C. Evans**
- 3:40** **520.** Kinetic-control effects towards persistent micelle templating. **A. Sarkar**, M. Stefik
- 4:00** **521.** Tuning of the aggregation number of platonic micelles with binary mixture of calix[4]arene surfactants. **J. Lee**, S. Fujii, R. Takahashi, K. Sakurai

- 4:20 **522.** Magnetite-loaded biocompatible diblock copolymer vesicles. **D.L. Beattie**, A. Sahota, C.J. Legge, O. Mykhaylyk, S.S. Staniland, S.P. Armes
- 4:40 **523.** Construction of artificial cells from galactopyranose-derived single-chain amphiphiles. **R.J. Brea Fernández**, A. Bhattacharya, N.K. Devaraj

SECTION C

San Diego Convention Center
Room 31B

Surface Chemistry

S. L. Tait, *Organizer*

O. Guseva, E. Tyrode, *Presiding*

- 2:00 **524.** Model predictions of phase transformation sequence in Al-oxide-hydroxide system in pure water by bulk and interface thermodynamics. **O. Guseva**, P. Schmutz, L.P. Jeurgens
- 2:20 **525.** Measuring the surface potential at water and pure liquid surfaces. **T. Adel**, S.M. Baumler, H.C. Allen
- 2:40 **526.** Probing mixed octadecanol/stearic acid monolayers at the air/water interface. **K. Judd**, P.S. Cremer
- 3:00 **527.** Do monovalent anions preferentially adsorb to extended hydrophobic surfaces exposing methyl groups?. **E. Tyrode**
- 3:20 **528.** Tracking the molecular organisation of water and alcohol mixtures at hydrophobic solid interfaces. **J.W. Foster**, H. Kusumaatmaja, K. Voitchofsky
- 3:40 Intermission.
- 4:00 **529.** Dilution effects on the behavior of thin ionic liquid films probed with electrochemistry and vibrational spectroscopy. **A. Horvath**, R.S. Anaredy, S.K. Shaw
- 4:20 **530.** Dual-responsive fluorinated ionic liquid infused slippery surfaces. **Q. Rao**, **Q. Zhang**, X. Zhan, F. Chen
- 4:40 **531.** Functional solid surface with liquid-like slippery feature for bubble/drop transport and self-assembly of nanoparticles. **X. Mao**, J. Tan, H. Zeng
- 5:00 **532.** Highly thermally stable hybrid coatings by fluoride rearrangement of phenylsilsesquioxanes and methyltrimethoxysilane. **W. Liu**, Y. Xiao, **x. zhang**

SECTION D

San Diego Convention Center
Room 31A

Targeted Delivery of Nanomedicines In Vivo

N. Feliu Torres, W. J. Parak, *Organizers*

P. del Pino, *Organizer, Presiding*

- 2:00 **533.** Understanding the fate and behaviour of nanoparticle in biological system. **C. Chen**, L. Wang, Y. Zhao
- 2:30 **534.** Silver nanoparticles toxicity and nanomedicine. **S. Liu**
- 3:00 **535.** Use of polymeric nanoparticle platform targeting the liver to induce Treg-mediated antigen-specific immune tolerance in a pulmonary allergen sensitization model. **T. Xia**
- 3:30 Intermission.
- 4:00 **536.** Towards tracking stem cells and macrophages with gold and iron oxide nanoparticles: Choice of the best suited particles. **N. Feliu Torres**
- 4:30 **537.** Drug delivery via polymer-drug conjugates for pancreatic ductal adenocarcinoma. **R. Sanyal**

What does Nanotechnology Have to do with Agriculture?

Sponsored by AGRO, Cosponsored by COLL

Surfactant & Colloid Science Applied to Formulations

Sponsored by AGRO, Cosponsored by COLL

TUESDAY EVENING – COLL

Future of Biomacromolecules at a Crossroads of Polymer Science & Biology

Sponsored by POLY, Cosponsored by BIOL, CARB, CELL, COLL, ENVR, MEDI, PHYS and PMSE

WEDNESDAY MORNING – COLL

SECTION A

San Diego Convention Center
Room 5B

Basic Research in Colloids, Surfactants & Interfaces

Molecular Behavior at Interfaces

R. Nagarajan, *Organizer*

U. Natarajan, *Presiding*

- 8:30 **538.** Surface pressure-induced crystallization behaviour of poly(caprolactone)-based mixed monolayers at the air/water interface. **B. Li**, A. Esker
- 8:50 **539.** It takes two to tangle: Nonionic polymer aggregation behavior at the oil/water interface

- as affected by varying surfactants. **R. Altman**, G.L. Richmond
- 9:10 540.** Bicarbonate charging of hydrophobic/water interfaces. **F. Ganachaud**, J. Bernard, X. Yan, A. Stocco
- 9:30 541.** Ion interactions with carboxylic acid monolayers: Surface charge, reversed affinities, and contact ion pairing as revealed by non-linear vibrational spectroscopy. **E. Tyrode**
- 9:50 542.** Effect of polymer charge and interface concentration on structure of isotactic poly(acrylic acid) PAA and isotactic poly(methacrylic acid) PMA at oil-water interface. **U. Natarajan**
- 10:20 543.** Dual actions of hydrotropes in bulk solution and at interface. **M.A. Anisimov**
- 10:40 544.** Molecule dynamics simulations of the trisiloxane surfactant monolayers at air-water and heptane-water interfaces. **X. Zhuang**, R. Ananth
- 11:00 545.** Surface dipoles give rise to the largest odd-even effects ever reported: Structure and wettability of CF_3 -terminated *n*-alkyl xanthic acid self-assembled monolayers. **H. Tran**, H. Lee, S. Sakunkaewkasem, L.T. Han, T. Yu, M. Valverde, M.D. Marquez, L. Grabow, T. Lee
- 11:20 546.** NSF's ChemMatCARS: National facility for liquid surface X-ray scattering. **W. Bu**

SECTION B

San Diego Convention Center
Room 6F

Surfaces & Interfaces in the Environment: Symposium in Honor of Vicki Grassian

Organic-Surface Interactions & Organic Aerosols

Cosponsored by ENVR and WCC

A. P. Ault, J. Baltrusaitis, *Organizers, Presiding*

- 8:30** Introductory Remarks.
- 8:35 547.** Five-isotope approach to tracking the origin and evolution of life. **M.H. Thiemens**, R. Shaheen, L. Mang
- 9:00 548.** Multiphase chemistry of reactive oxygen species in indoor environments and human surfaces. **M. Shiraiwa**
- 9:20 549.** Interfacial dissolved O_2 consumption by photolyzed aqueous pyruvic acid. **M.I. Guzman**, A.J. Eugene
- 9:40 550.** Aerosol spectroscopy and the dynamics of nanoparticle collisions. M.E. Miller, P. Kim, R.E. **Continetti**
- 10:00 551.** Condensed-phase photochemical processes in atmospheric particulate matter. **S.A. Nizkorodov**
- 10:20** Intermission.

- 10:30 552.** Molecular origin for cloud activation. **F. Geiger**
- 10:50 553.** Study of 3D morphology, phase state and viscoelastic properties of individual substrate-deposited particles. **A.V. Tivanski**
- 11:10 554.** Chemistry of atmospheric brown carbon. **A. Laskin**
- 11:40 555.** Old and new insights of heterogeneous and multiphase oxidative processes affecting the lifetimes of toxic organic substances in biomass burning and sea spray aerosol. **J.H. Slade**, S. Kruse, M. Shiraiwa, D.A. Knopf, A. Cooper

SECTION C

San Diego Convention Center
Room 31B

Surface Chemistry

S. L. Tait, *Organizer*

D. L. Patrick, L. Wong, *Presiding*

- 8:30 556.** Tuning surface properties in self-assembled monolayers of multi-functional boron clusters. **D.P. Goronzy**, K.M. Cheung, E. Avery, J. Staněk, J. Macháček, T. Base, P.S. Weiss
- 8:50 557.** Probing the electrochemical reductive stability of decanethiol/triazole-ferrocene mixed self-assembled monolayers on Au. **B.E. Bonsall**, C.C. McCrory
- 9:10 558.** Surface chemistry for modification and tuning of polymer CORALS. **A. Sidorenko**, P.B. Moore, C. McConnell
- 9:30 559.** Exploration of variables involved in surface pKa shifts of carboxylated carboranethiol self-assembled monolayers. **E. Avery**, D.P. Goronzy, J. Staněk, J. Macháček, T. Base, P.S. Weiss
- 9:50** Intermission.
- 10:10 560.** Biocatalytic parallelized scanning probe lithography for the additive fabrication of conjugated polymer structures. **L. Wong**, J. Hosford
- 10:30 561.** Combined experimental and triple-mode sorption modeling approach for sorption and diffusion in polymeric materials. **H.N. Sharma**, Y. Sun, E. Glascoe
- 10:50 562.** Bottom-up shape engineering of molecular single-crystals. **D.L. Patrick**, G.K. Reed, m. littleton, H.J. Doran
- 11:10 563.** Controlling assembly of layer-by-layer films via a small hydrogen-bonding molecule. A. Aliakseyeu, V. Selin, **R. Hlushko**, J. Ankner, S.A. Sukhishvili
- 11:30 564.** Multifunctional biocompatible nanocoatings of ionic fluorinated polyphosphazenes. **V. Albright**, A. Marin, A.K. Andrianov, S.A. Sukhishvili

SECTION D
San Diego Convention Center
Room 31A

Targeted Delivery of Nanomedicines In Vivo

P. del Pino, *Organizer*

N. Feliu Torres, W. J. Parak, *Organizers, Presiding*

- 8:30** **565.** Enzyme-responsive actively tumor-penetrating nanomedicine overcomes tumor diffusion barriers and produces potent anticancer efficacy. **Y. Shen**, Q. Zhou
- 9:00** **566.** Immunoreactions in the presence of nanostructures. **K. Riehemann**, H. Fuchs, K. Langer
- 9:30** **567.** Combination of cowpea mosaic virus and PD-1 blockade works synergistically to improve therapeutic efficacy. **C. Wang**, N.F. Steinmetz
- 10:00** Intermission.
- 10:30** **568.** Designed Au-TiO₂ nanoreactors for spatiotemporal controlled, NIR-promoted photocatalytic transformations inside living cells. **M. Correa-Duarte**
- 11:00** **569.** Withdrawn

SECTION E
San Diego Convention Center
Room 30E

Nanomaterials

Optimizing Nanostructure for Practical Applications

J. A. Hollingsworth, R. Nagarajan, *Organizers*

J. R. McBride, *Organizer, Presiding*

- 8:30** **570.** Nanoscale colocalization of fluorogenic probes reveals the role of oxygen vacancies in the photocatalytic activity of tungsten oxide nanowires. **B. Sadtler**
- 9:00** **571.** Synthesis and electrical properties of photoactive, two-dimensional SnS nanosheets. **A. Mews**, M. Kobylinski, C. Rumlieb, T. Tsangas, A. Kolditz, T. Kipp
- 9:30** **572.** Metal nanoclusters: New light harvesting antenna for solar energy conversion. **J. Bang**
- 9:50** **573.** Space-confined seeded growth of Au nanostructures for highly efficient photo-induced cancer therapy. **J. Chen**, Y. Yin
- 10:10** **574.** Solid plasmonic substrates synthesized using TFF purified colloidal silver for cancer detection by means of SERS analysis of blood plasma. V. Toma, G.F. Stiufluic, S. Nitica, R. Marginean, A.I. Moldovan, C.M. Lucaciu, **R.I. Stiufluic**
- 10:30** **575.** Electromagnetic field confinement in self-assembled anisotropic plasmonic nanoparticle superlattice. **L. Tay**, J. Hulse, S. Poirier, J. Fraser

- 10:50** **576.** Hierarchical assembly of gold nanoparticles on graphene nano platelets: Synthesis and characterization. **Y. Ren**, S. Bhusal, G. Kedziora, V. Varshney, A. Roy, D. Nepal

SECTION F
San Diego Convention Center
Room 30D

Formulation Strategies to Control the Physicochemical Parameters of Drug & Nucleic Acid Delivery Systems

K. Sakurai, *Organizer*

M. A. Ilies, *Organizer, Presiding*

- 8:30** **577.** Physical stability and fibrillation kinetics of teriparatide: Influence of conformational structure, product formulation, and the Hoffmeister ions. **M. Korang-Yeboah**, S. Ketcham, B. Bandaranayake, C.N. Cruz, M. Ashraf
- 9:00** **578.** Development of ROS-triggered degradable nanoparticles using oligoproline peptides as biomolecule delivery platform for plant cells. **R. Kawasaki**, K. Tsuchiya, K. Numata
- 9:30** **579.** Quantifying hyaluronic acid and metal-organic framework for biomedical applications using gas-phase electrophoresis. **D. Tsai**, H. Wang
- 10:00** **580.** Controlled synthesis of calcium carbonate nanoparticles and stimuli-responsive multilayered nanocapsules for oral drug delivery. **N. Elbaz**, A. Owen, S. Rannard, T. McDonald
- 10:30** **581.** Withdrawn
- 11:00** **582.** Improving the therapeutic efficacy of nucleic acids and small molecule drugs using stimuli-responsive nanostructures. **J.L. Rouge**
- 11:30** **583.** Formulation of carbonic anhydrase IX: Targeted drug delivery systems against hypoxic tumors. A. Shabana, U.K. Mondal, S. Akocak, **M.A. Ilies**

SECTION G
San Diego Convention Center
Room 30C

Basic Research in Colloids, Surfactants & Interfaces

Emulsions, Drops & Dispersions

R. Nagarajan, *Organizer*

S. Choi, *Presiding*

- 8:30** **584.** Surfactant-induced reorganization of the hydrophobic phase at nanoemulsion interfaces. **A. Carpenter**, G.L. Richmond

- 8:50 585.** Oil-in-oil Pickering emulsions stabilized solely by diblock copolymer nanoparticles. **M.J. Rymaruk**, S. Brown, C. Williams, S.P. Armes
- 9:10 586.** Understanding uniform, fast, and scalable buoyancy-driven macro-sized drop generations. **S. Choi**
- 9:40 587.** Phase stability and miscibility in alcohol microemulsions: Do reverse micelles form in ethanol/AOT/*n*-heptane systems?. **R. Ridley**, E. Alvarado, V. Vasquez, O. Graeve
- 10:00 588.** Two's company, three's a crowd: How ions tag along for the ride with SDS and PEI on a nanoemulsion surface. **E. Tran**, G.L. Richmond
- 10:20 589.** Effects of low-temperature hydrothermal treatment on the properties and removal of fine solids from nonaqueous extraction (NAE) bitumen. **M. Ahmed**, Q. Chen, X. Tan, Q. Liu
- 10:40 590.** How does end-group charge on the steric stabilizer block affect the formation and stability of Pickering nanoemulsions prepared using diblock copolymer nanoparticles?. **S.J. Hunter**, N.J. Penfold, O. Mykhaylyk, S.P. Armes
- 11:00 591.** Simple creams, complex structures. **D. Ahmadi**, D. Barlow, J. Lawrence

SECTION H

San Diego Convention Center

Room 33C

Theoretical & Experimental Investigations of Water Interactions with Materials

Cosponsored by ANYL

D. Donadio, *Organizer*T. Guo, *Organizer, Presiding*K. Bradford, *Presiding*

- 8:30 592.** Desiccant-based food drying for reduced carbon generation and improved food security. **K. Bradford**, J. Van Asbrouck, I. Donis-Gonzalez, T. Guo, D. Donadio
- 9:10 593.** NMR characterization of dehydration of zeolites by three heating methods. **T. Guo**
- 9:30 594.** Discerning the fundamental interactions of water with porous catalysts by *in situ* MAS NMR. **N.R. Jaegers**, M. Hu, M. Wang, V. Lebarbier Dagle, H. Wang, A.B. Padmaperuma, Y. Wang, J. Hu
- 10:10 595.** Drop manipulation on superhydrophobic surface with dielectrowetting. **J. yang**, X. Deng
- 10:30 596.** Electrified membranes for water treatment: Toward new experimental and theoretical tools. **D.S. Bergsman**, B.A. Getachew, A.P. Straub, J.J. Patil, B.D. Smith, J.C. Grossman
- 11:10 597.** Withdrawn

Biomaterials & Biointerfaces

S. Romero-Vargas Castrillon, *Organizer*M. Geoghegan, *Presiding*

- 8:30 598.** Charge and structure quantification of peptides at aqueous interfaces. **F. Geiger**, Q. Cui, N. Dalchand
- 8:50 599.** Dynamics of cellular membranes and their interactions with nanomaterials. P. Elvati, C. Lin, Y. Wang, **A. Violi**
- 9:10 600.** Force spectroscopy measurement of the adhesion of galactose to the human pathogen *Leishmania mexicana*. A.R. Hall, J. Blakeman, A.M. Eissa, P.M. Chapman, A.L. Morales-García, D.H. Dockrell, N.R. Cameron, M. Wiese, M.E. Rogers, **M. Geoghegan**
- 9:40 601.** Synthesis, characterization, and evaluation of a zwitterionic microgel for therapeutic protein delivery. **A. Erfani**, N.H. Flynn, C. Aichele, J.D. Ramsey
- 10:00 602.** Photodegradable hydrogels for retrieval of bacteria cells from screening interfaces. **R.R. Hansen**, N. Fattahi, N. Barua, P. Nieves-Otero, A. van der Vlies, T.G. Platt
- 10:20 603.** High throughput creation of water-in-water droplets in a microfluidic flow-focusing device. M. Jeyhani, V. Gnyawali, N. Abbasi, S.S. Tsai, **D. Hwang**
- 10:40 604.** Thermophoretic manipulation of the mechanical properties of biomaterials in microfluidics. **A. Kosmidis**, D. Vigolo, L.M. Grover, Y. Shen
- 11:00 605.** Tuning surface charge as a general approach to improving immobilized enzyme function on mixed lipid bilayers. **A.F. Chaparro Sosa**, K.J. Black, J. Kaar, D.K. Schwartz
- 11:20 606.** Molecular interactions at the cellulose-lignin interface explored via molecular simulation. **J.V. Vermaas**, M.F. Crowley, G. Beckham

Future of Biomacromolecules at a Crossroads of Polymer Science & Biology

Delivery Systems

Sponsored by POLY, Cosponsored by BIOL, CARB, CELL, COLL, ENVR, MEDI, PHYS and PMSE

Surfactant & Colloid Science Applied to Formulations

Sponsored by AGRO, Cosponsored by COLL

SECTION A

San Diego Convention Center
Room 5B

Basic Research in Colloids, Surfactants & Interfaces

Colloidal Materials

R. Nagarajan, *Organizer*
S. S. Datta, *Presiding*

- 2:00 **607.** Preparation and properties of fluoroalkyl end-capped vinyltrimethoxysilane oligomer/magnetite nanocomposites. **H. Sawada**, S. Okada, K. Yamashita
- 2:20 **608.** Synthesis of hybrid polystyrene-poly(organosiloxane) particles with complex architectures through use of organotrialkoxysilanes as surfmer. **P. Buskens**, D. Mann, M. Segers, H. Keul, M. Moller
- 2:40 **609.** Cracking and self-healing of shrinkable, granular materials. **H. Cho**, S.S. Datta
- 3:10 **610.** Preparation and application of fluoroalkyl end-capped vinyltrimethoxysilane oligomer/hexagonal boron nitride nanocomposites. **J. Saengkaew**, K. Yamashita, H. Sawada
- 3:30 **611.** Synthesis of nanoparticles in dispersion: Flow cell coupled analytics as a way to follow particle growth. **N. Meulendijks**, P. Buskens, R. van Ee, G. van Groenestijn, A. Volker, A.C. Voelker, R. Armenta, G. Pierre
- 3:50 **612.** Measuring the accessible surface area within the nanoparticle corona using molecular probe adsorption. **M. Park**, D. Salem, D. Parviz, X. Gong, K. Silmore, T. Lew, D.T. Khong, M.C. Ang, S. Kwak, M. Chan-Park, M. Strano
- 4:10 **613.** Polymer-based energetic composites with improved thermal conductivity through bioinspired interfacial engineering strategy. **G. He**
- 4:30 **614.** New insight into the role of Ag in the seed-mediated gold nanorods synthesis. **J. Zhu**, R. Lennox
- 4:50 **615.** Protection of organic molecular microcrystals encapsulated under two-dimensional materials. **W. Li**, N. Tierce, E. Bekyarova, C.J. Bardeen
- 5:10 **616.** Understanding interfacial interactions to unlock the potential of bioinspired nanomaterials. **S.V. Patwardhan**, J. Manning, M. Jorge, A. Centi, B. Walkley, J. Provis

SECTION B

San Diego Convention Center
Room 6FSurfaces & Interfaces in the Environment:
Symposium in Honor of Vicki Grassian

Nano in the Environment & Plenary Lecture

Cosponsored by ENVR and WCC

A. P. Ault, J. Baltrusaitis, *Organizers, Presiding*

- 2:00 Introductory Remarks.
- 2:05 **617.** Changes in the physiochemical properties of MoO₃ nanoparticles in aquatic systems. **D.F. Rodrigues**, S. Fanourakis, J.P. Bahamonde
- 2:25 **618.** Accelerating nano-EHS research: Applications in nano-chemistry and nano-toxicology. **C. Sayes**
- 2:45 **619.** Mineral growth, dissolution, and beyond: Iron oxide nanoparticles. J. Voelz, C. Johnston, M. Cruz Reyes, A. Soroush, J.A. Soltis, J.H. Strehlau, N.D. Burrows, A.M. Vindedahl, W. Arnold, **R. Penn**
- 3:05 **620.** Molecular level studies of carbon-based nanomaterials in aquatic environments. **H. Fairbrother**
- 3:25 **621.** Interfacial energy: Key to controlling calcium carbonate formation on environmentally-abundant surfaces. **Y. Jun**, Q. Li, Y. Zhu
- 3:45 Intermission.
- 3:55 **622.** Applications of nanotechnology for water treatment: Electrospun nanofibers as a platform for integrated treatment and monitoring. **D.M. Cwiertny**
- 4:15 **623.** Insight into the interactions of biomolecules and natural organic matter with mesoporous silica nanomaterials. **S.C. Larsen**
- 4:35 **624.** Physical chemistry of environmental interfaces. **V.H. Grassian**
- 5:25 Concluding Remarks.

SECTION C

San Diego Convention Center
Room 31B

Surface Chemistry

S. L. Tait, *Organizer*Y. Cardona Quintero, F. Kunc, *Presiding*

- 2:00 **625.** Multimethod quantification of nanomaterial surface functional groups. **F. Kunc**, Y. Sun, A. Brinkmann, G. Lopinski, L. Johnston, V. Balhara
- 2:20 **626.** Convergence of ensemble and single-molecule techniques to understand protein liquid chromatography. **A. Misiura**, H. Shen, C. Dutta, N. Moringo, L.D. Bishop, C.F. Landes

- 2:40 627.** Co-optimization of multifunctional surfaces using high-throughput surface patterning assays. **N. Alsharif**, T. Lawton, J.R. Uzarski, K.A. Brown
- 3:00 628.** Using non-standard N-heterocyclic carbenes to functionalize gold surfaces and analysis of their binding via SERS. **S. Strausser**, L. Sherman, J.P. Camden, D.M. Jenkins
- 3:20 629.** Surface energy determination comparison: Inverse gas chromatography and contact angle goniometry. **W. Skinner**, S. Manni
- 3:40** Intermission.
- 4:00 630.** Computational study of mechanism of different amino acids binding to Graphene sheet in gas phase with DFT. **M. Malhotra**, C.V. Kumar, J. Gascon
- 4:20 631.** Nerve-agent decomposition by polyoxometalates utilizing a correlated multimodal approach. **Y. Tian**, A. Plonka, A. Ebrahim, D.L. Collins-Wildman, C.L. Hill, A. Frenkel
- 4:40 632.** Functionalized porous silicon for the capture and detection of organophosphates from air. **B.R. Pimentel**, C.E. Wahl, A. Chaix, J.S. Ha, D.E. Hunka, M.J. Sailor, S. Cohen
- 5:00 633.** Adsorption of Sarin on dry, wet, and doped TiO₂(110) using density functional theory. **Y. Cardona Quintero**, R. Nagarajan

SECTION D

San Diego Convention Center
Room 31A

Targeted Delivery of Nanomedicines In Vivo

P. del Pino, *Organizer*

N. Feliu Torres, W. J. Parak, *Organizers, Presiding*

- 2:00 634.** Transition metal oxide nanostructures for a magnetic goal in nanomedicine. **V. Salgueirino**
- 2:30 635.** Fabrication of 3D plasmonic micro-structured super-crystals arrays. **N. Pazos-Perez**, R. Alvarez-Puebla
- 3:00 636.** Theranostic carcoded nanoparticles personalize cancer medicine by predicting the drug response in the primary tumor microenvironment and in brain metastasis. **A. Schroeder**
- 3:30** Intermission.
- 4:00 637.** Multimodal nanostructures as theragnostic agent in Alzheimer disease at early stages: PANA project. **M. Rodríguez-Pérez**, B. Pelaz, P. Aguiar, C. Correa, E. Polo, L. Vázquez-Vázquez, E. López-Arias, F. Campos, J. Castillo, P. del Pino, T. Sobrino
- 4:20 638.** Targeted delivery of supra-assembled nanocargoes *in vivo* to overcome the chemoresistance in colon cancer. **N. Thorat**, J. Bauer

- 4:40 639.** Investigating tantalum nanoparticles for X-ray CT and therapeutic use. **S. Chakravarty**, J.M. Hix, E.M. Shapiro

SECTION E

San Diego Convention Center
Room 30E

Nanomaterials

Synthesis of Metal & Metal Oxide Nanocrystals

J. R. McBride, R. Nagarajan, *Organizers*

J. A. Hollingsworth, *Organizer, Presiding*

- 2:00 640.** Two-phase synthesis of gold-copper bimetallic nanoparticles of tunable composition. **D. Hofmann**, C.J. Murphy
- 2:20 641.** Tuning the frequency of localized surface plasmon resonances. **C.R. Conti**, G.F. Strouse
- 2:40 642.** Syntheses of colloidal F:In₂O₃ cubes: Fluorine-induced faceting and infrared plasmonic response. **S. Cho**, S. Ghosh, Z. Berkson, J.A. Hachtel, J. Shi, X. Zhao, L. Reimnitz, C.J. Dahlman, Y. Ho, A. Yang, Y. Liu, J. Idrobo, B.F. Chmelka, D.J. Milliron
- 3:00 643.** Electrochromic niobium oxide nanorods. **C. Saez Cabezas**, G. Ong, S.L. Skjærvø, D.J. Milliron
- 3:20 644.** Lipase-catalyzed enzymatic biodegradation of carbon dots follows sequential oxidation pathways. **D. Sar**, I. Srivastava, D. Pan
- 3:40 645.** Green synthesis of palladium nanomaterials via biological templates using TMV and BSMV virus-like particles. **Y. Lee**, K. Lee, C.A. Scott, R. G. Susler, S. Loesch-Fries, K. Solomon, M.T. Harris
- 4:00 646.** Precision thermal and reaction control leads to selective formation of amphiphilic cationic gold clusters in the critical size range, n = 130-146 Au atoms [1.6-nm core diameter]. **M. Hoque**, A. Antonyamy, R. Whetten, K. Mayer
- 4:20 647.** Reshaping and sintering of 3D fcc metal nanocrystals: Stochastic atomistic modeling with realistic surface diffusion kinetics. **K. Lai**, J.W. Evans
- 4:40 648.** Site-selective carving and co-deposition: Transformation of Ag nanocubes into concave nanocrystals encased by Au-Ag alloy frames. **J. Ahn**, D. Wang, J. Zhang, Y. Ding, D. Qin
- 5:00 649.** Synthesis of Au-Pt coaxial nanotubes with high photothermal stability for chemo-photothermal therapy. **Q. Zhang**, Z. Nie

SECTION F
San Diego Convention Center
Room 30D

Basic Research in Colloids, Surfactants & Interfaces

Nanomaterials

R. Nagarajan, *Organizer*

C. Drew, *Presiding*

- 2:00 650. Enzymatically activated aggregation and cell-adhesion of peptide-nanoparticle conjugates selectively target tumor tissue with enhanced delivery efficiency. **H. Huang**, S. O'Brien, R. Ulijn
- 2:20 651. Molecular layer deposition: Mechanisms of vapor-phase organic thin-film synthesis. **D.S. Bergsman**, R.G. Closser, C.J. Tassone, B.M. Clemens, D. Nordlund, S.F. Bent
- 2:40 652. Amphiphilic conjugated polymers for nanoparticle stabilization. **S. Saxena**, J. Subbiah, P. Meier, A. Colsmann, W. Wong, D. Jones
- 3:00 653. Multiscale analysis of the doping-driven wettability of two-dimensional materials. **T. Tian**, S. Lin, S. Li, L. Zhao, E. Santos, C. Shih
- 3:20 654. Investigating physico-chemical properties of dynamically crosslinked nanopatterned hydrogels. **S. Heedy**, J. Luo, A.F. Yee
- 3:40 655. Withdrawn
- 4:00 656. Development of next-generation materials for hybrid electro-optic systems. **L.E. Johnson**, H. Xu, D.L. Elder, S.R. Hammond, Y. de Coene, K. Clays, L.R. Dalton, B.H. Robinson
- 4:20 657. Monodisperse magnetic silica hexapods. **J. Kim**, G. Yi
- 4:40 658. Additive-free processing of carbon nanotubes in cresols as dispersions, pastes, gels and dough. **K. Chiou**, J. Huang
- 5:00 659. Biocatalytic porous frameworks with reversible pH-gated speed regulation for smart micromotors. **S. Gao**, K. liang, V. Chen

SECTION G
San Diego Convention Center
Room 30C

Basic Research in Colloids, Surfactants & Interfaces

Polymer Particles & Gels

R. Nagarajan, *Organizer*

A. Mallia, *Presiding*

- 2:00 660. Characterization of core-shell latex particles by capillary electrophoresis. **M. Jing**, W. Gao, W. Young, L. Yin

- 2:20 661. CO₂-responsive polymer nanoparticles. **Y. Shieh**, F. Hu, P. Tai
- 2:40 662. Soft nanocomposite hydrogel microspheres with defined nanostructures. **D. Suzuki**, T. Watanabe, C. Song, K. Murata
- 3:00 663. Tuning composition and hydrophobicity of ionic statistical amphiphilic copolymers to control and predict copolymer particle size. **T.J. NEal**, O. Mykhaylyk, S. Spain
- 3:20 664. Structure property correlations, gelation, mechanical, and thermal properties of molecular gels derived from *N*-phenyloctadecanamides and *N*-(phenylalkyl)octadecanmides as molecular gelators. **A. Mallia**, K. Kanemitsu, J. Kim
- 3:50 665. Evaluation of thermoresponsive structural changes in hydrogel microspheres by high-speed atomic force microscopy. **Y. Nishizawa**, S. Matsui, K. Urayama, T. Kureha, M. Sibayama, T. Uchihashi, D. Suzuki
- 4:10 666. Formulation of new responsive and self-repairing magneto-capillary gels. **N.I. Morales Castellanos**, S. Roh, B. Bharti, S. Khan, O.D. Velev
- 4:30 667. New cationic sterically-stabilized diblock copolymer nanoparticles exhibit exceptionally high salt tolerance in aqueous media. **S. Byard**, A. Blanz, S.P. Armes
- 4:50 668. Preparation of fluorescent microspheres with conjugated polymers. **L. Fan**
- 5:10 669. Synthesis of well-defined, pyrrolidone-based homopolymers and stimulus-responsive diblock copolymers via RAFT aqueous solution polymerization of 2-(*N*-acryloyloxy) ethylpyrrolidone. **O. Deane**, S.P. Armes

SECTION H
San Diego Convention Center
Room 33C

Theoretical & Experimental Investigations of Water Interactions with Materials

Cosponsored by ANYL

T. Guo, *Organizer*

D. Donadio, *Organizer, Presiding*

D. S. Bergsman, *Presiding*

- 2:00 670. Competitive interactions in confined environments. **A.E. Clark**
- 2:40 671. Modeling of the hydration of nanoporous materials by machine learning. **M. Bauchy**
- 3:00 672. Computer modeling of water adsorption and water-mediated proton conduction in metal-organic frameworks. **F. Paesani**
- 3:40 673. Out-of-the-box implicit solvation at dielectric interfaces. **J. Filser**, M. Sinstein, C. Scheurer, S. Matera, K.U. Reuter, H. Oberhofer

SECTION A

San Diego Convention Center

Room 5B

Basic Research in Colloids, Surfactants & Interfaces

Applications of Novel Colloids

R. Nagarajan, *Organizer*T. Guo, *Presiding*

- 8:30** **685.** Preparation of fluorinated aliphatic diol/ phosphonic acids/magnetite composites: Application to separation of mixture of oil and water. **K. Yamashita**, Y. Kaneumi, T. Kijima, K. Kokin, H. Sawada
- 8:50** **686.** Synthesis of thermoresponsive block copolymer vesicles via polymerisation-induced self-assembly for oil thickening applications. **I.R. Dorsman**, S.P. Armes
- 9:10** **687.** Fabrication of Janus nanocups and selective loading with cargo. **X. Qiang**, A. Steinhaus, C. Chen, R. Chakroun, A. Gröschel
- 9:30** **688.** Synthesis and performance of nanoreactors from mesoporous silica. **T. Guo**
- 10:00** **689.** One-pot hydrothermal synthesis of benzalkonium-templated mesostructured silica antibacterial agents. **V. Dubovoy**, A. Ganti, T. Zhang, H. Al-Tameemi, J.D. Cerezo, J.M. Boyd, T.G. Asefa
- 10:20** **690.** Kinetic modeling of simple organophosphates hydrolysis using mixed metal nanofibers. **M.M. Allard**, Y. Zhu, C.C. Perry
- 10:40** **691.** Photothermal killing of *Escherichia coli* using gold nanorods and gold nanobipyramids. **S. Yougbare**, T. Kuo
- 11:00** **692.** Structure-dependent optical modulation of propulsion and collective behavior of acoustic/ light-driven hybrid microbowls. **S. Tang**, J. Wang
- 11:20** **693.** Photochemically patterned metal nanoparticle strontium barium niobate surfaces with tunable wettability, enhanced raman scattering and fluorescence emission. **E. Barnes**, L. Soblosky, E. Alberts, L. Johnson, J. Guy, A. Kumar

SECTION B

San Diego Convention Center

Room 6F

Basic Research in Colloids, Surfactants & Interfaces

- 4:00** **674.** Polarizable molecular simulations reveal how silicon-containing functional groups govern the desalination mechanism in nanoporous graphene. **L. Wang**, Y. Qiu, B. Schwegler
- 4:40** **675.** Water at charged interfaces: Localized vs. delocalized charges. **M. Sulpizi**

SECTION I

San Diego Convention Center

Room 29B

Biomaterials & Biointerfaces

S. Romero-Vargas Castrillon, *Organizer*N. Kornienko, *Presiding*

- 2:00** **676.** β -Diketonate-iron(III) complex: Versatile fluorine-19 MRI signal enhancement agent. **C. Wang**, H. Xu, S. Adams, W. Zhu, E. Ahrens
- 2:20** **677.** Inhibition of leukocyte adhesion in the presence of model particulate drug carriers. **W. Kelley**, P. Onyskiw, C. Fromen, O. Eniola-Adefeso
- 2:40** **678.** Interfacing enzymes with inorganic materials for semi-artificial photosynthesis. **N. Kornienko**
- 3:10** **679.** Photoconjugating affibodies to their receptor prevents their proteolytic degradation and preserves their activity: Strategy for gene-free cell modification. **S. Roy**, M. Brasino, A.H. Sanchez, J. Cha, A.P. Goodwin
- 3:30** **680.** Red/far-red light controlled bacteria-driven microrobots for cargo delivery and release. **I. Sentürk**, S.V. Wegner
- 3:50** **681.** Mining for peptides with affinity for a synthetic copolymer hydrogel nanoparticle: Compositional and structural contributions to affinity. **S. Lee**, I. Moody, Z. Zeng, E. Fleischer, G.A. Weiss, K.J. Shea
- 4:10** **682.** *In situ* surface modification of 3D printed emulsion inks. **E. Cosgriff-Hernandez**, D. Jenkins, P. Dhavalikar, M.S. Silverstein
- 4:30** **683.** Extracellular DNA provides structural integrity to a *Micrococcus luteus* biofilm. **J. Blakeman**, A. Morales-García, A. Hayward, J. Mukherjee, K. Gori, N. Lant, M. Geoghegan
- 4:50** **684.** Chirality engineering of supraparticles for controllable nanomedicine. **J. Yeom**, P. Guimaraes, H. Ahn, K. McHugh, M. Mitchell, C. Yun, A. Jaklenec, R. Langer

Future of Biomacromolecules at a Crossroads of Polymer Science & Biology

Biomaterials

Sponsored by POLY, Cosponsored by BIOL, CARB, CELL, COLL, ENVR, MEDI, PHYS and PMSE

Surfaces & Interfaces in the Environment

R. Nagarajan, *Organizer*

X. Yu, *Presiding*

- 8:30** **694.** Chemical, physical, and superstructural driving forces of aqueous interfacial phosphate recognition. **J.F. Neal**, W. Zhao, A.J. Grooms, M. Smeltzer, B. Shook, M. Zerkle, A.H. Flood, H.C. Allen
- 8:50** **695.** Heterogeneity in urban environmental films. **J. DeYoung**, J.S. Grant, S.K. Shaw
- 9:10** **696.** Viscosity increases in the core of phase separated particles after IEPOX uptake. **N.E. Olson**, Z. Lei, R.L. Craig, Y. Zhang, Y. Chen, J. Surratt, A.P. Ault
- 9:30** **697.** *In situ* molecular imaging of the air-liquid and liquid-liquid interface in the environment. **X. Yu**
- 10:00** **698.** Reflection-absorption infrared spectroscopy is not only a vibrational spectroscopy: Case of thin amorphous solid water (ASW) films. **J. Maurais**, P. Ayotte
- 10:20** **699.** Mineralogy dependent atmospheric processing of mineral dust aerosols and their impact on the growth of marine diatoms. **E. Hettiarachchi**, S. Ivanov, T. Kieft, R. Reynolds, H. Goldstein, B. Moskowicz, G. Rubasinghege
- 10:40** **700.** Phenol-water vapor deposition in long-term exposure: Different interfaces, similar sigmoid kinetics, and enhanced water retention. **M. Borisover**, N. Bukhanovsky, M. Lado
- 11:00** **701.** Photochemical reaction dynamics and absorption spectroscopy of environmentally important species. **D. Shemesh**, M. Luo, R. Gerber, V.H. Grassian
- 11:20** **702.** Design and formulation of an iodine-based antimicrobial coating for sporicidal and bactericidal activities. **O.V. Ezeh**, Y. Li, W. Han, K. Yeung
- 11:40** **703.** Surface chemistry of cerium oxide nanoparticles in an engineered UV/persulfate process with dissolved organic matter. **X. Wu**, Y. Rao, Y. Jun

SECTION C

San Diego Convention Center
Room 31B

Surface Chemistry

S. L. Tait, *Organizer*

J. M. Gorham, K. Tan, *Presiding*

- 8:30** **704.** NiAu single-atom alloys for selective C-C coupling. **P. Kress**, E.H. Sykes
- 8:50** **705.** Pair approximation of heterogeneous reaction networks. **C.A. Kim**, T.A. Van Voorhis

- 9:10** **706.** Atomic-scale characterization and reactivity of PtAg surface alloys. **D. Patel**, E.H. Sykes
- 9:30** **707.** Triaqua surface coordination complex on $\text{Co}_3\text{O}_4(111)$. **G. Yan**, T. Waehler, R. Schuster, M. Schwarz, C. Hohner, K. Werner, J. Libuda, P. Sautet
- 9:50** Intermission.
- 10:10** **708.** Role of functional groups for the synthesis of nanomaterials within metal organic frameworks materials. **K. Tan**, J. Cure, S. Jensen, L. Feng, H. Wang, J. Li, T. Thonhauser, H. Zhou, Y.J. Chabal
- 10:30** **709.** Challenges in surface chemical analysis in nanomaterial systems. **J.M. Gorham**, D. Gorka
- 10:50** **710.** Hydrophobic CeO_2 nanoparticles coating using polymer binder for enhanced adhesion capability. **S. Yasmeen**, R. Khan, H.B. Lee
- 11:10** **711.** Formation of tough latex films of polymeric microspheres crosslinked with rotaxane. **S. Hiroshige**, J. Sawada, D. Aoki, T. Takata, D. Suzuki
- 11:30** **712.** Molecular insights into surface ligand-dynamics and their impact on functionality of self-assembled nanoparticle superlattices. T. Patra, H. Chan, P. Podsiadlo, E. Shevchenko, S. Sankaranarayanan, **B. Narayanan**

SECTION D

San Diego Convention Center
Room 31A

Targeted Delivery of Nanomedicines In Vivo

N. Feliu Torres, W. J. Parak, *Organizers*

P. del Pino, *Organizer, Presiding*

- 8:30** **713.** Applications of SERS encoded particles. **R. Alvarez-Puebla**
- 9:00** **714.** "Smart" DNA-based materials for controlled release. **M. Vazquez**, C. Wang, S. Lilienthal, A. Fischer, W. Chen, I. Willner
- 9:30** **715.** Triple-labelling of polymer-coated quantum dots and adsorbed proteins for tracing their fate. **W.J. Parak**
- 10:00** Intermission.
- 10:30** **716.** Accessing intracellular targets using designed nanoplatforms. **S. Dhar**
- 11:00** **717.** Assessing the effect of surface chemistry on targeted delivery and cellular uptake of silica nanoparticle. **J. Joo**
- 11:20** **718.** Micromotors as targeted payload delivery platforms. **E. Karshalev**, B. Esteban-Fernández de Ávila, J. Wang
- 11:40** **719.** Stable J-aggregation of an aza-BODIPY lipid in a liposome for multimodal cancer imaging. **M. Cheng**, K.M. Harmatys, D.M. Charron, J. Chen, G. Zheng

SECTION E
San Diego Convention Center
Room 30E

Nanomaterials

Morphological Control of Colloidal Nanostructures

J. A. Hollingsworth, R. Nagarajan, *Organizers*

J. R. McBride, *Organizer, Presiding*

- 8:30** **720.** Study on surface interfacial regulation and properties of nanocomposites based on grafting of nano-Al. **C. Zeng**, F. Gong, J. Zhang
- 8:50** **721.** Electrically tunable liquid photonic crystals with highly saturated structural colors for display unit. **Q. Fu**, Y. Yin
- 9:10** **722.** Withdrawn
- 9:30** **723.** Monofacet-selective cavitation within solid-state silica-nanoconfinement towards Janus iron oxide nanocube. **N. Kumari**, I. Lee
- 9:50** **724.** Block copolymers in 3D confinement: Janus structures with complex topology. **A. Steinhaus**, X. Qiang, G. Quintieri, A. Gröschel
- 10:10** **725.** Fluorescent dye-encoded assemblies of amphiphilic Janus magnetoplasmonic nanoparticles: Cluster, lamellae, and vesicles. **D. Lu**, S. Hou, H. Duan
- 10:30** **726.** Assembly of rod-shaped hydrogel microspheres at the air/water interface. **K. Honda**, Y. Sazuka, K. Iizuka, S. Matsui, T. Uchihashi, T. Kureha, M. Shibayama, T. Watanabe, D. Suzuki
- 10:50** **727.** Complex inorganic nanomaterials by block terpolymer templating. **S. Tjaberings**, M. Heidelmann, A. Gröschel
- 11:10** **728.** Regioselective self-assembly of gold nanospheres and silver nanodiscs modulated by block copolymers with steric hindrance. **X. Lin**, Z. Nie
- 11:30** **729.** Controlled self-assembly of water-soluble, “hairy,” inorganic nanoparticles (HINPs) into supracolloids with defined valence. **K. Webb**, Z. Nie

SECTION F
San Diego Convention Center
Room 30D

Basic Research in Colloids, Surfactants & Interfaces

Interface Science

R. Nagarajan, *Organizer*

J. Samaniuk, *Presiding*

- 8:30** **730.** Complex behavior of metal surface corrosion and passivity in cellular automata-based simulations. J. Stepien, **J. Stafiej**

- 9:00** **731.** *Xylopi* *aethiopica* extract as green and eco-friendly corrosion inhibitor and its quantum chemical analysis. **N.E. Ibsi**
- 9:20** **732.** Dynamics of 2D materials with nanometer-scale thickness at fluid-fluid interfaces. **J. Samaniuk**, D. Goggin
- 9:50** **733.** On the temperature dependence of interfacial structure in liquid-liquid interface. **Z. Liu**, A.E. Clark
- 10:10** **734.** Water condensation on ionic liquid infused nanostructured surfaces. **Q. Ge**, S. Sett, N. Miljkovic, T. Zhang
- 10:30** **735.** Withdrawn
- 10:50** **736.** Effect of rigid red blood cells on platelet adhesion in flow. **A.L. Banka**, M. Gutierrez, T. Tanski, M. Shamoun, O. Eniola-Adefeso
- 11:10** **737.** Photoinduced changes in polymer-glass adhesion. **S. Mostafavi**, K.D. Clark, M. Sroda, J. Read De Alaniz, C.J. Bardeen
- 11:30** **738.** Quantifying the exposure time-dependent wetting properties of plasma-treated polymer surfaces. **A.R. White**, G. Whitlock, R. Henderson, G. Wills

SECTION G
San Diego Convention Center
Room 30C

Basic Research in Colloids, Surfactants & Interfaces

Colloidal Interactions

R. Nagarajan, *Organizer*

T. Wei, *Presiding*

- 8:30** **739.** Lipid and complex coacervates interactions. **F. Pir-Cakmak**, A. Grigas, C.D. Keating
- 8:50** **740.** Probing interactions between surfactants and hydrophobically modified starch nanoparticles by fluorescence. Q. Zhang, D. Kim, **J. Duhamel**
- 9:20** **741.** Small molecule segregation from poly(vinyl alcohol) films. **R. Fong**
- 9:40** **742.** Morphology, texture and stability of spin dewetted 5CB nematic liquid crystal droplets. **P. Dhara**, R. Mukherjee
- 10:00** **743.** Characterization of particle charge from aerosol generation process: Impact on infrared signatures and material reactivity. **E.M. Durke**, M. McEntee, M. He, S. Dhaniyala
- 10:20** **744.** Interfacial behavior of amino acid residues on gold surfaces studied with electrical spectroscopy and atomistic reaxFF simulations. M. Sajib, W. Jean-Baptiste, K. Chin, **T. Wei**
- 10:50** **745.** Tuning the interaction energies between lipid head groups and planar substrates. **C. Liu**, S. Sun, D.R. Melendez, P.S. Cremer

- 11:10 746.** Revisiting the colloidal fundamentals and exploring nanofilm formation of water-dispersible polyesters. **S. Islam**, O.D. Velev

SECTION H
San Diego Convention Center
Room 33C

Theoretical & Experimental Investigations of Water Interactions with Materials

Cosponsored by ANYL

D. Donadio, T. Guo, *Organizers*

M. Sulpizi, L. Wang, *Presiding*

- 8:30 747.** Water interactions with striped phases of amphiphiles on 2D materials. **S.A. Claridge**
- 9:10 748.** Understanding an active role for water in zeolite-hydrocarbon reactions. **J.L. White**, K. Chen, M. Abdolrahmani, S. Crossley, D.E. Resasco, S. Horstmeier, B. Wang
- 9:50 749.** Water adsorption in zeolites: Insight from multiscale modeling. **D. Donadio**, S. Chen, T. Guo
- 10:10 750.** Understanding material and component level properties on the performance of MOF-based atmospheric water harvesting systems. **S.R. Rao**, A. LaPotin, H. Hyunho Kim, E.N. Wang
- 10:50 751.** Interplay between specific-ion effects and confinement in the aqueous electric double layer. **C. Zhan**, T. Pham, M. Ceron, S. Hawks, B. Wood, M. Stadermann, P. Campbell

Biomaterials & Biointerfaces

S. Romero-Vargas Castrillon, *Organizer*

H. Sakai, *Presiding*

- 8:30 752.** Design of synthetic polymer nanoparticulates for metalloproteinase inhibition. **M. Nakamoto**, D. Zhao, K.J. Shea
- 8:50 753.** New polymer formulations for cryostorage of biologics. **A.E. Fayter**, M.I. Gibson, M. Hasan
- 9:10 754.** Electron mediators shuttling between erythrocytes and liposomes encapsulating hemoglobin (artificial red cells) to reduce methemoglobin by using abundant glycolytic electron energies. **H. Sakai**
- 9:40 755.** pH-Response tunable mixed-charged polymers for reversible adsorption and desorption of proteins. **Y. Hiruta**, K. Sawada, T. Kaku, Y. Tokura, S. Shiratori, D. Citterio
- 10:00 756.** Determination of the adsorption orientation of amyloid beta 1-40 monomer over nano-gold colloidal particles' surfaces. **K. Yokoyama**
- 10:20 757.** Discovery of anti-mycobacterial copolymers using a photo-chemical combinatorial platform. **S. Richards**, M.I. Gibson
- 10:40 758.** Probing the nano-bio interface of hydroxyapatite with solid-state MAS NMR. **Y. Li**, B. Addison, G.P. Holland
- 11:00 759.** Collagen thin film adhesion mediated by mussel-inspired catecholamine surface primers. **G. Degen**, E. Valois, G. Lindsey, R. Andresen Eguiluz
- 11:20 760.** Targeting *S. aureus* in osteoblast infection employing antibody linked metallic nanoparticles. **T. Abdulrehman**, S.M. Qadri, Y. Haik

COMP

DIVISION OF COMPUTERS IN CHEMISTRY

H. Woodcock and J. Shen, *Program Chairs*

SUNDAY MORNING – COMP

SECTION A

Omni San Diego Hotel
Gallery 2

Immersive Virtual Reality for Molecular Design

Cosponsored by CHED, CINF and COMSCI

R. S. Paton, L. Whitehead, *Organizers, Presiding*

- 8:30** 1. Development of a virtual reality interface for molecular simulations-driven interactive ensemble-based drug design. J. Juarez-Jimenez, S. Llabres, **J. Michel**
- 9:10** 2. Nanome: Next generation molecular visualization, collaboration, and design. E. Leija, S. McCloskey, **K. Wang**
- 9:50** 3. Development of a virtual reality platform for effective communication in drug discovery. L. Kingsley, G. Spraggon
- 10:30** Intermission.
- 10:50** 4. Computational modeling of Novichok interaction with acetylcholinesterase in VR. **Z. Radic**
- 11:30** 5. Use of VR for molecular structures. **J. Boström**

SECTION B

Omni San Diego Hotel
Gallery 3A

Advances in Multiscale Computational Modeling of Biomass Conversion Processes

R. Assary, V. Glezakou, S. Kim, *Organizers, Presiding*

- 8:30** Introductory Remarks.
- 8:35** 6. Overview of the US Department of Energy's consortium for computational physics and chemistry. **G.J. Leong**, J. Parks
- 9:00** 7. Computational studies of catalytic biomass conversion. **D.A. Dixon**
- 9:30** 8. Catalytic mechanisms of butanediol conversion by metal phosphates. J. Alegre Requena, Y. Guan, X. Huo, J. Stunkel, S. Kim, D. Vardon, **R.S. Paton**
- 10:00** Intermission.

- 10:15** 9. Multiscale modelling approach for the electrochemical hydrogenation of organic compounds. **R. Rousseau**, V. Glezakou, M. Lee, D.C. Cantu, S. Akhade, M. Nguyen, S. Yuk, D. Zhang
- 10:45** 10. Multiscale modeling of hierarchical transport and chemical reaction in porous catalyst particles in fluidized and packed bed reactor systems. **P. Ciesielski**, V.S. Bharadwaj, B. Pecha, H. Sitaraman, L. Bu, A. Lattanzi, X. Gao, W. Rogers
- 11:15** 11. Toward the optimal design of molybdenum carbide catalysts for vapor phase upgrading of bio-oil. **H. Doan**, M. Zhou, R. Assary

SECTION C

Omni San Diego Hotel
Gaslamp 1

Quantum Mechanics

A. E. DePrince, H. P. Hratchian, *Organizers*

H. Harb, *Presiding*

- 8:30** 12. Impact of protein conformational changes and electrostatics on a BLUF photoreceptor. **J.J. Goings**, S. Hammes-Schiffer
- 9:00** 13. Catalytic structure and function of CRISPR-Cas9 revealed by *ab initio* quantum mechanics/molecular mechanics (QM/MM) simulations. **G. Palermo**
- 9:30** 14. Effect of ions on absorption spectra of green fluorescent protein (GFP) chromophore in aqueous solution. **S.V. Shedje**, T.J. Zuehlsdorff, M. Servis, A.E. Clark, C. Isborn
- 10:00** Intermission.
- 10:15** 15. Quantum mechanics of how solvents alter the identity of chemical bonds. D.R. Widmer, **B.J. Schwartz**
- 10:45** 16. Bond orders: Definition, evaluation, and physical meaning. **G. Knizia**, S. Bintrim
- 11:15** 17. Rovibrational spectroscopy of magnesium acetylide (MgCCH) and its detection in the interstellar medium. J.E. Burns, Q. Cheng, R.C. Fortenberry, **N.J. Deyonker**
- 11:45** 18. Static and dynamic approaches to computing spectral lineshapes. **T.J. Zuehlsdorff**, A. Montoya Castillo, J. Napoli, T. Markland, C. Isborn

SECTION D
Omni San Diego Hotel
Gaslamp 2

Advances in Multiscale Modeling

Financially supported by Schrödinger
W. G. Noid, J. Shelley, *Organizers*
J. Li, *Organizer, Presiding*

- 8:30 Introductory Remarks.
8:35 19. Recent advances in coarse-graining. **G.A. Voth**
9:05 20. Relative entropy design of coarse-grained protein models. **M. Shell**, T. Sanyal
9:35 21. Systematic coarse-graining for thermodynamic properties and inhomogeneous systems. **W.G. Noid**
10:05 Intermission.
10:20 22. Consistent representation of structural and dynamical properties from coarse-grained simulation models. **J.F. Rudzinski**, T. Bereau
10:50 23. Developing transferable coarse-grained potentials for the prediction of multiproperties of polymer systems. **H. Guo**
11:20 24. Integrating dynamic ionization into membrane permeation free energy landscapes and macroscopic permeability calculations. Z. Yue, **J.M. Swanson**

SECTION E
Omni San Diego Hotel
Gaslamp 3

Use of Predictive Computational ADME Tools to Enable Drug Discovery

F. Broccatelli, *Organizer*
D. F. Ortwine, *Organizer, Presiding*

- 8:30 Introductory Remarks.
8:35 25. 30 years of computational ADME: What have we learned?. **N. Hosea**
9:05 26. Comparison of matched molecular pairs, matched molecular series and machine learning models for the optimization of ADME endpoints. **C. Keefer**
9:35 27. Building a stronger *in silico* ADME program through partnership. **K.E. Desino**
10:05 Intermission.
10:20 28. Estimation of membrane permeation using implicit membrane models and machine learning. **B. Dutagaci**, S. Brocke, A.D. Mackerell, M. Feig
10:50 29. Advancing the quan/qual partnership for chemical design. **C. Kochansky**
11:20 30. Anticipating and addressing solubility and precipitation problems computationally. **R.D. Clark**, R. Fraczkiewicz

Computational Quantum Chemistry: From Promise to Prominence: A Symposium in Honor of Henry F. Schaefer

Sponsored by PHYS, Cosponsored by COMP

SUNDAY AFTERNOON – COMP

SECTION A
Omni San Diego Hotel
Gallery 2

Role of Water Phase in Molecular Biology: Importance of Water in Folding, Binding & Transport Phenomena

Modeling Protein-Ligand Recognition in Aqueous Environment: Present & Future

E. Alexov, C. Chang, R. Luo, *Organizers*
H. Muddana, *Presiding*

- 1:30 Introductory Remarks.
1:35 31. Modeling water in molecular recognition and drug design. **M.K. Gilson**
2:05 32. Ligand-protein pose and affinity predictions: New perspectives and lessons learned from the drug design data resource (D3R). **R.E. Amaro**
2:35 33. Water, water everywhere, nor any drop to drink. **M.S. Head**
3:05 Intermission.
3:20 34. Molecular diffusion in biology. **J. McCammon**
3:50 35. Machine learning identifies chemical drivers of enzyme catalysis. N. Seelam, B.M. Bonk, J.W. Weis, **B. Tidor**
4:20 36. Modeling ligand-CDK8/CycC unbinding free energy barriers for designing drugs with preferred binding kinetics. **C. Chang**, Z. Tang, S. Chen, H.D. Pandey

SECTION B
Omni San Diego Hotel
Gallery 3A

Advances in Multiscale Computational Modeling of Biomass Conversion Processes

R. Assary, V. Glezakou, S. Kim, *Organizers, Presiding*

- 1:30 37. PETase: Engineering and characterization of a plastic “eating” enzyme. **H.L. Woodcock**, G. Beckham, J. McGeehan
2:00 38. Unraveling the oxidative coupling of methanol on Au(111) using first-principles-based kinetic modelling. R. Réocreux, I. Fampiou, **M. Stamatakis**

- 2:30** 39. Computational fluid dynamic modeling and simulation of biomass pyrolysis vapor-phase upgrading process at reactor scale. **X. Gao**, T. Li, W. Rogers, R. Panday, C. Li, H. Ashfaq, B. Hughes
- 3:00** Intermission.
- 3:15** 40. Computational scale-up of packed bed reactor and process for catalytic upgrading of pyrolysis vapors using COMSOL. **B. Adkins**, J. Parks, K. Lisa, K. Smith
- 3:45** 41. Predicting hydroxymethylfurfural (HMF) formation rate in sugar upgrading through investigation of Lewis acid and organic solvent effects. **Y. Kim**, H.M. Pilath, D. Robichaud, D.K. Johnson, S. Kim
- 4:05** 42. First-principle based microkinetic study of water effect in aldol condensation reaction on MgO(111) surface. **M. Zhou**, L.A. Curtiss, R. Assary
- 4:25** Concluding Remarks.

SECTION C

Omni San Diego Hotel
Gaslamp 1

Molecular Mechanics

J. Shen, *Organizer*

R. Teo, *Presiding*

- 1:30** 43. From *ab initio* data to high-dimensional potential energy surfaces: Nuts and bolts of generating a general many-body potential energy function. **S.E. Brown**, F. Paesani
- 1:50** 44. Effective fragment potentials made faster. **L.V. Slipchenko**, K.B. Bravaya, E. Epifanovsky
- 2:10** 45. Modeling hydrogen-oxygen combustion via programmable potentials. **A.M. Avila**, **L. Bertels**, **M.P. Head-Gordon**, **I. Meziar**
- 2:30** 46. Advanced electrostatic potential based methods to derive atomic charges and polarizabilities. **M. Schauerperl**, P.S. Nerenberg, L. Wang, D.L. Mobley, C.I. Bayly, M.K. Gilson
- 2:50** 47. MBX: Next generation molecular dynamics. **M. Riera Riambau**, D. Smith, A.C. Simmonett, F. Paesani
- 3:05** Intermission.
- 3:20** 48. Implementing polarizable Gaussian multipole model for molecular dynamics simulations. H. Wei, **R. Qi**, R. Luo
- 3:40** 49. Modeling vibrational Stark effects using polarizable force fields: KSI as an exemplar. **J.W. Essex**, R.T. Bradshaw, S. Fried
- 4:00** 50. Assessing the performance of various binding-free-energy-prediction approaches on kinase/ligand complexes: Importance of the density-functional theory tight-binding method and atomic-charge calculations. **M. Ghaani**, O. Barker, N. English

- 4:20** 51. Accuracy vs. efficiency? Towards ACKS2-based polarization in force fields. **P. Gütlein**, H. Oberhofer, K.U. Reuter, J. Blumberger

SECTION D

Omni San Diego Hotel
Gaslamp 2

Advances in Multiscale Modeling

Financially supported by Schrödinger

J. Li, W. G. Noid, J. Shelley, *Organizers*

J. F. Rudzinski, *Presiding*

- 1:30** 52. Polymer electrolytes statistics and thermodynamics. **M. Olvera De La Cruz**
- 2:00** 53. Multiscale modeling for the materials and pharmaceutical industries. **J. Shelley**
- 2:30** 54. Molecular and mesoscale modeling for mechanical issues in composite interfaces. **N.E. Iwamoto**
- 3:00** Intermission.
- 3:15** 55. Structure and dynamics of macromolecular systems on multiple scales. **M. Guenza**
- 3:45** 56. Coarse-grained electron transfer model for reactive force fields. **I. Leven**, T.L. Head-Gordon
- 4:15** 57. Coarse-graining electrons: Nonreactive many-body force fields for molecular dynamics. T.L. Head-Gordon, **A. Das**

SECTION E

Omni San Diego Hotel
Gaslamp 3

Use of Predictive Computational ADME Tools to Enable Drug Discovery

F. Broccatelli, *Organizer*

D. F. Ortwine, *Organizer, Presiding*

- 1:30** Introductory Remarks.
- 1:35** 58. Dose optimization concepts in drug design. **F. Broccatelli**
- 2:05** 59. Integration of machine learning models for ADME to enable drug discovery: Deep neural network vs. support vector machine. **P. Desai**
- 2:35** 60. Incorporating ADME/Tox parameters in optimising multiobjective molecular design. **N. Brown**
- 3:05** Intermission.
- 3:20** 61. Cross-company evaluation of *in silico* approaches to predict microsomal or hepatocyte binding. **S. Winiwarter**
- 3:50** 62. Rationally controlling the chameleonic properties of beyond Rule of 5 (bRo5) compounds. **G. Caron**, G. Ermondi

- 4:20 63. Beyond ADME QSAR: Adapting physiologically-based PK simulations to lead optimization. **E.J. Martin**, B.D. Madej, M. Bolger, R. Clark, P.R. Daga

Computational Quantum Chemistry: From Promise to Prominence: A Symposium in Honor of Henry F. Schaefer

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SUNDAY EVENING – COMP

Computational Methods for Lanthanides & Actinides: Theory & Applications

Sponsored by NUCL, Cosponsored by COMP

MONDAY MORNING – COMP

SECTION A Omni San Diego Hotel Gallery 2

Role of Water Phase in Molecular Biology: Importance of Water in Folding, Binding & Transport Phenomena

Modeling Protein-Ligand Recognition in Aqueous Environment: Present & Future

E. Alexov, C. Chang, R. Luo, *Organizers*
M. S. Head, *Presiding*

- 8:30 64. Using structure to identify protein-protein and drug protein interaction networks. **B.H. Honig**
- 9:00 65. Challenges and improvements in modeling protein-ligand interactions. **D.L. Mobley**
- 9:30 66. Solvation structure and thermodynamic mapping (SSTMap): Open-source software package for the analysis of water in molecular dynamics trajectories. K. Haider, A. Cruz, S. Ramsey, M.K. Gilson, **T.P. Kurtzman**
- 10:00 Intermission.
- 10:15 67. Role of interfacial water in protein-ligand binding: Classical density functional perspective. **R.M. Levy**
- 10:45 68. Computational crystal structure and polymorph prediction. **H. Muddana**
- 11:15 69. Molecular simulation: Methodology advancements and applications to drug discovery. **R. Luo**
- 11:45 70. Constraining evolution —> Avoiding drug resistance: Lessons from viruses. **C.A. Schiffer**
- 12:15 Concluding Remarks.

SECTION B

Omni San Diego Hotel
Gallery 3A

Women Make COMP

Cosponsored by PROF and WCC
K. Armacost, M. C. Nagan, *Organizers*
G. Palermo, *Organizer, Presiding*

- 8:30 Introductory Remarks.
- 8:35 Panel Discussion.
- 8:50 Discussion.
- 8:55 71. Development of rare-event sampling methods for biomolecular transport systems. **N. Roussey**, A. Dickson
- 9:00 72. Tailoring the variational implicit solvent method (VISM) for new challenges: Heterogeneous hydration in biomolecular recognition. **C. Gravina Ricci**, B. Li, L. Cheng, J. Dzubiella, J. McCammon
- 9:05 73. Computational methodologies for the accurate simulation of Raman intensities in the low-frequency vibrational spectra of molecular crystals. **S.J. Dampf**, T.M. Korter
- 9:10 74. Structural basis for ligand modulation of the CCR2 conformational landscape. **B.C. Taylor**, C.T. Lee, R.E. Amaro
- 9:25 75. Identifying and quantifying allosteric pathways from molecular simulations. **H. Klem**, P. Lake, R.B. Davidson, R.S. Paton, M. McCullagh
- 9:30 76. Structural and dynamic properties of A β ₂₁₋₃₀ with experiments and simulations. **D.B. Amirkulova**, M. Chakraborty, A. White
- 9:35 77. Targeting alpha isoform specificity in human topoisomerase II. **J.A. Akkarapattiakal Kuriappan**, N. Osheroff, M. Devivo
- 9:50 78. Elucidation of the mechanism for ethene hydrogenation over single metal cation catalysts: Combined modeling and experimental study. **H. Shabbir**, S.L. Pellizzeri, M. Ferrandon, I. Kim, M. Delferro, A.B. Martinson, R.B. Getman
- 9:55 79. Iridium(I) catalyzed α -C(sp³)-H alkylation of saturated azacycles: Experiment and theory. **P. Verma**, N. Chekshin, J. Yu
- 10:00 80. Putting force fields to the test: Mutual interaction of aminoacids, lipids, and carbohydrates with GPI-anchored proteins inserted into lipid bilayers and membranes. **P. Banerjee**, R. Lipowsky, M. Santer
- 10:05 81. Charge density in enzyme active site as a descriptor of electrostatic preorganization. **A. Alexandrova**, M. Eberhart
- 10:20 Intermission.
- 10:30 82. Towards a wavelength sensitive detector, based on ICD in a system of coupled quantum wells. **T.G. Goldzak**, N. Moiseyev

- 10:45 83.** Hot ground state photochemistry of aldehydes in the atmosphere. **M. Corrigan**, B. Welsh, S. Kable, M. Jordan
- 10:50 84.** Investigating the mechanical perturbations of asymmetric lipid bilayers on mechanosensitive Piezo ion channels through multiscale approach. **W. Jiang**, W.M. Botello-Smith, H. Zhang, J. Lacroix, Y.L. Luo
- 10:55 85.** Enhancing side chain rotamer sampling using non-equilibrium candidate Monte Carlo. **K.H. Burley**, S.C. Gill, N.M. Lim, C. Goulding, D.L. Mobley
- 11:00** Panel Discussion.
- 11:15 86.** Computational probing of the force-biased potential energy surface: Uncovering nonintuitive mechanochemical reaction pathways. **A.K. Roessler**
- 11:20 87.** Enzyme engineering to computationally predict stereoselective products for biocatalysts. **S. Lenka**, P. Buteler, R.R. Watkins, J.D. Stewart, A.E. Roitberg
- 11:25 88.** Towards the *de novo* design of functional metalloproteins. **K. Belsare**, W.F. Degrado, N. Polizzi
- 11:30 89.** Machine-learning-aided *in silico* drug discovery: Machine-learning-based atom parameterization program for molecular mechanics force fields. **M. Charles**
- 11:45 90.** Molecular simulation to accelerate discovery of $\alpha_v\beta_6$ integrin inhibitors. **E. Guest**, S. Oatley, S.J. MacDonald, J.D. Hirst
- 11:50 91.** Solvent design strategies from computation and statistical modeling. **L.C. Gallegos**, J. Alegre Requena, R.S. Paton
- 11:55 92.** Understanding and correcting DFT errors in transition metal chemistry. **F. Liu**, H.J. Kulik
- 12:00 93.** Computational flavor chemistry: Towards the rational design of chemosensory GPCR-targeted food ingredients and drug candidates. **A. Di Pizio**, L. Waterloo, M. Behrens, P. Gmeiner, M. Niv

SECTION C
Omni San Diego Hotel
Gaslamp 1

Quantum Mechanics

A. E. DePrince, H. P. Hratchian, *Organizers*
A. Zamani, *Presiding*

- 8:30 94.** Halogen-bonding interactions: Revised benchmarks and a new assessment of exchange vs. dispersion. **B.M. Wong**, L. Anderson, F. Aquino, A.E. Raeber, X. Chen
- 9:00 95.** Compressibility of intramolecular dispersion interactions. **C.J. Mackie**, J. Gonthier, M.P. Head-Gordon

- 9:30 96.** Accurate prediction of electronic coupling for hole and electron transfer problems using DFT-based approaches. **Y. Mao**, T. Markland
- 10:00** Intermission.
- 10:15 97.** Conformational exploration of aromatic amino acids: Assessment of DFT levels by comparison of vibrational frequencies with experimental data. **T. Dinadayalane**, D.A. Daggag
- 10:45 98.** Methane combustion studied using the *ab initio* nanoreactor approach combined with kinetic modeling. **J. Meisner**, X. Zhu, H. Hirai, K. Thompson, T.J. Martinez
- 11:15 99.** Modeling the photodetachment processes of lanthanide oxide and boride clusters. **H. Harb**, H.P. Hratchian
- 11:40 100.** Spin state ordering in metal-based compounds using the localized active space self-consistent field method. **R. Pandharkar**, M. Hermes, C.J. Cramer, L. Gagliardi

SECTION D
Omni San Diego Hotel
Gaslamp 2

Advances in Multiscale Modeling

Financially supported by Schrödinger
J. Li, J. Shelley, *Organizers*
W. G. Noid, *Organizer, Presiding*

- 8:30 101.** Combining enhanced sampling with machine learning in the generation of high-dimensional free energy landscapes of complex molecular systems. **M.E. Tuckerman**
- 9:00 102.** Machine learning of coarse-grained molecular dynamics force fields. **F. Noe**, C. Clementi
- 9:30 103.** Coarse-graining molecular models with machine learning and experimental data. **C. Clementi**
- 10:00** Intermission.
- 10:15 104.** Nanoscale simulations to enable mRNA delivery. **M.L. Hall**
- 10:45 105.** High-throughput molecular dynamics of drug-membrane thermodynamics. **T. Berau**
- 11:15 106.** Bridging the scales: Machine learning directed macro-to-micro scale simulation to model KRAS initiation of cancer. **T.S. Carpenter**, F.C. Lightstone, D.V. Nissley, F. Streitz, H. Ingolfsson
- 11:45 107.** Top-down multiscale modeling to design nanomaterials from peptide self-assembly. **J. Li**

SECTION E
Omni San Diego Hotel
Gaslamp 3

Recent Advances in Kinase Drug Discovery: A Joint Venture Between Medicinal, Biological & Computational Chemists

Cosponsored by MEDI
L. Whitehead, *Organizer*
J. Shen, *Organizer, Presiding*

- 8:30 **108.** In pursuit of elusive allosteric pathways in protein kinases. **A.P. Kornev**
- 9:00 **109.** Harnessing allostery for selective targeting of Aurora kinase A in cancer. **N. Levinson**
- 9:30 Intermission.
- 9:40 **110.** Innovative technologies packages for kinase drugs with diverse inhibition modes. **L. Neumann, D. Witte**, L. Lercher, K. von König, E. Schneider
- 10:10 **111.** Conformational plasticity and covalent hotspots: New computational tools for assisting targeted kinase inhibitor design. **J. Shen**, C. Tsai, R. Liu

Frontiers in Interdisciplinary Research: New Paradigms for Integration of Theory & Experiment

Sponsored by BIOL, Cosponsored by COMP, ORGN and PHYS

Computational Quantum Chemistry: From Promise to Prominence: A Symposium in Honor of Henry F. Schaefer

Sponsored by PHYS, Cosponsored by COMP

MONDAY AFTERNOON – COMP

SECTION A
Omni San Diego Hotel
Gallery 2

Role of Water Phase in Molecular Biology: Importance of Water in Folding, Binding & Transport Phenomena

Membrane Systems & Water Phase

E. Alexov, C. Chang, R. Luo, *Organizers*
A. V. Onufriev, *Presiding*

- 1:30 **112.** Water facilitated proton transport in biomolecular systems: Remarkably complex and collective phenomenon. **G.A. Voth**

- 2:00 **113.** How proteins use hydration as a kinetic control knob in coupled ion exchange. **J.M. Swanson**
- 2:30 **114.** Modeling studies of water interaction with magnesium and calcium ions and inhibitors in selective ion channels. **M.G. Kurnikova**
- 3:00 Intermission.
- 3:15 **115.** Ras signaling: PI3K and Raf activation at the membrane. **R. Nussinov**, M. Zhang, H. Jang
- 3:45 **116.** Preferential solvation of membrane surfaces in the presence of protein crowders. **M. Feig**

SECTION B
Omni San Diego Hotel
Gallery 3A

Women Make COMP

Cosponsored by PROF and WCC
M. C. Nagan, G. Palermo, *Organizers*
K. Armacost, *Organizer, Presiding*

- 1:30 Panel Discussion.
- 1:45 **117.** DNA can do it! Catalytic mechanism of the 8-17 DNAzyme. **S. Ekesan**, D.M. York
- 1:50 **118.** Linking multiscale data analyses, ligand- and structure-based modeling to explore ligand interactions with hepatic organic anion transporting polypeptides. **A. Tuerkova**, S. Jain, U. Norinder, C. Özvegy-Laczka, G. Szakács, B. Zdrzil
- 1:55 **119.** BioSimSpace: Interoperable molecular software framework. **A. Mey**, L.O. Hedges, C. Woods, J. Michel
- 2:00 **120.** Excited states of the photosystem II reaction center. **M. Kavanagh**, I.R. Gould, L. Barter
- 2:05 **121.** Women in science: What can you do to close the gap?. **A. Krylov**
- 2:20 **122.** Electron transfer in transition metal complexes. **H. Carson**, T. Keane, J.A. Weinstein, A.J. Meijer
- 2:25 **123.** Linking the ligand modulation of the binding site to the function of HCN ion channels. **F. Tofoleanu**, B. Brooks
- 2:30 **124.** Structural basis for group 1 influenza fusion inhibition by Arbidol characterized with a cell-scale, ensemble based Markov state model. **S.E. Kochanek**, R.E. Amaro
- 2:35 **125.** Deriving a modern fixed partial charge set for the nucleic acids using the IPolQ scheme. **E.A. Rosenzweig**, D.S. Cerutti, D.A. Case
- 2:50 Intermission.
- 3:05 **126.** On the many roles played by lipids in the activation TRPV1, the noxious heat and capsaicin receptor. **E. Gianti**, A. Yazici, M.A. Kasimova, T. Rohacs, M.L. Klein, V. Carnevale

- 3:20 **127.** MD in protein design: Investigation of binding determinants for design strategies and screening. **E. Pecora de Barros**, J. Schiffer, A.A. Vorobieva, J. Dou, D. Baker, R.E. Amaro
- 3:25 **128.** Extending molecular kinetics modeling tools to nonreversible dynamics. **B.E. Husic**
- 3:30 **129.** Efficient prediction of binding affinity for reversible covalent inhibitors. **H. Zhang**, W. Jiang, P. Chatterjee, P. Edwards, Y.L. Luo
- 3:35 **130.** Modelling the aggregation-induced emission phenomena: Challenge for computational chemistry. **L. Le Bras**, L. de Thieulloy, C. Adamo, A. Perrier
- 3:50 **131.** Computational investigation of reaction selectivity in non-heme Fe(II) and alpha-ketoglutarate dependent halogenase SyrB2. **R. Mehmood**, H. Qi, A.H. Steeves, H.J. Kulik
- 3:55 **132.** Multi-task modeling of antiviral activity for small organic compounds. **E.A. Sosnina**, S. Sosnin, D.I. Osolodkin, M. Fedorov
- 4:00 **133.** Brownian dynamic study of an enzyme metabolon in the TCA cycle: Substrate kinetics and channeling. **Y.M. Huang**, G. Huber, N. Wang, S.D. Minter, J. McCammon
- 4:05 **134.** Mechanistic insights into photodecarboxylation of fatty acids from classical and QM/MM simulations. **A. Walker**, T.J. Lane, H. van den Bedem, T.J. Martinez
- 4:20 **135.** Modeling actinide chemistry with spin-orbit coupled auxiliary field quantum Monte Carlo. **H. Hao**, R. Nanguneri, B. Marston, B.M. Rubenstein
- 4:25 **136.** Transcription initiation machinery functional dynamics and genetic disease. **C. Yan**, T. Dodd, J.A. Tainer, S.E. Tsutakawa, I.N. Ivanov
- 4:30 Panel Discussion.
- 4:45 Discussion.
- 4:50 Concluding Remarks.

SECTION C

Omni San Diego Hotel
Gaslamp 1

Quantum Mechanics

A. E. DePrince, H. P. Hratchian, *Organizers*
A. Abou Taka, *Presiding*

- 1:30 **137.** Multicomponent wave function based methods for describing nuclear quantum effects in molecular systems. **F. Pavosevic**, S. Hammes-Schiffer
- 2:00 **138.** Simulating photoionisation phenomena in DNA/RNA pyrimidine nucleobases. **J. Segarra-Martí**, T. Tran, T.A. Mackenzie, M. Bearpark
- 2:30 Intermission.

- 2:45 **139.** MolSSI quantum chemistry archive project. **D. Smith**, L. Naden, D. Altarawy
- 3:15 **140.** Understanding the vibrational solvatochromism of the ester carbonyl vibration in dilute PCBM solutions. **Y. Yu**, L. Shi
- 3:45 **141.** Computational NMR characterization of chiral Au₂₅(SMeBut)₁₈⁰. **S. Gelpi Dominguez**, J. Gascon

SECTION D

Omni San Diego Hotel
Gaslamp 2

Advances in Multiscale Modeling

Financially supported by Schrödinger
J. Li, W. G. Noid, *Organizers*
J. Shelley, *Organizer, Presiding*

- 1:30 **142.** Atomistic and coarse-grained analyses of membrane remodeling by proteins and nanoparticles. **Q. Cui**
- 2:00 **143.** Simulations at multiple scales reconcile lipid membrane structure with the barrier function of mammalian skin. **G. Fiorin**, C.M. MacDermaid, R. Devane, M.L. Klein
- 2:30 **144.** Multiscale modeling of mechanochemistry during protein synthesis: Challenges and insights. **E. O'Brien**, C. Deutsch, S. Leininger
- 3:00 Intermission.
- 3:15 **145.** Coarse-grained models for liquid-liquid phase separation of intrinsically disordered proteins. **T.L. Head-Gordon**
- 3:45 **146.** Coarse-grained models of cellular environments to study dynamics and phase behavior. **M. Feig**
- 4:15 **147.** Multiscale simulations of G-protein coupled receptors. **P. Carloni**
- 4:45 Concluding Remarks.

SECTION E

Omni San Diego Hotel
Gaslamp 3

Recent Advances in Kinase Drug Discovery: A Joint Venture Between Medicinal, Biological & Computational Chemists

Cosponsored by MEDI
J. Shen, *Organizer*
L. Whitehead, *Organizer, Presiding*

- 1:15 **148.** What makes a kinase promiscuous for inhibitors?. S. Hanson, G. Georghiou, M.K. Thakur, J. Rest, W.T. Miller, J.D. Chodera, **M. Seeliger**
- 1:40 **149.** How, when and why do small molecules unbind: Insights from predictive all-atom simulations. **P. Tiwary**

MONDAY EVENING – COMP

SECTION A

San Diego Convention Center

TBD

Sci-Mix

H. L. Woodcock, *Organizer*

8:00 - 10:00

156. Water purification with nanoscale Turing structures. **R. Chakraborty**
212, 213, 214, 215, 216, 225, 229, 231, 233, 238, 240, 242, 247, 249, 255, 260, 263, 264, 271, 274, 278, 281, 282, 286, 294, 302, 308, 309, 310, 311, 312, 313, 314, 315, 316, 347, 348, 349, 391, 392, 393, 394, 403, 404, 405, 406, 407, 409, 410, 411.
See Subsequent Listings.

TUESDAY MORNING – COMP

SECTION A

Omni San Diego Hotel

Gallery 2

Role of Water Phase in Molecular Biology: Importance of Water in Folding, Binding & Transport Phenomena

Enzyme Mechanisms & pH-Dependence Processes

E. Alexov, C. Chang, R. Luo, *Organizers*
M. Feig, *Presiding*

- 8:30** **157.** Simulations and force fields with quantum mechanics/molecular mechanics and machine learning. **W. Yang**
- 9:00** **158.** Importance of modeling water in enzyme function elucidation and protein-ligand scoring function development. **Y. Zhang**
- 9:30** **159.** Exploring pH- and redox-dependent properties of biomolecules. **A.E. Roitberg**
- 10:00** Intermission.
- 10:15** **160.** Role of aqueous pH in modulating biological function. **C.L. Brooks**
- 10:45** **161.** How ligand protonation state controls water in protein-ligand binding. **J. Shen**, J. Henderson
- 11:15** **162.** Modeling pKa without solute-water boundary: DelPhiPKa and its applications to protein-protein binding. **S. Pahari**, E. Alexov

- 2:05** **150.** Allosteric regulation and reversible covalent drug design for serine/threonine kinase. **Y.L. Luo**, W. Botello-Smith
- 2:30** Intermission.
- 2:45** **151.** Targeting the r-spine: Design, synthesis, and biological evaluation of novel type I½ p38α MAP kinase inhibitors with excellent selectivity, high potency, and prolonged target residence time. Implication for cancer- and CNS-applications. **S.A. Laufer**, H.K. Wentsch, N.M. Walter, M. Laemmerhofer, R. Buijsman, D. Rauh, L. Zender
- 3:10** **152.** Application of ensemble based simulations and machine learning for the prediction of binding free energies and personalized drug selection. S. Wan, **P.V. Coveney**
- 3:35** **153.** Leveraging synthetically-aware enumeration strategies and free energy simulations in drug discovery campaigns. **J.L. Knight**, K. Konze, P. Bos, S. Bhat, R. Abel, L. Wang
- 4:00** **154.** Modeling covalent modifiers of kinase proteins. E. Awoonor-Williams, **C.N. Rowley**
- 4:25** **155.** Connection between protein conformational dynamics and catalysis in protein kinases: Insights from multiscale simulations. **K. Nam**

Frontiers in Interdisciplinary Research: New Paradigms for Integration of Theory & Experiment

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Sponsored by PHYS, Cosponsored by COMP

Metabolomics in Forensics: Applications, Technical Barriers & Emerging Approaches for Chemical Identification Using In Silico Reference Libraries

Sponsored by ANYL, Cosponsored by COMP

SECTION B
Omni San Diego Hotel
Gallery 3A

Drug Design

Novel Methods & Lightning Talks

Y. Tseng, *Organizer*

M. R. Landon, *Organizer, Presiding*

- 8:30** **163.** Drug discovery by molecular dynamics: Role of the free energy landscape. **S. Leoni**, A. Casini
- 8:55** **164.** Electrostatic-field and surface-shape similarity for ligand-based drug design. **A.N. Jain**, A.E. Cleves
- 9:20** **165.** PickR: Pick diverse R-groups for library design using 3D electrostatics and shape. **P. Tosco**, M.D. Mackey, T. Cheeseright
- 9:45** Intermission.
- 10:00** Discussion.

SECTION C
Omni San Diego Hotel
Gaslamp 1

Exploring Transition Metal Chemistry & Spectroscopy with Quantum Chemistry

C. M. Aikens, N. Mayhall, *Organizers*

H. P. Hratchian, *Organizer, Presiding*

- 8:30** **166.** Theoretical studies of spectroscopic properties of transition metal complexes. **J. Autschbach**
- 9:05** **167.** Computational EPR spectroscopy of transition metal complexes with DMRG. **E. Sayfutyarova**, G.K. Chan
- 9:40** **168.** Magnetic anisotropy in mono- and binuclear complexes: Theoretical insight and prospects. **N. Guihéry**, R. Maurice, B. Cahier, N. Suaud
- 10:15** Intermission.
- 10:35** **169.** Towards a uniform black-box framework for computing magnetic properties: Theory and applications to single molecular magnets. **A. Krylov**
- 11:10** **170.** Diffuse and magnetic Dyson orbitals in the Rydberg anions and solvated-electron precursors of transition-metal chemistry. **J.V. Ortiz**
- 11:45** **171.** Embedding relativistic 2-component Kohn-Sham density functional theory in a non-relativistic quantum environment. **C. Hoyer**, D. Williams-Young, C. Huang, X. Li

SECTION D
Omni San Diego Hotel
Gaslamp 2

Protein Degradation Computational Design

L. Xiao, *Organizer, Presiding*

- 8:30** Introductory Remarks.
- 8:40** **172.** Principles of small molecule mediated ubiquitin ligase targeting. **E.S. Fischer**
- 9:10** **173.** Design and optimization of targeted protein degraders: Leveraging computational tools. **Y. Che**
- 9:40** **174.** Computational modeling of PROTAC-mediated ternary complexes: Applications and insight. **M.L. Drummond**
- 10:10** Intermission.
- 10:30** **175.** Development and validation of a computational modeling workflow to characterize the structure of bi-functional degraders-protein-protein ternary complex. **D.R. Weiss**, P. Novick, A.C. Parente, M. Lawrenz, D.W. Robbins, A. Kelly, M.G. Cardozo
- 11:00** **176.** PROTAC-mediated protein degradation: New therapeutic modality. **G. Burslem**

SECTION E
Omni San Diego Hotel
Gaslamp 3

Recent Advances in Kinase Drug Discovery: A Joint Venture Between Medicinal, Biological & Computational Chemists

Cosponsored by MEDI

L. Whitehead, *Organizer*

J. Shen, *Organizer, Presiding*

- 8:30** **177.** Exploring chemical space to discover novel BRD4 inhibitors. **C. Lemmen**
- 9:00** **178.** Is using a 2D drawing application to design for kinase selectivity an oxymoron?. **P. Tosco**, M.D. Mackey, T. Cheeseright, H. Jubb
- 9:30** **179.** Kinase atlas: Predicted regulatory hot spots in kinases. **S. Vajda**, C. Yueh, D. Kozakov
- 10:00** Intermission.
- 10:15** **180.** Multi-target pharmacology of kinase inhibitors, beneficial off-targets and allosteric sites. **R. Abagyan**, I. Kufareva, K. Chahal, D. Shi
- 10:45** **181.** Rational design of cross-gene family multitarget kinase inhibitors for multi-indication polypharmacology. **L. Xie**
- 11:15** **182.** Strategies to design conformation-specific kinase inhibitors. **A. Schlessinger**

Computational Quantum Chemistry: From Promise to Prominence: A Symposium in Honor of Henry F. Schaefer

Sponsored by PHYS, Cosponsored by COMP

TUESDAY AFTERNOON – COMP

SECTION A

Omni San Diego Hotel
Gallery 2

Role of Water Phase in Molecular Biology: Importance of Water in Folding, Binding & Transport Phenomena

Biomolecular Recognition

E. Alexov, C. Chang, R. Luo, *Organizers*
W. Jiang, *Presiding*

- 1:30** **183.** Long-timescale protein motion coupled solvation dynamics. **W. Yang**
- 2:00** **184.** Simulation of amyloid formation and propagation. **U. Hansmann**
- 2:30** **185.** Energy-flow perspective on activated dynamics in biomolecules. **A. Ma**
- 3:00** Intermission.
- 3:15** **186.** Why some atomistic simulations are very sensitive to the water model. **A.V. Onufriev**
- 3:45** **187.** Revealing the essential role of protein-protein interactions in viral capsid assembly. **Y. Xian, C. Karki, L. Li**
- 4:15** **188.** Effect of water on the entropy of protein-protein binding. **A. Chakravorty, J. Higham, E. Alexov, R.H. Henchman**

SECTION B

Omni San Diego Hotel
Gallery 3A

Drug Design

Novel Methods & Lightning Talks

Y. Tseng, *Organizer*
M. R. Landon, *Organizer, Presiding*

- 1:30** **189.** MDockPeP2: Predicting protein-peptide complex structures by accounting for peptide flexibility in long peptides. **X. Xu, X. Zou**
- 1:55** **190.** Dynamic docking to investigate thermodynamics and kinetics of drug-target binding. **A. Cavalli**
- 2:20** **191.** Design in 2D, model in 3D: Live 3D pose generation from 2D sketches. **P. Tosco, M.D. Mackey, T. Cheeseright**

- 2:45** **192.** Protein-ligand binding mode prediction from the apo-protein structure using a molecular dynamics-based pocket generation approach. **M. Araki, Y. Okuno**
- 3:10** Intermission.
- 3:25** Discussion.

SECTION C

Omni San Diego Hotel
Gaslamp 1

Exploring Transition Metal Chemistry & Spectroscopy with Quantum Chemistry

C. M. Aikens, H. P. Hratchian, *Organizers*
N. Mayhall, *Organizer, Presiding*

- 1:30** **193.** Magnetic properties and hyperfine tensors of TbPc₂-type single-molecule magnets. **K. Park**
- 2:05** **194.** Density-functional perturbation theory for excited states from constrained DFT. **D.A. Strubbe**
- 2:40** **195.** Calculations of transition metal clusters and complexes using self-interaction corrected energy functional. **H. Jonsson**
- 3:15** Intermission.
- 3:35** **196.** Interfacial proton-coupled electron transfer at nanoparticles and electrodes composed of transition metals. **S. Hammes-Schiffer**
- 4:10** **197.** Computational catalysis on amorphous silicates. **M. Caricato**

SECTION D

Omni San Diego Hotel
Gaslamp 2

Protein Degradation Computational Design

L. Xiao, *Organizer, Presiding*

- 1:30** Introductory Remarks.
- 1:35** **198.** New activities for cereblon modulators: Low molecular weight inducers of targeted protein degradation. **P. Chamberlain**
- 2:05** **199.** Reimagining druggability using chemoproteomic platforms. **D. Nomura**
- 2:35** **200.** Inhibition and degradation of drug targets using bioPROTAC mRNAs: Novel approach with broad therapeutic potential. **S. Ng, J. Chang, S. Lim, R. Khoo, P. Gopal, B. Henry, A. Partridge**
- 3:05** Intermission.
- 3:25** **201.** Targeting the undruggables: Design of highly potent and efficacious STAT3 degraders with absolute selectivity over other STAT proteins. **S. Wang**
- 3:55** **202.** Targeted protein degradation. **A. Phillips**
- 4:25** Concluding Remarks.

SECTION E

Omni San Diego Hotel
Gaslamp 3

Molecular Mechanics

J. Shen, *Organizer*

P. Buteler, *Presiding*

- 1:30** **203.** Tracking the allosteric signaling in CRISPR-Cas9 by leveraging accelerated molecular dynamics, solution NMR and artificial intelligence. **G. Palermo**, V.S. Batista, G.P. Lisi
- 1:50** **204.** Computational quest of full-length apobec3B. **O. Demir**
- 2:10** **205.** Mechanical coupling in the nitrogenase complex. **Q. Huang**, L.E. Johnson, B. Ginovska, S. Raugei
- 2:30** **206.** Temperature-modulated allostery in the IGPS enzyme of a thermophile. **F. Tofoleanu**, U. Morzan, J. Loria, A. Chaudhuri, B. Brooks, V.S. Batista
- 2:50** **207.** Molecular dynamics study on the stability of G-quadruplexes in the presents of incorporated mono-valent metal ions and small drug molecules. **U. Schnupf**, M. Caterino, A. Cesaro, J. Brady
- 3:10** Intermission.
- 3:20** **208.** Dissociation mechanism of processive cellulases explored through molecular simulation. **J.V. Vermaas**, R. Kont, G. Beckham, M.F. Crowley, M. Sandgren, J. Ståhlberg, P. Våljamäe, B. Knott
- 3:40** **209.** From Markov state models to absolute binding free energies. **B. Xie**, D.D. Minh
- 4:00** **210.** Binding free energies computed using emerging force fields from the Open Force Field Initiative. **D. Slochower**, N.M. Henriksen, M.K. Gilson
- 4:20** **211.** Markov models of functional dynamics of histone methyltransferases by millisecond-timescale molecular simulation and chemical probing. **R.P. Wiewiora**, S. Chen, M. Luo, J.D. Chodera

Elucidating Reaction Mechanisms with Computational & Experimental Chemistry

Sponsored by CMA, Cosponsored by COMP and PROF

TUESDAY EVENING – COMP

SECTION A

San Diego Convention Center
TBD

Chemical Computing Group Graduate Student Travel Awards

K. N. Kirschner, C. L. Simmerling, *Organizers*

6:00 - 8:30

- 212.** Unraveling functional hole hopping pathways in the [4Fe4S]-containing DNA primase. **R. Teo**, A. Migliore, D.N. Beratan
- 213.** Development of excited state quantum chemistry methods capable of describing photodissociation of single bonds. **D. Hait**, A. Rettig, M.P. Head-Gordon
- 214.** Multifidelity methods for the design of transition metal complexes. **J.P. Janet**, H.J. Kulik
- 215.** Rapid RNA structure determination through cryo-EM, high-throughput biochemistry, and computational modeling. **K. Kappel**, K. Zhang, Z. Su, G. Pintilie, W. Chiu, R. Das
- 216.** High fidelity ultra-coarse-graining of soft matter systems. **J. Jin**, G.A. Voth

SECTION A

San Diego Convention Center
TBD

COMP Poster Session

H. L. Woodcock, *Organizer*

6:00 - 8:30

- 217.** Electron transfer model for reactive force fields. **I. Leven**, T.L. Head-Gordon
- 218.** Bottom-up coarse graining of inhomogeneous environments. **M. Delyser**, W.G. Noid
- 219.** Capturing the H₂-metal interaction in the M-MOF-74 series using classical polarization. **T. Pham**, K. Forrest, B. Space
- 220.** Compound libraries on Chemspace: An approach to chart useful regions in available chemical space. **Y. Moroz**, O. Gavrylenko
- 221.** Crystal-structure prediction via basin-hopping global optimisation employing tiny periodic simulation cells and multipole expansion. **C. Burnham**, P. Samanta, M. Ghaani
- 222.** Degradation of high energy molecules using biological reduction: Rational way to reach bioremediation. **S. Agüero**
- 223.** Building upon a mean field platform for excited state quantum chemistry. **J. Shea**, E. Neuscamman

- 224.** Design and integration of mutual supply network for ethylene feedstock. **Q. Li**
- 225.** Predicting protein degradation through computational modeling of PROTAC-mediated ternary complexes. **M.L. Drummond**
- 226.** Docking study of thymine-dimer containing DNA decamer on translesion DNA polymerase zeta from *Dictyostelium discoideum*. **D. He**, S.K. Mauldin
- 227.** Computational exploration of spectroscopic and electronic properties of various 2,7-disubstitutions of 4,10-dihydropyrrolo[3',2':9,10]phenanthro[4,5-*efg*]indole (DPPAI). **B. Wex**
- 228.** Consistent method to calculate diffusion coefficients from molecular dynamics simulation. **D. Yu**
- 229.** Predicting protein-ligand binding affinity with gnina. **P. Francoeur**, D. Koes
- 230.** Classification and analysis of privileged scaffolds in protein families. **O.B. Scott**, A.E. Chan, X. Zhang
- 231.** Assessment and preparation of crystal structures for drug design. **C. Williams**
- 232.** Protocol for the analysis of vibrational circular dichroism spectra of small molecules using Gaussian and MOE. **A. Ajamian**
- 233.** Application of extended Hückel theory to pharmacophore modeling. **A. Ajamian**
- 234.** Computational analysis of the dimer interface of p53 bound to DNA. **T. Qiu**
- 235.** Prediction of fluorescence and absorbance of cytidine analogues using time-dependent density functional theory (TDDFT). **S. Bachori**, A. Cooksy
- 236.** Development of massively parallel software for quantum chemistry calculations: SMASH. **K. Ishimura**
- 237.** New red-emitting phosphor $K_{3-x}Rb_xSiF_7:Mn^{4+}$: DFT study and its synthesis. **S. Jang**, J. Park, C. Kim, H. Chang
- 238.** Molecular dynamics study of the hydrophobic effect in ethanol-water mixtures. **B. Liu**, T. Ichiye
- 239.** Meta-dynamics-based conformational sampling with semi-empirical tight-binding methods. **P. Pracht**, S. Grimme
- 240.** Quantum cluster growth: Explicit approach towards solvation free energies. **S. Spicher**, S. Grimme
- 241.** Geometric approach toward identifying stable parameters for network Hamiltonians governing amyloid fibril formation. **G. Grazioli**, Y. Yu, C.T. Butts
- 242.** Fragment-based *de novo* design targeting FABP5 and nSMase2. **L.E. Prentis**, P. Shanbhogue, Y.A. Hannun, R.C. Rizzo
- 243.** Enhanced sampling of hydration states and binding modes in protein-ligand structures with nonequilibrium candidate Monte Carlo simulations. **M.L. Samways**, H. Bruce Macdonald, J.W. Essex
- 244.** Protein-ligand pose and affinity prediction: Case study on BACE1 cyclic ligand dataset in D3R Grand Challenge 4. **C. Yang**, J. Lu, Y. Yang, Y. Zhang
- 245.** Modelling electric double layers at metal/water interfaces from density functional theory based molecular dynamics. **J. Le**, J. Cheng
- 246.** Conformational analysis and small molecule ligand recognition of the human-specific CHRFAM7A nicotinic receptor implicated in neuropsychiatric disorders. **D. LIU**, J. de Souza Cunha, A. Bronowska
- 247.** Examination of factors affecting the accuracy of quantum chemical frequency calculations for first-row transition metal compounds. **A. Abou Taka**, L.M. Thompson, H.P. Hratchian
- 248.** Effect of chemical functionalization on the thermal transport in the boron nitride nanosheets/polyvinyl alcohol composite. **J. Lu**, R. Sun, C.P. Wong
- 249.** Evaluation of alchemical non-equilibrium free energy calculations. **H. Baumann**, D.L. Mobley
- 250.** DFT study on the relative stabilities of double nitrogen doped graphene systems. **N.F. Alzaaqi**, T. Dinadayalane
- 251.** Cooperativity effects in multivalent systems: Case study. **A.J. Achazi**, L.K. von Krbek, M. Solleder, M. Weber, C.A. Schalley, B. Paulus
- 252.** Dynamics and molecular interactions of ssDNA in nucleic acid biosensors with varied surface properties. **T. Cholko**, S. Kaushik, C. Chang
- 253.** Revealing the optoelectronic properties of non-fullerene acceptors and benzodithiophene based polymer donors: Molecular dynamics simulation approach. **J.K. Roy**, A. Golius, J.R. Leszczynski
- 254.** Intermolecular interactions in human HDAC8 crystal structures and the stability of binding modes of co-crystallized inhibitors. **K. Yelekci**, A.I. Uba
- 255.** LASSOing the atom-typing problem: Statistical method for ligand force field model selection. **J.J. Cherian**, R.T. McGibbon, P. Angelikopoulos, A.G. Taube, J.L. Klepeis, B. Cole, D.E. Shaw
- 256.** How does glycosylation affect small molecule binding on influenza? Roles of electrostatics and sterics examined through Brownian dynamics simulations. **C. Seitz**, L. Casalino, G. Huber, J. McCammon, R.E. Amaro
- 257.** Density functional theoretical study on the C-Cl oxidative addition reaction at POP Rh center. **S. Hwang**

- 258.** Computational insights in generation mechanism of metal-hydrides. **H. Li**
- 259.** Investigating the effects of mutations and post-translational modifications on intrinsic EGFR dynamics using molecular simulations in improved solvation model. **M. Kondal**, A. Ahmad, J. de Souza Cunha, A. Bronowska
- 260.** Next generation of ADMETox dashboard for drug discovery: Learnings and recommendations. **B. Bhatarai**, G. Gerebtzoff, J. Berghausen
- 261.** Conformational analysis and investigation of energetics of the human AhR PAS-B domain: Impact on druggability. **S. Reznikov**, J. de Souza Cunha, A. Bronowska
- 262.** Explicit solvent effects on the excited state of p-phenylene vinylene. **D.A. Tracy**, A.E. Roitberg
- 263.** Force field complexity assessed via Bayesian inference and reversible jump Monte Carlo sampling. **O. Madin**, R. Messerly, M.R. Shirts
- 264.** Targeting glioblastoma cancer stem cell derived neurospheres: From phenotypic screen to target identification. **S. Bahmanyar**, D.S. Mortensen, V. Plantevin-Krenitsky, b. whitefield, E. Torres, V.H. Grant, J. Parnes, J. Brazeau, J. Young, K. Leftheris, S.E. Swift, B. Gaffney, D. Zhu, D. Mikolon, G. Deyanat-Yazdi, L. Wong, T. Tran, J. Boylan, A. Wurmser
- 265.** D3R Grand Challenge 4: Pose prediction and affinity ranking for BACE-1 inhibitors using ligand similarity and MM-GBSA calculations. **L. El Khoury**, S. Sasmal, D.L. Mobley
- 266.** Data analysis of various homo-peptide repeats in proteins associated with degenerative diseases. **Q. Price**, D. Tandabany
- 267.** Effects of electrostatic fields on the stability and reactivity of iron-sulfur clusters. **S. Gaughan**, J.D. Hirst, A. Croft, C.M. Jaeger
- 268.** How does prenylated flavin mononucleotide biosynthesis occur? Computational study. **S. Zaczek**, A. Dybala-Defratyka
- 269.** Band-gap opening and optical properties of graphene binding with low-concentration fluorine. **Y. Duan**, B. Chorpening, C. Stinespring
- 270.** Influenza virus glycosylation: Impact on virulence and transmissibility revealed by all-atom mesoscale simulations. **L. Casalino**, C. Seitz, M.O. Altman, I.A. Wilson, R.E. Amaro
- 271.** D3R Grand Challenge 4: Blind prediction of protein-ligand poses and affinity predictions. **Z. Gaieb**, C. Parks, M. Chiu, H. Yang, C. Shao, P. Walters, R.A. Lewis, S.D. Bembenek, S.K. Burley, R.E. Amaro, M.K. Gilson
- 272.** Controlling emission energies in functionalized carbon nanotubes. **B.J. Gifford**, S.K. Doorn, S. Tretiak
- 273.** Modeling coordinated conformational changes and interaction networks in alpha subunit of tryptophan synthase. **Y. Bosken**, D.D. Boehr, C. Chang
- 274.** MB-nrg doesn't work by accident!. **C. Egan**, B. Bizzarro, M. Riera, F. Paesani
- 275.** Computational predictions of drug binding kinetics with a multiscale molecular dynamics, Brownian dynamics, and milestoning approach. **B.R. Jagger**, C.T. Lee, R.E. Amaro
- 276.** viewSq: VMD module for visualizing and quantifying periodic atomic ordering underlying static structure factors from molecular dynamics simulations. **T. Mackoy**, B. Kale, M.E. Papka, R.A. Wheeler
- 277.** Structure-property relationship of high-spin state donor-acceptor (DA) polymers: Computational study. **M. Sabuj**, O. Muoh, N. Rai
- 278.** Improving force fields by identifying and characterizing small molecules with parameter inconsistencies. **J. Ehrman**, V.T. Lim, C.C. Bannan, N. Thi, D. Kyu, D.L. Mobley
- 279.** Multi-state QM/QM extrapolation of UV/Vis absorption spectra with point charge embedding. **K. Zhang**, S. Ren, M. Caricato
- 280.** Modeling crystallization pathways of polymorphic materials: Enhanced sampling techniques and method development. **T.D. Janicki**, J.R. Schmidt
- 281.** Curious case of DMSO: A computational study. **L. Olive**, E.V. Dornshuld, C.E. Webster
- 282.** Virtual screening and *de novo* drug design with machine learning. **C. Parks**, Z. Gaieb, R.E. Amaro
- 283.** Identification and characterization of small molecule inhibitors of Zika virus glycoprotein E. **S. Telehany**, M. Humby, D. McGee, A. Jacobs, R.C. Rizzo
- 284.** Connecting wave function and ensemble DFT methods through inversion of model systems. **V. Martinetto**, A. Pribram-Jones
- 285.** Efficient fitting of a density function theory energy curve using active learning. **T. Loeffler**, H. Chan, S. Sankaranarayanan
- 286.** Optimizing Lennard-Jones parameters by coupling nano- and macroscale target data using user-guided numerical algorithms. **R. Strickstock**, M. Huelsmann, D. Reith, K.N. Kirschner
- 287.** Withdrawn
- 288.** Mechanisms for the transduction of light and chemical energy into molecular motion. **M. Feng**, M.K. Gilson
- 289.** Probing binding modes of dye molecules on semiconductor surface and their dynamics. **M. Huda**, N. Rai

- 290.** Computational investigations on the structure-function relationship of rubisco activase from tobacco. **P. Khakbaz**, D. Shukla
- 291.** Thermal adiabatic connection for the uniform gas. **B. Harding**, A. Pribram-Jones
- 292.** Waterkit: Fast method for estimating receptor desolvation free energy. **J. Eberhardt**, S. Forli
- 293.** Comparing the stability of the sarcin/ricin domain and A-form RNA using adaptively biased molecular dynamics. **J.M. Imamoto**, M.F. Bruist
- 294.** Effects of spin contamination on the potential energy surfaces of water splitting catalysis by tungsten-oxide clusters. **A. Zamani**, H.P. Hratchian
- 295.** Reduced RAM access algorithm for molecular orbital electron repulsion integrals with resolution of the identity applied in post Hartree-Fock methods. **J. Lew Yee**, R. Flores Moreno, J. Martín del Campo Ramírez
- 296.** Calculating 1-octanol/water and hexadecane/water partition coefficients for small molecules. **S. Sasmal**, A. Nguyen, D.L. Mobley
- 297.** Molecular insights into the activity and structural impacts of enzymes across the changing pH environment in marine aerosol particles. **N.A. Wauer**, A. Dommer, R.E. Amaro
- 298.** Effects of the crystal packing of homo-halogenated benzenes on their electronic properties. **K. Pearce**, B. Schatschneider
- 299.** Fitting improper torsion parameters for atomistic force fields. **J. Maat**, C.C. Bannan, V.T. Lim, D.L. Mobley, B. Tjanaka, L. Wang, C.I. Bayly
- 300.** Intrinsic conductivity and small polaron formation in normal spinel ZnFe₂O₄ from first-principles. **R. Leano**, T. Smart, Y. Ping
- 301.** Computational models for activated human MEK1: Identification of key active site residues and interactions. **K.R. Sabsay**, R.T. Lee, L.M. Ravatt, J.P. Oza, A. Ringer McDonald
- 302.** Towards improved accuracy in calculation of binding thermodynamics. **S. Kantonen**, H. Muddana, M.K. Gilson
- 303.** New integrator framework for GROMACS. **P.T. Merz**, M.J. Abraham, M.R. Shirts
- 304.** Determining the effect of hydration shell on the spectra of proteolysis targeting chimera MD-224 by efficiently sampling conformations using the effective stochastic potential method. **J. Scher**, A. Chakraborty
- 305.** Characterization of active site and distal residues in the human ornithine transcarbamylase. **S. Watson**, P.J. Beuning, M. Ondrechen
- 306.** Mechanistic study of isotactic propylene oxide polymerization by a flexible bimetallic Cr(III) catalyst. **A.K. Roessler**
- 307.** Assessment for the inclusion of liquid-phase chemistry in automatic kinetic model generation. K. De Ras, **R. Van de Vijver**, F.H. Vermeire, G.B. Marin, K. Van Geem
- 308.** Withdrawn
- 309.** Many-body effect in the selectivity of calcium-binding proteins. **Z. Jing**, P. Ren
- 310.** Withdrawn
- 311.** Computational design of foldamer based water channels. **S. Houshyar Azar**, V. Pophristic, Z. Liu
- 312.** Natural transition orbitals for complex 2-component TDDFT. **J.M. Kasper**, X. Li
- 313.** Excited state calculations using multiconfiguration pair-density functional theory: Successes and challenges. **P. Sharma**, V. Bernales, D.G. Truhlar, L. Gagliardi
- 314.** Multiconfigurational pair-density functional theory: Strong-correlation method in quantum chemist's toolbox. **M. Mostafanejad**, A.E. DePrince
- 315.** Deciphering biomolecular corona formation on coated nanoparticles through all-atom molecular dynamics and dissipative particle dynamics simulations. **G. Chong**, M. Wu, I.U. Foreman-Ortiz, C. Allen, E. Tollefson, E.E. Carlson, J.A. Pedersen, C.J. Murphy, R. Hernandez
- 316.** Using coarse-graining and maximum entropy method to study A β aggregation. **D.B. Amirkulova**
- 317.** Building accurate and fast implicit solvation models. **I.S. Tolokh**, A. Mukhopadhyay, A.V. Onufriev
- 318.** Towards predictive chromatography: Computationally directed separations for efficient drug design and production. **L.D. Bishop**, N. Moringo, A. Misiura, C.F. Landes
- 319.** SkeleDock: New scaffold docking based algorithm. **A. Varela Rial**, G. De Fabritiis
- 320.** LigVoxel: Inpainting binding pockets using 3D-convolutional neural networks. **A. Varela Rial**, G. De Fabritiis
- 321.** Reactive docking: HTVS of covalent binders for *in silico* proteomics. **S. Forli**, G. Bianco, K.M. Backus
- 322.** Drug design using virtual reality: Free energy calculation of pathways generated from interactive molecular dynamics. **S.R. Hare**, D.R. Glowacki, B.K. Carpenter
- 323.** Exploration of the potential of mean force (PMF) method applied to the study of protein:ligand binding using the movable type method. **L. Westerhoff**, Z. Zheng, K.M. Merz
- 324.** Predicting plasticity of ligand-unbinding transition states for a library of minutes-scale k_d inhibitors. **S.D. Lotz**
- 325.** Non-covalent interactions in carbonyl complexes of Mn: Theoretical QTAIM study. **J.F. Van Der Maelen**, J. Ruiz

- 326.** Withdrawn
- 327.** Mechanism of spin-dependent electron transfer on ferromagnetic interfaces: *Ab initio* study. **S. Ghan**, K.U. Reuter, H. Oberhofer
- 328.** Electronic structure of metal-organic frameworks. **R. Chakraborty**, J.R. Long, M.P. Head-Gordon
- 329.** Spin-flip EOM-CCSD investigation of g-tensors in spin-frustrated systems. **S. Kaehler**, A. Krylov
- 330.** Beyond property prediction: What can machine learning do for virtual screening of transition metal complex space?. **J.P. Janet**, C. Duan, A. Nandy, H.J. Kulik
- 331.** Quantum mechanical studies of the depolymerization of lignin by the ZnCl₂: Ethylene glycol deep eutectic solvent (DES). **A. Landera**, A. George, L. Das, J. Gladden
- 332.** Automated generation of metal-doped amorphous silica clusters. **A. Jystad**, P.N. Wimalasiri, W.H. Thompson, M. Caricato
- 333.** Streamlining the exploration of chemical space for aqueous molecular metal oxides as thin film precursors. **A.J. Achazi**, P. Miro
- 334.** Exploring magnetic responses of transition metal complexes. **S. Sun**, X. Li
- 335.** Strong correlation in transition metals with adaptive sampling configuration interactions. A. Aldossary, **R. Chakraborty**, N. Tubman, D. Hait, M.P. Head-Gordon
- 336.** Multiconfigurational calculations on bimetallic decorated NU-1000 for C–H activation and comparison with DFT. **C. Gaggioli**, J. Sauer, L. Gagliardi
- 337.** Spin-flip Bethe–Salpeter equation approach and applications to simple molecular systems. **B.A. Barker**, D.A. Strubbe
- 338.** Computational study of the reactivity and stability of dinuclear heterogeneous catalysts on metal oxide supports. **K. Yang**, V.S. Batista
- 339.** Computational investigation of domain registration of membrane rafts. **P.B. Moore**, N. Chen
- 340.** Mechanistic elucidation of transition metal-catalyzed bond activations by quantum chemical simulation. **X. Hong**
- 341.** Chemical activation and allosteric modulation of mechanosensitive Piezo1 channel. **Y.L. Luo**
- 342.** Advancing nonadiabatic molecular dynamics methods and software for condensed matter and nanoscale systems. **A.V. Akimov**
- 343.** Clean and simple wave function interpretation with intrinsic bond orbitals: From [F–H–F]– to proton coupled electron transfer in enzymes. **G. Knizia**
- 344.** On the role of noncovalent interactions in the initial aggregation of dipeptide-based nanostructures. **M.L. Mayes**, L. Perreault, B. Visayas
- 345.** Absolute binding free energies from binding free energies to multiple rigid receptor conformations. **D.D. Minh**
- 346.** Withdrawn
- 347.** Enhanced sampling methods to resolve thermodynamics and kinetics of slow and rare biophysical processes. **H. Vashisth**
- 348.** Identifying metrics governing the non-native structure evolution in ionic liquid-ionic liquid mixtures from molecular simulations. **J. Shah**, U. Kapoor
- 349.** Modeling electron detachment in metal oxide and metal boride clusters. **H.P. Hratchian**
- 350.** Combinatorial reaction searches on the PES using KinBot. **R. Van de Vijver**, J. Zádor, G.B. Marin, K. Van Geem
- 351.** Modelling nonelectrostatic solute-solvent interactions in continuum embedding. C. Hille, S. Ringe, **J. Filser**, M. Deimel, C. Kunkel, W.E. Acree, K.U. Reuter, H. Oberhofer
- 352.** Excitation energies from linear response theories with localized orbitals scaling correction in density functional theory. **J. Li**, N. Su, Y. Jin, W. Yang
- 353.** Application of computational reaction modeling to the development of pharmaceuticals. **C. Lam**
- 354.** How to fix CO₂ with four amino acids: Enoyl-CoA carboxylase/reducase QM/MM study. **E. Vohringer-Martinez**, D. Saez
- 355.** Understanding the nature of weak interactions between functionalized boranes and N₂/O₂, promising functional groups for gas separations. **J. Townsend**, K.D. Vogiatzis
- 356.** Efficient and accurate estimation of free energy profiles for Kemp elimination reactions. **X. Pan**, Y. Mei, Y. Shao
- 357.** Theoretical design and analysis of high-spin state donor-acceptor (DA) polymers. **M. Sabuj**, M. Huda, N. Rai
- 358.** Towards density functional approximations from coupled cluster correlation energy densities. J. Margraf, **C. Kunkel**, K.U. Reuter
- 359.** Withdrawn
- 360.** Performance of Dunning, Jensen, and Karlsruhe basis sets on computing relative energies and geometries of minima and transition states. **K.N. Kirschner**, D. Reith, W. Heiden
- 361.** Impurities limit the capacitance of carbon-based supercapacitors. **T.T. Duignan**, X. Zhao
- 362.** *In silico* prediction of O⁶-methylguanine-

- DNA methyltransferase inhibitory potency of base analogs with QSAR and machine learning methods. **S. Guohui**, T. Fan, X. Sun, Y. Hao, X. Cui, L. Zhao, T. Ren, Y. Zhou, R. Zhong, Y. Peng
- 363.** Scaling up quantum chemistry simulation: Error control and automation. **F. Liu**, H.J. Kulik
- 364.** Modeling the interaction between EG₆ coated gold nanoparticles and cytochrome c. **C.A. Daly**, C.R. Allen, N. Rozanov, G. Chong, J.A. Pedersen, C.L. Haynes, E.E. Carlson, R. Hernandez
- 365.** Exploring large combinatorial chemical spaces to accelerate drug discovery with multisite λ -dynamics. **J.Z. Vilseck**, R. Hayes, N. Sohail, K. Armacost, C.L. Brooks
- 366.** Improvement of the GEM polarizable water model: Importance of the dispersion energy. **S. Naseem Khan**, G.A. Cisneros
- 367.** Design principles for gas activation, storage, and transport in metal organic frameworks. **R. Chakraborty**, J.R. Long, M.P. Head-Gordon
- 368.** Withdrawn
- 369.** Computational structure prediction of arylamide foldamer helices encapsulating monosaccharides. **S. Makeneni**, Z. Liu, V. Pophristic
- 370.** Computational study of water oxidation on metal oxide surfaces and its implication for efficient solar fuel production. **K. Yang**, V.S. Batista
- 371.** Withdrawn
- 372.** Investigating the role of linkers in the conformation of triazine-based sequence-defined polymers. **S. Ahn**, J.W. Grate
- 373.** Quantum calculations of reactions on interstellar ice-covered surfaces. **A. Lamberts**
- 374.** Improvements in symmetry-adapted perturbation theory (SAPT): Accurate separation of polarization and charge transfer terms. **S. Naseem Khan**, N. Gresh, A.J. Misquitta, J.A. Piquemal
- 375.** Methane activation by an iron atom supported on graphene. **C. Wu**, I.D. Gates
- 376.** Secret dance in Parkinson's disease: *In situ* structure determination of a pathological mutant of LRRK2 bound to microtubules. **M. Audagnotto**, K. Lasker, R. Watanabe Castillon, R.E. Amaro, R. Buschauer, J. Bohning, D. Boassa, S.S. Taylor, E. Villa
- 377.** Using domain-aware machine learning to forecast aqueous iodine reactions. **J. Bilbrey**, C. Ortiz Marrero, M. Schram, R. Rallo
- 378.** Modeling the effects of protein mutations towards target specificity in CRISPR/Cas9-based genome editing. **A. Ray**, R. Di Felice
- 379.** Absolute binding free energy predictions for heat shock protein 90 (Hsp90) complexes. **L. El Khoury**, J. Hariyanto, D.L. Mobley
- 380.** Parameterization of lamotrigine using quantum mechanical calculations. **S. Darancou**, S.T. Shipman
- 381.** On the origin of circularly-polarized luminescence from achiral polymers. **B. Laidlaw**, T. Penfold
- 382.** Withdrawn
- 383.** Sampling binding modes of flexible ligands using nonequilibrium candidate Monte Carlo. **S. Sasmal**, D.L. Mobley
- 384.** Pressure and temperature effects in *Escherichia coli* and *Moritella profunda* dihydrofolate reductase. **Q. Huang**, J.M. Rodgers, R.J. Hemley, T. Ichiye
- 385.** From structure to molecular flux: Predicting compound permeability in Gram-negative bacteria. **S. Acosta-Gutierrez**
- 386.** Protracted colored noise dynamics in polymer simulation. A. Peters, B. Nation, C. Henderson, **P.J. Ludovice**
- 387.** Probing the early stage of aggregation of low molecular weight gelator (12-hydroxyoctadecanamide) in organic solvents. **M. Huda**, N. Rai
- 388.** Molecular dynamics simulations reveal the mechanism of agonist ligand binding to ERR α . **L. Hegazy**
- 389.** Highly efficient conformational sampling of *in vivo* SERCA activator CDN1163 for determination of thermal and solvent effects on its excited state properties. **J. Scher**, A. Chakraborty
- 390.** Divergent ligand binding mechanisms in *Arabidopsis thaliana* and *Striga hermonthica* strigolactone receptors. **J. Chen**, D. Shukla
- 391.** Microphysical climate-relevant properties of model marine aerosols surfaces explored with GPU-accelerated all-atom molecular dynamics. **A. Dommer**, R.E. Amaro
- 392.** Exploring sequence-to-sequence learning methods for end-to-end, complete protein structure prediction. **J. King**, P. Francoeur, D. Koes
- 393.** Rational engineering of CRISPR-based genome editors using computational methods. **K. Rallapalli**, F. Paesani
- 394.** Molecular basis of glucose transport in plants. **B. Selvam**, D. Shukla
- 395.** Characterizing the structural and chemical features of biological short hydrogen bonds. S. Zhou, **L. Wang**
- 396.** Molecules mimicking atoms: Case of solvated electron precursors. I. Ariyaratna, N. Khan, N. Almeida, **E. Miliordos**
- 397.** Embedded cluster density approximation for exchange-correlation energy. **C. Huang**
- 398.** Evidence for nitrogen-fluorine halogen

bonding in silver-initiated fluorination reactions. **S. Bidwell**, A.M. Hua, S. Baker, R. Baxter, H.P. Hratchian
399. Using computational chemistry to understand genomes. C.L. Mills, L.A. Ruffner, P.J. Beuning, **M.J. Ondrechen**

400. Improving precision in absolute binding free energy calculations by increasing the number of alchemical intermediates. **B. Xie**, D.D. Minh

401. Assessing the conformational equilibrium of carboxylic acid via quantum mechanical and molecular dynamics studies on acetic acid. **V.T. Lim**, C.I. Bayly, L. Fusti-Molnar, D.L. Mobley

402. Rapid evaluation of protein hydration layer dynamics using hydration shell structure. **J.N. Dahanayake**, E. Shahryari, K.M. Roberts, M.E.

Heikes, C. Kasireddy, K.R. Mitchell-Koch

SECTION A

San Diego Convention Center
TBD

NVIDIA GPU Award

M. E. Berger, C. L. Simmerling, *Organizers*

6:00 - 8:30

403. Efficient implementation of flexible integral-based Generalized Born implicit solvent model. **Y. Wang**, C.L. Brooks

404. GPU-accelerated constant pH and redox potential molecular dynamics: Exploring electrochemistry in AMBER. **V.D. Cruzeiro**, A.E. Roitberg

405. Revealing ALK-drug resistance mechanisms using GPU-driven molecular dynamics sampling. **Z. Zhao**, P. Bourne

406. Accelerating MM/PBSA calculation of protein-ligand binding on graphics processing units. **R. Qi**, A. Luo, H. Wei, R. Luo

407. Improving REMD efficiency with Monte Carlo moves using a structure reservoir. **K. Kasavajhala**, K. Lam, C.L. Simmerling

SECTION A

San Diego Convention Center
TBD

OpenEye Outstanding Junior Faculty Award

C. L. Simmerling, *Organizer*

6:00 - 8:30

408. Hierarchical simulation: Two different approaches and their applications to design complex biomaterials. X. Zhao, J. Ferrell, C. Liao, **J. Li**

409. Computational modeling of polariton chemistry. **J. Yuen Zhou**

410. Exploring graphene oxide-water interfaces: Computational investigation. **R. Kumar**

411. Wepy: Tool for exploring rough free energy landscapes. S.D. Lotz, N. Donyapour, N. Roussey, T. Dixon, **A. Dickson**

SECTION A

San Diego Convention Center
TBD

Wiley Computers in Chemistry Outstanding Postdoc Award

M. Cavalleri, C. L. Simmerling, *Organizers*

6:00 - 8:30

412. Photochemistry of conjugated systems with “black-box” multireference methods. **E. Sayfutyarova**, S. Hammes-Schiffer

WEDNESDAY MORNING – COMP

SECTION A

Omni San Diego Hotel
Gallery 2

Role of Water Phase in Molecular Biology: Importance of Water in Folding, Binding & Transport Phenomena

Biomolecular Recognition

E. Alexov, C. Chang, R. Luo, *Organizers*
A. Ma, *Presiding*

8:30 **413.** Can Google’s Alphafold discover new drugs?.
G. Wei

9:00 **414.** Predicting direct and water-mediated interactions in protein-protein complexes. **X. Zou**

9:30 **415.** Accelerating convergence of free energy computations with Hamiltonian simulated annealing of water. **W. Jiang**

10:00 Intermission.

10:15 **416.** Regulating protein-protein interactions by phosphorylation: New mechanism involving solvated electrostatic interactions. **C.B. Post**, D.P. Hua, C. Feng

10:45 **417.** Predicting metal ion dehydration in RNA structures. **S. Chen**

11:15 **418.** Roles of water molecules and shapes of compounds and DNA sequences in the design and analysis of sequence-specific minor groove complexes. **W. Wilson**, A. Paul, N. Harika, P. Guo, A. Kumar, D.W. Boykin

SECTION B
Omni San Diego Hotel
Gallery 3A

Drug Design

Free Energy Methods

M. R. Landon, Y. Tseng, *Organizers*
V. D. Cruzeiro, *Presiding*

- 8:30** **419.** No one-size-fits-all: Evaluation of free energy methods for drug discovery campaigns. **K. Armacost**, X. Yan, Z. Guo, E. Metwally, H. Gunaydin, B. Sherborne
- 8:55** **420.** Rigorous free energy perturbation approach to estimating relative binding affinities between ligands with multiple protonation and tautomeric states. **C. de Oliveira**, H. Yu, W. Chen, R. Abel, L. Wang
- 9:20** **421.** Assessing the role and impact of force field and charge model selection on free energy calculations using the movable type (MT) method. **O. Borbulevych**, Z. Zheng, L. Westerhoff
- 9:45** **422.** Computational design of a binding mode flip for the validation of a novel class of potent tri-vector cyclophilin inhibitors. A. De Simone, C. Georgiou, H. Ioannidis, A. Gupta, J. Juarez-Jimenez, D. Doughty-Shenton, E.A. Blackburn, M. Wear, J.P. Richards, P. Barlow, N. Carragher, M. Walkinshaw, A. Hulme, **J. Michel**
- 10:10** Intermission.
- 10:25** **423.** Exploring protein–ligand interactions using multilayer molecules-in-molecules (MIM) fragmentation-based approach. B. Thapa, **K. Raghavachari**
- 10:50** **424.** Free energy calculations with thermodynamic integration in MOE using AMBER. **M. Ebert**
- 11:15** **425.** Exploring combinatorial chemical spaces with a discrete-Gibbs sampler-based -dynamics approach. **J.Z. Vilseck**, X. Ding, R. Hayes, C.L. Brooks
- 11:40** **426.** Development and validation of a relative Free Energy Perturbation (FEP) workflow. **P. Raman**

SECTION C
Omni San Diego Hotel
Gaslamp 1

Exploring Transition Metal Chemistry & Spectroscopy with Quantum Chemistry

C. M. Aikens, N. Mayhall, *Organizers*
H. P. Hratchian, *Organizer, Presiding*

- 8:30** **427.** Addressing limitations of density functional theory for transition metal chemistry. **S. Mallikarjun Sharada**

- 9:05** **428.** Transition metal catalysts with complex electronic properties. **P.M. Zimmerman**
- 9:40** **429.** Automated generation of benchmark sets guided by a Bayesian decision maker. **C.J. Stein**, J. Proppe, T. Gaudin, R.J. Hickman, M.P. Head-Gordon, A. Aspuru-Guzik
- 10:05** Intermission.
- 10:25** **430.** Automated selectivity predictions for transition metal catalyzed reactions. **S.E. Wheeler**, V.M. Ingman, A.J. Schaefer
- 11:00** **431.** *In-situ* automated analysis and control of transition metal chemistry simulation. **F. Liu**, C. Duan, H.J. Kulik
- 11:35** **432.** Effect of localized states on exciton transfer in colloidal quantum dots. **T.G. Goldzak**, A.R. Mclsaac, T.A. Van Voorhis

SECTION D
Omni San Diego Hotel
Gaslamp 2

Molecular Mechanics

J. Shen, *Organizer*
E. Pecora de Barros, *Presiding*

- 8:30** **433.** Importance of data selection for machine learning-based atomistic potentials. **J.S. Smith**, B.T. Nebgen, N. Lubbers, S. Tretiak, K. Barros
- 9:00** **434.** Machine learning coarse-grained model for water. **H. Chan**, M. Cherukara, B. Narayanan, T. Loeffler, C. Benmore, S.K. Gray, S. Sankaranarayanan
- 9:20** **435.** Dynamic modes of ignition phenomena: Learning chemistry from data. **C. Brown**, R. Mohr, M. Alaghemandi, J. Green, I. Mezić
- 9:40** **436.** Topological coarse-graining: Building ultra efficient computer models of aggregation using network Hamiltonians. **G. Grazioli**, Y. Yu, M. Unhelkar, R.W. Martin, C.T. Butts
- 10:00** **437.** Automated protein coarse-grained force field optimisation using free energy simulations. **J. Caceres-Delpiano**, L. Wang, J.W. Essex
- 10:15** Intermission.
- 10:25** **438.** NAMD 2.13 and beyond: New features, larger systems, and faster GPU simulations. **J. Maia**, D. Hardy, B. Radak, J. Ribeiro, J. Stone, E. Tajkhorshid
- 10:45** **439.** Knowledge-based statistical scoring function for protein-DNA interactions with enhanced generalization for structural variation. **L. Qiu**
- 11:05** **440.** Rapid graph-based determination of mechanical coupling in proteins. **L.E. Johnson**, Q. Huang, B. Ginovska, A. Fenton, S. Rauegi
- 11:25** **441.** Physical validity in molecular simulations. **P.T. Merz**, M.R. Shirts

- 11:45 **442.** Benchmarking quantum chemistry methods for accurate fixed-charge electrostatic models. A. Zhou, M. Schauperl, L. Wang, **P.S. Nerenberg**
- 12:05 **443.** Accessible molecular modeling environment with VMD and NAMD. **J. Ribeiro**, E. Tajkhorshid

SECTION E

Omni San Diego Hotel
Gaslamp 3

Molecular Mechanics: Molecular Simulations for Materials Design

C. M. Aikens, J. Shen, *Organizers*
S. J. Dampf, *Presiding*

- 8:30 **444.** From quantum to continuum: Multi-scale modelling of nanocomposites. **P.V. Coveney**
- 9:00 **445.** Charge transport networks in amorphous organic semiconductors. **M. Matta**, R.J. Gowers, C.T. Chapman, G.C. Schatz
- 9:20 **446.** Solid-state electrolytes: Li-metal interfaces. **J.M. Seminario**, D.E. Galvez-Aranda
- 9:40 **447.** Metashooting: Tool for Investigating mechanisms of material conversion. **S. Leoni**
- 10:00 Intermission.
- 10:20 **448.** Advances in atomistic methods for materials chemistry. **S.B. Sinnott**
- 10:50 **449.** Withdrawn
- 11:10 **450.** Modeling variations in the composition of ionic liquid-solvent mixtures confined inside nanopores. **A. Fang**, A. Smolyanitsky
- 11:30 **451.** Molecular modeling of ionic liquid-based electrolytes. S. Schweizer, **D. Firaha**, M. Neumann, J. Hill
- 11:50 **452.** Influence of electronic polarization on the structure of ionic liquids. **J.G. McDaniel**

Computational Quantum Chemistry: From Promise to Prominence: A Symposium in Honor of Henry F. Schaefer

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Interface between Experiments & Modeling in Unraveling the Physical & Chemical Properties of Charged Droplets

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SECTION A

Omni San Diego Hotel
Gallery 2

Computational Studies of Water

T. P. Kurtzman, D. J. Sindhikara, *Organizers*
K. M. Hunter, *Presiding*

- 1:30 **453.** Empirical models of water at interfaces and around solutes. **T. Ichiye**
- 2:00 **454.** Role of the hydrogen bond network on the anomalies of water. **F. Martelli**
- 2:25 **455.** Role of entropy in connecting protein solvent shell structure and hydration dynamics. **J.N. Dahanayake**, K.R. Mitchell-Koch
- 2:45 **456.** Understanding the structure and dynamics of water confined inside metal-organic frameworks. **K.M. Hunter**, F. Paesani
- 3:00 **457.** Structural and thermodynamic information content of the three-body angle distribution of liquid water. **J. Monroe**, M. Shell
- 3:15 Intermission.
- 3:30 **458.** Polarizability, infrared, and Raman spectra of water from first-principles simulations using the SCAN exchange-correlation functional. M. LaCount, **F. Gygi**
- 4:00 **459.** Useful relationships between localized vibrational modes and anharmonic entropy. **S. Lu**, P.M. Zimmerman
- 4:20 **460.** Proton transport through carbon nanotubes: Multi-level quantum mechanics/molecular mechanics simulations with NAMD. **M. Spivak**, N. Aluru, E. Tajkhorshid
- 4:35 **461.** Solvation free energy calculations with quantum mechanics/molecular mechanics and machine learning models. **P. Zhang**, L. Shen, W. Yang

SECTION B

Omni San Diego Hotel
Gallery 3A

Drug Design

Applications of Machine Learning

M. R. Landon, Y. Tseng, *Organizers*
S. Lenka, *Presiding*

- 1:30 **462.** Mathematical deep learning for drug discovery. **G. Wei**
- 1:55 **463.** Combining structure-based convolutional neural networks and ligand-based methods to address kinase selectivity. **A. Rossi**, J. Sorenson, I. Wallach

- 2:20 **464.** High-throughput drug design and lead optimization with PlayMolecule. **F. Chevalier**, G. De Fabritiis
- 2:45 Intermission.
- 3:00 **465.** Systematic target deconvolution: Are we there yet?. **G. Zahoranszky-Kohalmi**, R. Guha, M.G. Cyr, C. Danchik, S. Fang, M. Henderson, A. Zakharov
- 3:25 **466.** Leveraging machine learning and the Free-Wilson approach in lead optimization: Efficient discovery of a new chemical class modulating the GABA_A α_5 receptor. **O. Hucke**, M. Bieler, J. Larsen, T. Dyhring, T.A. Jacobsen, K.S. Nielsen, H. Schauerte, Y. Cui, S. Peters, N. Heine, C. Eickmeier, R. Arban, F. Montel
- 3:50 **467.** Developing Kernel, a virtual assistant for medicinal chemistry discovery teams at Eli Lilly. **M.P. Baumgartner**, L. Vidler

SECTION C

Omni San Diego Hotel

Gaslamp 1

Exploring Transition Metal Chemistry & Spectroscopy with Quantum Chemistry

C. M. Aikens, H. P. Hratchian, *Organizers*N. Mayhall, *Organizer, Presiding*

- 1:30 **468.** Computational studies of the properties of transition metal and metal oxide clusters. **D.A. Dixon**
- 2:05 **469.** Accurate models of reaction mechanisms to understand activity and selectivity of catalytic organometallic complexes. R.C. Chapleski, S.B. Isbill, **S. Roy**
- 2:40 **470.** Combined methodological approach for configuration interaction of orthogonal and non-orthogonal SCF solutions. **A.D. Mahler**, L.M. Thompson
- 3:05 Intermission.
- 3:25 **471.** Quantum chemistry of strongly correlated transition metal systems with the Adaptive Sampling Configuration Interaction Self Consistent Field (ASCI-SCF) method. **D. Hait**, D.S. Levine, N. Tubman, K.B. Whaley, M.P. Head-Gordon
- 3:50 **472.** CASPT2 molecular geometries and electronic structures of transition metal complexes. **B. Vlaisavljevich**
- 4:25 **473.** When should we use relativistic methods for transition metals?. **X. Li**

Material Science

Light-Matter Interaction in Materials: MOFs & Separations

C. M. Aikens, *Organizer*H. Carson, *Presiding*

- 1:30 **474.** Design of new thermally activated delayed fluorescence materials for oled applications. R. Ozek, **V. Aviyente**, S. Catak, A. Monari
- 1:50 **475.** Theoretical insights into the mechanisms of aggregation-induced emission and photo/thermal E/Z isomerization of a cyanostilbene derivative. **N. Yamamoto**
- 2:10 **476.** Finding the right building blocks for molecular optimization: Mining a database of organic semiconductors. **C. Kunkel**, C. Schober, J.T. Margraf, K.U. Reuter, H. Oberhofer
- 2:30 **477.** Unlocking the electronic genome of functionalized polycyclic aromatic hydrocarbon molecules and crystals. C. Mora, S. Jezowski, K. Pearce, C. Pacheco, A. Cosley, H. Oberhofer, **C.U. Pomona**
- 2:50 **478.** Charge transfer in metal/organic semiconductor interfaces from quantum chemical calculations. **O. Ozelik**, F. Paesani
- 3:10 **479.** Chemistry of remotely separated species hybridized by strong light-matter coupling. **M. Du**, R. Florentino Ribeiro, L.A. Martínez-Martínez, Z. Hu, V.M. Menon, J. Yuen-Zhou
- 3:30 Intermission.
- 3:50 **480.** DFT+U within a numeric atom centered orbital framework and its intricacies. **M. Kick**, K.U. Reuter, H. Oberhofer
- 4:10 **481.** Metal-organic frameworks: From database to supramolecular effects in complexation. **A. Mitrofanov**, V. Korolev, E. Marchenko, N. Eremin, N. Andreadi, P. Matveev, N. Borisova, A. Eliseev, V. Tkachenko
- 4:30 **482.** Towards computational materials design of metal-organic framework semiconductors. **C.J. Muschielok**, H. Oberhofer
- 4:50 **483.** Efficient simulation of aerosol filtration. **D.R. Rottach**, Z. Lei
- 5:10 **484.** Computational modeling of mixing solids as high-performance CO₂ sorbents for capture technology. **Y. Duan**

SECTION E
Omni San Diego Hotel
Gaslamp 3

Molecular Mechanics: Conformational Dynamics of Receptors, Ion Channels & Transporters

J. Shen, *Organizer*

K. H. Burley, *Presiding*

- 1:30** 485. Understanding the early stages of rhodopsin activation by combining simulations and experiments. L. Salas Estrada, **A. Grossfield**
- 2:00** 486. What molecular dynamics simulations tell us about GPCRs. T.R. Clark, **P. Ibrahim**
- 2:20** 487. Allosteric transport in ion channels and receptors. S. Milenkovic, I. Bodrenko, **M. Ceccarelli**
- 2:40** 488. Understanding conformational plasticity in GPCR selective pathway activation. **S. Acosta-Gutierrez**, F.L. Gervasio
- 3:00** Intermission.
- 3:10** 489. Inactive state of dopamine D₂ receptor has multiple conformations. **L. Shi**
- 3:40** 490. Accelerated molecular dynamics samples slow conformational changes in apo REV-ERB α . **L. Hegazy**
- 4:00** 491. Understanding ligand selectivity in bitter taste receptors using multiscale molecular dynamics simulations. F. Fierro, A. Giorgetti, P. Carloni, W. Meyerhof, **M. Alfonso-Prieto**

Computational Quantum Chemistry: From Promise to Prominence: A Symposium in Honor of Henry F. Schaefer

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THURSDAY MORNING – COMP

SECTION A
Omni San Diego Hotel
Gallery 2

Computational Studies of Water

T. P. Kurtzman, D. J. Sindhikara, *Organizers*

S. Yue, *Presiding*

- 8:30** 492. Role of water in protein-ligand binding: Water locations, network binding free energies, and

- structure-activity relationships by grand canonical Monte Carlo. **J.W. Essex**, H. Bruce Macdonald, C. Cave-Ayland, G. Ross, M.L. Samways, R. Taylor
- 9:00** 493. Development and applications of water-pharmacophore. **A. Cho**, S. Jung, T.P. Kurtzman
- 9:30** 494. Equilibration of buried water molecules to enhance protein-ligand binding free energy calculations. **I.Y. Ben-Shalom**, C. Lin, T. Kurtzman, R. Walker, M.K. Gilson
- 9:50** 495. Development of a novel water model for molecular dynamics for IDPs: Presenting the CAIPi3P model. **J. de Souza Cunha**, F.S. Zariquiey, A. Bronowska
- 10:05** Intermission.
- 10:20** 496. All-atom molecular dynamics simulation of hygroscopicity in atmospheric aerosols. **D. Roston**
- 10:40** 497. New coarse-grained model for water with improved thermodynamic and structural properties: Bottom-up many-body projected water (BUMPer). **J. Jin**, G.A. Voth
- 10:55** 498. Direct inversion approach to local permittivity at liquid-liquid interfaces. **D. Egger**, C. Scheurer, K.U. Reuter
- 11:10** 499. Dynamic properties of aqueous electrolyte solutions from nonpolarizable, polarizable, and scaled-charge models. **S. Yue**, A. Panagiotopoulos

SECTION B
Omni San Diego Hotel
Gallery 3A

Material Science

2D Materials, Machine Learning, Phase Behavior & Surfaces

C. M. Aikens, *Organizer*

M. Du, *Presiding*

- 8:30** 500. Atomic and electronic structure of the edges of bulk and monolayer tin disulfide (SnS₂). **T. Yan**
- 8:50** 501. Uncovering the kinetics of sulfurization of molybdenum trioxide by elemental sulfur in the growth of two-dimensional molybdenum disulfide by powder vaporization. **T. Tsafack**, **S.F. Bartolucci**, **J.A. Maurer**
- 9:10** 502. Proper first-principles approach on charge-discharge behavior of 2D hetero-structure electrodes. **K. Yim**, C. Lee, R. Tamarany, H. Kim, C. Yoo, H. Yoon, P. Kim
- 9:30** 503. Computational study of MXene/epoxy nanocomposite interface and mechanical properties. **Y. Sliozberg**, J. Andzelm, L. Nataraj, C. Hatter, Y. Gogotsi, A. Hall
- 9:50** 504. Artificial intelligence guided material design and characterization. **T. Loeffler**, H. Chan, S. Sankaranarayanan

- 10:10 505.** Application of machine learning in separation processes using graphene-supported metallic clusters. **J. Zhang**, M. Nguyen, V. Glezakou
- 10:30** Intermission.
- 10:50 506.** Generating metastable phase diagrams of carbon using machine learning. **S. Srinivasan**, T. Loeffler, H. Chan, J. Wen, D. Luo, S. Sankaranarayanan
- 11:10 507.** Anisotropic growth of Pt on Pd nanocubes promotes direct synthesis of hydrogen peroxide. **M. Kim**, G. Han, X. Xiao, J. Song, H. Kim, J. Ahn, S. Han, K. Lee, T. Yu
- 11:30 508.** Assessing the structural stabilities of novel uranium materials with DFT and bond valence calculations. **A. Shields**, T.L. Spano, B.B. Anderson, R. Kapsimalis, A. Miskowicz, J.L. Niedziela
- 11:50 509.** First-principles guided discovery of novel bimetallic catalysts for direct synthesis of hydrogen peroxide. **S. Han**, B. Yeo, D. Kim
- 12:10 510.** Surface charge density and structure for coated gold nanoparticle models. **G. Chong**, E.D. Laudadio, M. Wu, C.J. Murphy, R.J. Hamers, R. Hernandez

SECTION C

Omni San Diego Hotel
Gaslamp 1

Quantum Mechanics

A. E. DePrince, H. P. Hratchian, *Organizers*
S. Bidwell, *Presiding*

- 8:30 511.** Advances in electron propagator theory. **H.H. Corzo**, M. Díaz-Tinoco, J.V. Ortiz
- 9:00 512.** Designed optically multiadaptive materials. **C.B. Rinderspacher**, R.H. Lambeth
- 10:00** Intermission.
- 10:15 513.** Reformulated analytical gradients for dynamically weighted complete active space self-consistent field. **W.J. Glover**
- 10:45 514.** CASPT2 geometries and energies of Fe(II) spin-crossover complexes. **B.A. Finney**, B. Vlasisavljevich
- 11:15 515.** Efficient semiempirical excited electronic state methods for photochemical studies of large systems. **C. Bannwarth**, T.J. Martinez

SECTION D

Omni San Diego Hotel
Gaslamp 2

Molecular Mechanics

J. Shen, *Organizer*
B. C. Taylor, *Presiding*

- 8:30 516.** Withdrawn

- 8:50 517.** Interaction of proteins with polyelectrolytes: Comparison of theory to experiment. **X. Xu**, M.M. Ballauff, J. Dzubiella
- 9:10 518.** Progresses in molecular dynamics simulation-directed rational design of intelligent nanoreceptors for chemosensing. X. Sun, L. Riccardi, F. De Biasi, F. Rastrelli, F. Mancin, **M. Devivo**
- 9:30 519.** Decryption of the diverse and complex movements in molecular machines. **W. Cai**, H. Fu, X. Shao
- 9:50 520.** Simulation of structure/property relationships in block copolymer photoresists for directed self-assembly. A. Peters, B. Nation, C. Breaux, J. Delony, C. Henderson, **P.J. Ludovice**
- 10:10** Intermission.
- 10:30 521.** Effect of tacticity and charge on solubilization free energy of synthetic anionic polyelectrolyte in water by molecular dynamics simulations. R. Chockalingam, **U. Natarajan**
- 10:50 522.** Computer led design of functional arylamide foldamers. **Z. Liu**, V. Pophristic, S. Makeneni, S. Houshyar Azar, P. Reagan, R. D'Elia
- 11:10 523.** 2D nanomembranes by design using lipid-like peptoids. **M.D. Baer**
- 11:30 524.** Nanoscale isolated island polymer brushes: Simulation study. **P.B. Moore**, A. Sidorenko

SECTION E

Omni San Diego Hotel
Gaslamp 3

Molecular Mechanics: Conformational Dynamics of Receptors, Ion Channels & Transporters

J. Shen, *Organizer*
A. Dommer, *Presiding*

- 8:30 525.** Molecular mechanisms of ion permeation and gating in ion channels. **R. Pomes**
- 9:00 526.** Computational study of changes in conformational dynamics of Piezo1 induced by Yoda 1 agonist binding and membrane tension. **W.M. Botello-Smith**, W. Jiang, Y.C. Lin, H. Zhang, Y.L. Luo, J. Lacroix, A. Ozkan
- 9:20 527.** Elucidating molecular mechanisms of anion channelrhodopsins to design new optogenetics tools. **J.M. Paggi**, R.O. Dror
- 9:40 528.** Exploring the acid resistance mechanism of electrogenic amino acid antiporters in food-borne pathogens using computational experiments. **M. Prevost**, G. Roos, E. Krammer
- 10:00** Intermission.
- 10:10 529.** Understanding coupled ion exchange in ClC antiporters from the kinetic landscape of Cl⁻/H⁺ exchange. **J.M. Swanson**

THURSDAY AFTERNOON – COMP

Computational Quantum Chemistry: From Promise to Prominence: A Symposium in Honor of Henry F. Schaefer

Sponsored by PHYS, Cosponsored by COMP

- 10:40 530.** Substrate-induced conformational transitions of the human serotonin transporter. **M. Chan**, B. Selvam, D. Shukla
- 11:00 531.** Structure and dynamics of the wild-type and mutant ABC transported CFTR as gleaned from MD simulations. **H. Senderowitz**, N. Khazanov, L. Simchaev, M. Zhenin

Computational Quantum Chemistry: From Promise to Prominence: A Symposium in Honor of Henry F. Schaefer

Sponsored by PHYS, Cosponsored by COMP

Chemometric Analysis for Aqueous Sample

Sponsored by ANYL, Cosponsored by COMP and ENVR

Interface between Experiments & Modeling in Unraveling the Physical & Chemical Properties of Charged Droplets

Sponsored by ANYL, Cosponsored by COMP, ORGN and PHYS

COMSCI COMMITTEE ON SCIENCE

M. Fisher, *Program Chair*

SUNDAY MORNING – COMSCI

Immersive Virtual Reality for Molecular Design

Sponsored by COMP, Cosponsored by CHED, CINF and COMSCI

TUESDAY MORNING – COMSCI

SECTION A

Omni San Diego Hotel
Grand Ballroom B

Water for Two Worlds

Technologies for Tomorrow

Cosponsored by MPPG

M. G. Kociolek, *Organizer*

T. H. Boyer, K. Linden, P. K. Westerhoff, *Presiding*

- 8:00** Introductory remarks.
- 8:10** **1.** Assessing the impact of wildfires on water quality and treatment. **F.L. Rosario**
- 8:45** **2.** Opportunities for building-scale urine diversion and challenges for implementation. **T.H. Boyer, D. Saetta**
- 9:20** **3.** Catalytic converters for water treatment. **M.S. Wong, K.N. Heck, S. Garcia-Segura, P.K. Westerhoff**
- 9:55** Intermission.
- 10:05** **4.** Electrochemistry at the membrane/water interface. **D. Jassby, X. Zhu**
- 10:40** **5.** Nanobubble technologies offer opportunities to improve water treatment. **P.K. Westerhoff, A. Atkinson, O. Apul, S. Garcia-Segura, O. Schneider**
- 11:15** **6.** Be prepared to address the challenges for two water supplies in China: Urban and rural communities. **C. Chen, P. Lin, X. Wu, X. Zhang**

TUESDAY AFTERNOON – COMSCI

SECTION A

Omni San Diego Hotel
Grand Ballroom B

Water for Two Worlds

Lighting the Way to Safe Water

Cosponsored by MPPG

M. G. Kociolek, *Organizer*

T. H. Boyer, K. Linden, P. K. Westerhoff, *Presiding*

- 1:30** Introductory Remarks.
- 1:35** **7.** Global drivers of antimicrobial resistance. **P.J. Vikesland, A. Pruden**
- 2:10** **8.** Thinking outside the treatment plant: UV for water distribution system disinfection. **K. Linden, N. Hull, V. Speight**
- 2:45** Intermission.
- 2:55** **9.** Water disinfection in rural areas demands unconventional solar technologies. **C. Chu, E. Ryberg, S.K. Loeb, M. Suh, J. Kim**
- 3:30** **10.** Photothermal membrane water treatment for two worlds. **Y. Jun, X. Wu, D. Ghim, Q. Jiang, S. Cao, S. Singamaneni**
- 4:05** **11.** Toward realizing multifunctionality: Photoactive and selective adsorbents for the removal of inorganics in water treatment. **L.N. Pincus, J.B. Zimmerman, A.W. Lounsbury**

CPRC

COMMITTEE ON PUBLIC RELATIONS AND COMMUNICATIONS

SUNDAY AFTERNOON – CPRC

**Celebrating Sir Martyn Poliakoff: From Blue
Matrix to Green Chemistry & Everything in
Between**

Sponsored by MPPG, Cosponsored by CPRC

CPRM

COMMITTEE ON PATENTS AND RELATED MATTERS

SUNDAY MORNING – CPRM

**Nothing New Under the Sun: The Practical
Challenges of Patent Novelty Searching**

Sponsored by CINF, Cosponsored by CHAL and CPRM

CTA

COMMITTEE ON TECHNICIAN AFFAIRS

SUNDAY MORNING – CTA

I&EC General Papers

Sponsored by I&EC, Cosponsored by CTA

SUNDAY AFTERNOON – CTA

I&EC General Papers

Sponsored by I&EC, Cosponsored by CTA

TUESDAY EVENING – CTA

I&EC General Posters

Sponsored by I&EC, Cosponsored by CTA

SUNDAY MORNING – ENFL

SECTION A

San Diego Convention Center
Room 23A2D Materials & Beyond: Innovative Materials,
Assemblies & Devices for Energy & FuelV. Barone, L. Hu, M. Song, *Organizers*Y. Lin, Y. Zhu, *Organizers, Presiding*

- 9:00 Introductory Remarks.
- 9:05 1. Controllable asymmetric functionalization of graphene oxide nanosheets in mass quantity. **W. Wang**, S. Chang
- 9:20 2. Catalytic cracking of JP-10 nanofluids with Pt nanoparticles over functionalized graphene oxide sheets. X. Jia, L. Wang, X. Zhang, **G. Liu**
- 9:35 3. Graphene-based supports decorated with functional transition metal oxides for hydrogen storage. Z. Gohari, Y. Yurum, **A. Yurum**
- 9:50 4. Electrodeposited niobium oxide films for electrical energy storage. **R.M. Penner**
- 10:25 5. Electronic structure underlying electrochemistry of 2D materials. **Y. Liu**
- 10:40 Intermission.
- 10:50 6. 2D semiconductor optoelectronics. **A. Javey**
- 11:25 7. Organic materials “beyond graphene” in electronic devices. **M. Bojdys**
- 11:40 8. Shape of things to come for 2D materials: Pentagonal layered PdSe₂ for electronics. **K. Xiao**, A. Oyedele, S. Yang, L. Liang, A. Puretzky, B. Sumpter, M.F. Chisholm, C. Rouleau, A. Li, D. Geohegan
- 12:05 9. Structure and properties of 2D semiconducting transition metal dichalcogenides grown by CVD for energy applications and opto-electronics. **J. Warner**
- 12:30 10. Unified understanding of the dielectric nature of 2D materials via electronic polarizability. **T. Tian**, D. Scullion, E. Santos, C. Shih

SECTION B

San Diego Convention Center
Room 23B

Advancing Innovative Battery Technologies

B. Liu, H. Pan, D. Wang, K. Xu, *Organizers*C. Ban, S. Meng, *Presiding*

- 9:00 Introductory Remarks.
- 9:05 11. Interfacial phenomena in all solid-state batteries. **S. Meng**
- 9:35 12. Innovations in processing of ceramics for solid-state batteries. **M. Doeff**
- 10:05 13. SnO/SnO₂ p-n junction interface design for high rate lithium-ion batteries. **J. Lee**
- 10:25 Intermission.
- 10:45 14. Interface science and engineering for stabilizing electrochemical materials. **C. Ban**
- 11:15 15. Layer-by-layer assembly and *in situ* multimodal analysis of electrochemical interfaces. **V. Murugesan**, V. Prabhakaran, S. Roy, K.T. Mueller
- 11:45 16. High-throughput computational design of electrode-electrolyte interface for solid-state lithium ion batteries. **C. Wang**, T. Mueller

SECTION C

San Diego Convention Center
Room 23CAtomic-level Understanding & Design of
Materials & Processes for Energy ApplicationsH. Zhuang, *Organizer*Y. Liu, *Organizer, Presiding*

- 9:00 Introductory Remarks.
- 9:05 17. Withdrawn
- 9:35 18. Fe_xNi_{1-x}O(H)_y nanoparticles for alkaline electrocatalysis: Understanding the chemical structure of complex nanocatalysts. **L.F. Greenlee**, P. Acharya, J. Chen, R.H. Manso
- 10:05 19. Design, synthesis, and characterization of organic semiconductors with high charge carrier mobility. W. Feng, T. Testoff, X. Zhou, **L. Wang**

- 10:35** **20.** Synthesis and evaluation of dipicolinic acid (DPA)-based interwell tracers for reservoir surveillance. **R. Shi**, G. Thomas, S. Chang, H. Ow
- 11:05** Intermission.
- 11:20** **21.** Understanding the surface dynamics of hydrogen and CO in the electrochemical reduction of CO₂. **M. Schreier**, M. Graetzel, Y. Surendranath
- 11:50** **22.** Glass transitions in water-lean CO₂ capture solvents: Influence of dynamic changes in mesoscopic structure. **D.J. Heldebrant**, J. Banuelos, D. Malhotra, M. Lee, M. Nguyen, D. Zhang, D.C. Cantu, V. Glezakou, R. Rousseau, T. Headen, R. Dalgliesh
- 12:20** **23.** Atomic layer deposition of FeS_x, CoS_x, and NiS_x for electrocatalysis. **X. Wang**

SECTION D

San Diego Convention Center
Room 24A

Hybrid Energy Techniques: Catalysts to Vehicle

V. Li, Q. Zhen, *Organizers*

S. Bashir, J. L. Liu, *Organizers, Presiding*

- 9:00** Introductory Remarks.
- 9:05** **24.** Ascorbate fuel cells with carbon electrodes and the role of isomers toward the oxidation of small organic molecules such as ascorbate. **J. Haan**, O. Muneeb, I. Chino, K. Hendrix
- 9:30** **25.** Unbiased solar H₂ production with current density up to 23 mA/cm² by swiss-cheese black Si coupled with wastewater bioanode. **W. Vakki**, **M. Fairchild**, **J. Gu**
- 9:55** **26.** Advanced coupling of energy storage and photovoltaics. **Q. Qiao**
- 10:20** **27.** Withdrawn
- 10:45** **28.** Current energy mix and techno-economic analysis of concentrating solar power (CSP) technologies. **N. Huda**
- 11:10** **29.** Electrocatalyst for improved performance of proton exchange membrane fuel cells. **J.L. Liu**
- 11:35** **30.** Should we be burning coal, gas or developing PV?. **S. Liu**, **J.L. Liu**
- 12:00** Concluding Remarks.

SECTION E

San Diego Convention Center
Room 24B

Innovative Chemistry & Materials for Electrochemical Energy Storage

H. Chen, W. Kan, F. Lin, W. Xu, *Organizers*

R. J. Clement, *Organizer, Presiding*

T. Liu, W. Wang, *Presiding*

- 9:00** Introductory Remarks.
- 9:05** **31.** Mining redox active materials for energy storage. **T. Liu**
- 9:35** **32.** Expanding cell potential of metal picolinamide redox carriers for flow cell applications. **G. Andrade**, **I. Popov**, **P. Yang**, **E.R. Batista**, **B.L. Davis**
- 9:50** **33.** Determining molecular design parameters for quinones used in organic redox flow batteries. **A. Nirmalchandar**, **A. Murali**, **B. Yang**, **S.G. Prakash**, **S.R. Narayan**
- 10:05** **34.** Redox-active organic substrates with potential applications in lithium ion and flow batteries. **A. Dumitrascu**, **A. Porath**, **A. Rajewski**, **J.G. Gillmore**, **T.F. Guarr**
- 10:20** **35.** Molecular engineering towards extremely high-potential catholyte for non-aqueous redox flow battery. **Y. Yan**, **S.G. Robinson**, **M.S. Sigman**, **M.S. Sanford**
- 10:35** **36.** Advanced redox flow battery technologies. **W. Wang**
- 11:05** Concluding Remarks.
- 11:10** Intermission.
- 11:25** Introductory Remarks.
- 11:30** **37.** Plasma exfoliation graphene wrapped MXene for supercapacitors application. **K. Wang**, **Q. Fan**
- 11:45** **38.** Novel silver nanoparticle deposition on a reduced graphene oxide composite for energy storage. **H.R. Tinker**, **Z. Guo**, **C.E. Knapp**
- 12:00** **39.** Hierarchical porous frameworks derived from covalent triazine frameworks for high mass loading supercapacitors. **D. Baumann**, **X. Duan**
- 12:30** **40.** 3D structure of MnO₂ nanowire for supercapacitor application. **A.H. Ghanim**, **J. Koonce**, **S. Mubeen**
- 12:45** Concluding Remarks.

SECTION F

San Diego Convention Center
Room 24C

Energy & Fuels Lectureship Award in Honor of Mark Thomas

Energy & Fuels Joint Excellence Publication Award

D. Dadyburjor, D. J. Heldebrant, H. Lin, *Organizers*

M. A. Reynolds, R. S. Weber, *Organizers, Presiding*

- 9:00** Introductory Remarks.
- 9:10** **41.** Adsorption at low concentrations: Environmental aspects and importance. **E. Suuberg**
- 9:40** **42.** Methane absolute adsorption in shale reservoirs: Central challenges arising from dual heterogeneity. **Z. Jin**

- 10:10** 43. From kerogen precursors to hydrocarbon expulsion: Insights from atomistic simulations. **J. Leyssale**
- 10:40** 44. Isolation and reactivity of kerogen prepared by various methods. **A. Chaffee**
- 11:10** 45. High-pressure methane adsorption and characterization of pores in Posidonia shales and isolated kerogens. T. Rexer, E.J. Mathia, A.C. Aplin, **K.M. Thomas**
- 11:55** Discussion.
- 12:40** Concluding Remarks.

SECTION G

San Diego Convention Center
Room 25A

Hybrid Organic-Inorganic Semiconductors for Energy

Hybrid Perovskite Materials

M. C. Beard, Y. Yan, *Organizers, Presiding*

- 9:00** Introductory Remarks.
- 9:05** 46. Intricacies of halide ion mobility in metal halide perovskites. **P.V. Kamat**, R. Scheidt
- 9:35** 47. Two-dimensional organic-inorganic hybrid perovskites: Phases, orientation, and organic cations. **W. You**, J. Hu, L. Yan
- 10:05** 48. Unique defect properties in metal halide perovskites. **Y. Yan**
- 10:35** Intermission.
- 10:45** 49. Dynamic disorder dominates delocalization transport and recombination in halide perovskites. **J.B. Asbury**
- 11:15** 50. Perovskite for photocatalytic organic synthesis. X. Zhu, J. San Martin, **Y. Yan**
- 11:45** 51. Solar quantum cutting using ytterbium-doped metal-halide perovskites. **D.R. Gamelin**
- 12:15** 52. Understanding photocatalytic reaction on CsPbBr₃ nanocrystals through ultrafast spectroscopy and surface design. **H. Lu**, M.C. Beard
- 12:35** Concluding Remarks.

SECTION H

San Diego Convention Center
Room 25B

Understanding of Energy Materials with Advanced Computation & Characterization

L. Cheng, *Organizer*

T. Li, H. Zhao, *Organizers, Presiding*

- 9:00** Introductory Remarks.
- 9:05** 53. *In-situ* and *operando* characterization of battery materials using synchrotron x-ray and neutron diffraction techniques. **Y. Ren**

- 9:35** 54. Power of *in-situ* X-ray methods to understand energy materials. **R.E. Winans**, T. Li, S. Lee, S. Lee
- 10:05** 55. Heterogeneous reactions in battery electrodes under dynamic cycling. **K.W. Chapman**
- 10:35** Intermission.
- 10:50** 56. Investigating the tetragonal/cubic phase transformation using *in situ* high-energy x-ray diffraction. H. Nguyen, T. Li, **Z. Chen**
- 11:20** 57. Application of *in-situ* advanced x-ray spectroscopy on energy materials. **C. Sun**
- 11:50** 58. Unraveling the mechanism of energy storage in batteries. **P. Chupas**
- 12:20** 59. Design, synthesis, and application of 3D graphene for energy conversion and storage. **Y.H. Hu**
- 12:40** Concluding Remarks.

Catalysis at Metal-Support Interfaces

Sponsored by CATL, Cosponsored by ENFL

Future Insights into Syngas Conversion Catalysis: Symposium in honor of Burtron H. Davis

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

Solvent Effects in Metal-Catalyzed Reactions

Sponsored by CATL, Cosponsored by ENFL and PHYS

Advances in Catalysis with Ceria & Other Reducible Oxides

Model Ceria Catalyst

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

SUNDAY AFTERNOON – ENFL

SECTION A

San Diego Convention Center
Room 23A

2D Materials & Beyond: Innovative Materials, Assemblies & Devices for Energy & Fuel

L. Hu, Y. Lin, M. Song, *Organizers*

V. Barone, Y. Zhu, *Organizers, Presiding*

- 2:00** Introductory Remarks.
- 2:05** 60. Strategies for chemical modification of semiconducting 2D metal chalcogenides: Functionalization, transformation, and self-assembly. **Q. Wang**

- 2:30** **61.** Pillared structure design of MXene with controlled interlayer spacing for high performance lithium/sodium-ion storage. **J. Luo**, W. Zhang, X. Tao, W. Li
- 2:45** **62.** 2D MXenes as building blocks for assembly of high performance electrodes. **M. Beidaghi**
- 3:10** **63.** 3D bicontinuous nanoporous graphene for energy conversion and storage. **M. Chen**
- 3:40** **64.** Functional 2D materials for high-performance Li/S batteries. **Y. Zhang**
- 4:05** Intermission.
- 4:10** **65.** High rate charge storage mechanisms in MXenes. **Y. Gogotsi**, J. Tang, T. Mathis, N. Kurra
- 4:40** **66.** Ultracapacitive energy storage using 2D nanomaterials under extreme conditions. **H. Park**
- 5:05** **67.** Enabling dense and porous electrodes by holey graphene. **Y. Lin**, J.W. Connell
- 5:30** **68.** Optimized processing of carbon nanotube fibers for increased electrical conductivity. **V. Gangoli**, C. Barnett, A.R. Barron
- 5:45** **69.** Laser annealing improves photoelectrochemical activity of ultrathin MoSe₂ photoelectrodes. **L. WANG**, J. Sambur

SECTION B

San Diego Convention Center
Room 23B

Advancing Innovative Battery Technologies

B. Liu, H. Pan, D. Wang, K. Xu, *Organizers*
C. S. Johnson, H. Peng, *Presiding*

- 2:00** **70.** Energy storage and conversion in 1D devices. **H. Peng**
- 2:30** **71.** One-dimensional nanomaterials for emerging energy storage. **L. Mai**
- 3:00** **72.** Structural engineering of high-performance electrodes for potassium ion storage. **J. Xu**
- 3:20** Intermission.
- 3:40** **73.** Developing flexible energy storage devices for wearable electronics. **G. Shen**
- 4:10** **74.** Where are sodium-ion batteries headed? An analysis of their future. **C.S. Johnson**
- 4:40** **75.** Pillared MXene with ultralarge interlayer spacing as a stable matrix for high performance sodium metal anodes. **J. Luo**, X. Tao, W. Li

SECTION C

San Diego Convention Center
Room 23C

Atomic-level Understanding & Design of Materials & Processes for Energy Applications

Y. Liu, *Organizer*
H. Zhuang, *Organizer, Presiding*

- 2:00** Introductory Remarks.
- 2:05** **76.** Towards atomic intercalation of the entire periodic table. **K.J. Koski**
- 2:35** **77.** Polymer-templated, porous composites for energy storage. **Y. Zhu**
- 3:05** **78.** Design and synthesis of 2D transition metal carbides and nitrides (MXenes). K. Hantanasirisakul, X. Xiao, P. Urbankowski, B. Anasori, T. Tan, N. Frey, V. Shenoy, **Y. Gogotsi**
- 3:35** Intermission.
- 3:50** **79.** Energy conversion using inorganic nanolayers made from a single element. **F. Geiger**, T.F. Miller, E. Lozier, M. Boamah
- 4:20** **80.** Design of electrocatalysts at atomic scale. P. Papa Lopes, N. Becknell, D. Jung, D. Strmcnik, N. Markovic, **V. Stamenkovic**
- 4:50** **81.** Small molecule molybdenum sulfide compounds as low-cost hydrogen-evolution catalysts. R. Lalisce, B.R. Garrett, S.M. Polen, Y. Wu, **C.M. Hadad**
- 5:20** **82.** Surface reconstruction of ternary oxide catalysts: Does surface facet still matter?. **Z. Wu**

SECTION D

San Diego Convention Center
Room 24A

Hybrid Energy Techniques: Catalysts to Vehicle

S. Bashir, V. Li, Q. Zhen, *Organizers*
J. L. Liu, *Organizer, Presiding*
S. Liu, *Presiding*

- 2:00** Introductory Remarks.
- 2:05** **83.** Electrochemical Interfaces for energy conversion and storage. **D. Strmcnik**, N. Markovic, P. Papa Lopes, V. Stamenkovic
- 2:50** **84.** Transition of nanomaterials chemical synthesis to manufacturing. **R. Wang**, H. Li, P. Papa Lopes, D. Strmcnik, N. Markovic, V. Stamenkovic
- 3:35** **85.** Materials for fuel cells and batteries in hybrid vehicles. **P. Papa Lopes**, D. Strmcnik, N. Markovic, V. Stamenkovic
- 4:20** Intermission.
- 4:25** **86.** Withdrawn
- 5:10** **87.** Design of photovoltaics based manufacturing system using computer-aided design (CAD). **J.S. Aguilar**
- 5:55** Concluding Remarks.

SECTION E
San Diego Convention Center
Room 24B

Innovative Chemistry & Materials for Electrochemical Energy Storage

R. J. Clement, W. Kan, F. Lin, W. Xu, *Organizers*

H. Chen, *Organizer, Presiding*

J. Guo, *Presiding*

- 2:00** Introductory Remarks.
- 2:05** **88.** Multialkali ion intercalation reactions make feasible higher energy density cathodes. **M.S. Whittingham**
- 2:45** **89.** Plasma-polymerized C₆₀ as an elastic matrix integrated Sn nanoparticles anode for lithium-ion batteries. **R.E. Ardhi**, G. Liu, M. Tran, C. Hudaya, J. Kim, J. Lee
- 3:00** **90.** Flexible, fiber-shaped, high-performance energy storage devices. **B. Wang**
- 3:15** **91.** Low-cobalt cathodes for lithium-ion batteries. **A. Manthiram**
- 3:45** **92.** Ion-conducting protective layer for NCA cathodes to enhance the capacity and stability of Li-ion batteries. A. Yigitalp, A. Tasdemir, S. Alkan Gürsel, **A. Yurum**
- 4:00** Intermission.
- 4:15** **93.** Electrodeposited lithium and sodium battery electrodes. **P.V. Braun**
- 4:45** **94.** Silicon-carbon composite anode materials towards practical standards. **J. Guo**
- 5:15** **95.** Superconcentrated aqueous electrolytes: Electrochemistry and applications in rechargeable batteries. **D. Belanger**
- 5:30** **96.** Intrinsically flexible redox-active polyurethanes for electrochemical energy storage. **D.G. Mackanic**, Y. Cui, Z. Bao
- 5:45** Concluding Remarks.

SECTION F
San Diego Convention Center
Room 24C

Sustainable Energy & Water via Innovative Electrocatalytic, Photocatalytic & Hybrid Catalytic Systems

Y. Cheng, F. Jiao, G. Wu, *Organizers*

C. Liu, Y. Shao, *Organizers, Presiding*

- 2:00** Introductory Remarks.
- 2:05** **97.** Metal nitride incorporated perovskite-type novel cathode catalysts for electrocatalytic ammonia production at atmospheric pressure. **U.S. Ozkan**, S. Gunduz, D.J. Deka, A. Co

- 2:35** **98.** Electrochemical nitrogen reduction to ammonia on transition metal nitrides. **B. Xu**
- 3:05** **99.** Developing base metal electrocatalysts for CO₂ valorization and N₂ fixation. **T. Liu**
- 3:35** **100.** Multifunctional electrocatalysts for chemical transformation: Oxygen reduction reaction (ORR), hydrogen evolution reaction (HER) and electrocatalytic hydrogenation (ECH) reaction. **Y. Shao**
- 4:05** Intermission.
- 4:10** **101.** Enzymatic bioelectrocatalysis for energy conversion applications. **S.D. Minteer**
- 4:40** **102.** Photocatalysis in semiconductor biohybrid systems. **P. Yang**, **S. Cestellos-Blanco**
- 5:10** **103.** Mimicking protein interactions for photodriven nitrogenase activation. **A. Harris**, A. Harguindey, R. Patalano, S. Roy, O. Yehezkeli, A.P. Goodwin, J. Cha
- 5:35** **104.** Micro-structured electrode enabling O₂-incompatible biological nitrogen reduction in air. **S. Lu**, X. Guan, C. Liu

SECTION G
San Diego Convention Center
Room 25A

Hybrid Organic-Inorganic Semiconductors for Energy

Hybrid Perovskite Materials

M. C. Beard, Y. Yan, *Organizers, Presiding*

- 2:00** Introductory Remarks.
- 2:05** **105.** High-efficiency inorganic CsPbI₃ perovskite solar cells. **Y. Zhao**
- 2:35** **106.** Lattice dynamics in methylammonium lead iodide. **M. Toney**
- 3:05** **107.** Ambient Kelvin probe force microscopy with sub 15 nm spatial resolution for nano-electrical characterizations of perovskite. **X. Xu**, D. Jakob
- 3:35** Intermission.
- 3:45** **108.** Defect chemistry of tin vs. lead-halide perovskites. **F. De Angelis**
- 4:15** **109.** Passivation of magic sized clusters and quantum dots of metal halide perovskites using conductive ligands to enhance charge transfer. **J.Z. Zhang**
- 4:45** **110.** Photoexcitation dynamics in perovskite solar cells. **R. Long**
- 5:05** Concluding Remarks.

SECTION H
San Diego Convention Center
Room 25B

Understanding of Energy Materials with Advanced Computation & Characterization

H. Zhao, *Organizer*

L. Cheng, T. Li, *Organizers, Presiding*

- 1:00** Introductory Remarks.
- 1:05** **111.** $\text{Li}_4\text{Ti}_5\text{O}_{12}$ (LTO) antimatter meets defects: Combined theoretical and experimental approach. **C. Grosu**, P. Jakes, S. Seidlmayer, W. Egger, C. Hugenschmidt, J. Granwehr, R. Eichel, K.U. Reuter, C. Scheurer
- 1:25** **112.** Solvation structure transition in $\text{Mg}(\text{TFSI})_2$ aqueous solution. **Z. Yu**, L. Cheng
- 1:45** **113.** Bridging electronic and atomistic scales in modeling energy-relevant reactive interfaces using machine learning. **B. Narayanan**, H. Chan, M. Cherukara, F. Sen, K. Sasikumar, S.K. Gray, M. Chan, S. Sankaranarayanan
- 2:15** **114.** *Ab initio* simulations of XAS spectra for Li-rich transition metal oxides. **B. Taudul**, M. Doublet
- 2:35** Intermission.
- 2:50** **115.** Understanding pseudocapacitive energy storage in MXenes and oxides. **D. Jiang**
- 3:20** **116.** Quantitation and visualization of static structure factor peaks for a phosphonium-based ionic liquid. **T. Mackoy**, R.A. Wheeler
- 3:50** **117.** Understanding proton transfer in MXene-confined water from first principles. **Y. Sun**, D. Jiang
- 4:10** **118.** Multiscale modeling of carrier transport in photocatalytic systems towards enhanced charge separation. **V. Pasumarthi**, M. Dupuis, T. Liu, C. Li
- 4:30** **119.** Optimal design of petroleum refinery configuration using a model-based mixed-integer programming approach with practical approximation. **T.A. Albahri**, C.S. Khor, **M. Elsholkami**, **A. Elkamel**
- 4:50** Concluding Remarks.

Catalysis at Metal-Support Interfaces

Sponsored by CATL, Cosponsored by ENFL

Future Insights into Syngas Conversion Catalysis: Symposium in honor of Burtron H. Davis

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

Solvent Effects in Metal-Catalyzed Reactions

Sponsored by CATL, Cosponsored by ENFL and PHYS

Advances in Catalysis with Ceria & Other Reducible Oxides

Theory of Ceria Catalysts

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

MONDAY MORNING – ENFL

SECTION A
San Diego Convention Center
Room 23A

2D Materials & Beyond: Innovative Materials, Assemblies & Devices for Energy & Fuel

V. Barone, L. Hu, Y. Zhu, *Organizers*

Y. Lin, M. Song, *Organizers, Presiding*

- 8:00** Introductory Remarks.
- 8:05** **120.** Electrocatalytic activity of two-dimensional nanosheets of magnetic metal phosphorus trichalcogenides. **F. Wang**, J. He, S. Jin
- 8:20** **121.** Synthesis of graphene/ SnO_2 passivation layer to enhance the charge collection in perovskite solar cells. **H. Javed**, R. Fatima, A. Mahmood
- 8:35** **122.** Can phosphorus-doped graphene be a good anode for Na-ion batteries? First-principles study. **E. Paek**
- 9:00** **123.** Graphene oxide liquid crystal based functional assembled structures for energy applications. **S. Kim**
- 9:30** **124.** Computational materials discovery for energy applications. **V. Barone**
- 9:55** Intermission.
- 10:00** **125.** Exploring the synthesis and applications of graphene for energy storage. **R.B. Kaner**, X. Chang, A. Huang, C. Wang, M. Muni, H. Wang, M.F. El-Kady
- 10:30** **126.** Flexible energy storage: Zinc-based batteries. **C. Zhi**
- 10:55** **127.** 2D materials for electrode, electrolyte, and electrode/electrolyte interfacial design of safe Li batteries. **R. Yassar**
- 11:20** **128.** Impact-resistant electrolyte with nanofillers for safe Li-ion batteries. **Y. Zhu**
- 11:45** **129.** Photoelectrochemical microscopy of ultrathin liquid junction solar cells. **J. Sambur**

SECTION B
San Diego Convention Center
Room 23B

Advancing Innovative Battery Technologies

B. Liu, H. Pan, D. Wang, K. Xu, *Organizers*

B. Helms, W. Xu, *Presiding*

- 8:00** **130.** Nonflammable localized high concentration electrolytes for lithium ion batteries. **W. Xu**, X. Cao, H. Jia, X. Ren, J. Zhang
- 8:30** **131.** Advancing Li-metal battery technology. **Q. Hu**
- 9:00** **132.** *In situ* characterization of fluorinated compounds at the lithium metal interface. **J. Lopez**, Y. Zhang, Y. Shao-Horn
- 9:20** Intermission.
- 9:40** **133.** Preventing Li depletion and pulverization by monolithic SEI layer generated in fluorinated orthoformate based electrolytes. X. Cao, X. Ren, I. zou, M. Engelhard, W. Huang, H. Wang, B. Matthews, H. Lee, C. Niu, B. Arey, Y. Cui, C. Wang, J. Xiao, J. Liu, W. Xu, **J. Zhang**
- 10:10** **134.** Chemomechanical factors dictating the uniformity of lithium metal plating at high rate with nanostructured solid-ion conductors. **B. Helms**, C. Fu, V. Venturi, Z. Ahmad, A. Ells, V. Viswanathan
- 10:40** **135.** High-energy Li metal pouch cells with limited anode swelling and long stable cycles. **C. Niu**, H. Lee, S. Chen, W. Xu, J. Zhang, J. Xiao, J. Liu

SECTION C

San Diego Convention Center
Room 23C

Atomic-level Understanding & Design of Materials & Processes for Energy Applications

Y. Liu, *Organizer*

H. Zhuang, *Organizer, Presiding*

- 8:00** Introductory Remarks.
- 8:05** **136.** Advanced electrocatalysts for CO₂ and CO reduction. D. Raciti, Y. Wang, **C. Wang**
- 8:35** **137.** Oxygen-evolution catalyst design for polymer-electrolyte-membrane electrolysis. **S.W. Boettcher**, R. Krivina
- 9:05** **138.** Element-specific restructuring of transition metal phosphide and sulfide nanoparticles under electrochemical water-splitting conditions. **H. Wang**
- 9:35** **139.** Elucidating biofuel sooting tendencies and mechanisms with reactive molecular dynamics and density functional theory. **R. Messerly**, B. Etz, H. Kwon, P. St. John, Y. Xuan, S. Kim
- 10:05** Intermission.
- 10:20** **140.** Electro-adsorption and oxygen evolution on well-defined oxide surfaces: Progress in theory-experiment convergence. D. Kuo, **J. Suntivich**
- 10:50** **141.** Synthetic design of materials for energy applications. **R.E. Schaak**
- 11:20** **142.** Understanding the electronic structure of 2D materials for energy applications. **Y. Liu**

SECTION D

San Diego Convention Center
Room 24A

Hybrid Energy Techniques: Catalysts to Vehicle

S. Bashir, V. Li, Q. Zhen, *Organizers*

J. L. Liu, *Organizer, Presiding*

J. Fu, *Presiding*

- 8:00** Introductory Remarks.
- 8:05** **143.** Academic publishing: Communication among editors, reviewers, publishers and authors. Publishing with fuel. **E. Suuberg**, J. Fu
- 8:25** **144.** Academic publishing: Communication among editors, reviewers, publishers and authors. Publishing with progress in energy and combustion science, or publishing with joule. **H. Wang**, **P. Earis**, J. Fu
- 8:45** Intermission.
- 8:55** **145.** Academic publishing: Communication among editors, reviewers, publishers and authors. Publishing with fuel processing technology or publishing with etransportation. **C. Li**, **C. Mi**, J. Fu
- 9:15** **146.** Academic publishing: Communication among editors, reviewers, publishers and authors. Publishing with Elsevier's fuel and energy or publishing with Springer energy journals. **Y. Sun**, **S. Pauly**, J. Fu
- 9:35** Concluding Remarks.

SECTION E

San Diego Convention Center
Room 24B

Innovative Chemistry & Materials for Electrochemical Energy Storage

R. J. Clement, W. Kan, F. Lin, W. Xu, *Organizers*

H. Chen, *Organizer, Presiding*

M. Doublet, S. Ong, *Presiding*

- 8:00** Introductory Remarks.
- 8:05** **147.** Computational vs. conceptual approaches to battery materials. M. Saubanere, M. Ben Yahia, **M. Doublet**
- 9:05** **148.** Understanding surface densified phases in Ni-rich layered compounds. **P. Xiao**, T. Shi, W. Huang, G. Ceder
- 9:20** **149.** Design of all-solid-state alkali-ion batteries: From materials to interfaces. **S. Ong**
- 9:50** Intermission.
- 10:05** **150.** Li-stuffed garnet-type electrolytes for all-solid-state batteries. **V. Thangadurai**
- 10:35** **151.** Interface stability between Li_{1.4}Al_{0.4}Ti_{1.6}(PO₄)₃ and cathode for all solid-state lithium-ion batteries. **J. Choi**, C. Yu, V. Anandan, J. Kim

- 10:50 152.** Single-ion conducting polymer electrolytes toward a stretchable solid-state battery. **P. Cao**, B. Li, G. Yang, S. Zhao, T. Liu, F. Lin, Z. Du, D. Wood, A.P. Sokolov, J. Nanda, T. Saito
- 11:20 153.** Electrochemically stable all-solid-state sodium metal battery enabled by chemically engineered solid electrolytes. **E. Matios**, H. Wang, W. Li
- 11:35 154.** Cathode interfacial resistance in lithium-sulfur batteries under lean electrolyte condition. **Y. Zhao**, J. Guo
- 11:50** Concluding Remarks.

SECTION F

San Diego Convention Center
Room 24C

Sustainable Energy & Water via Innovative Electrocatalytic, Photocatalytic & Hybrid Catalytic Systems

Y. Cheng, Y. Shao, G. Wu, *Organizers*
F. Jiao, C. Liu, *Organizers, Presiding*

- 8:00** Introductory Remarks.
- 8:05 155.** Effect of the electrolyte on electrochemical CO₂ reduction. **K. Chan**
- 8:35 156.** Rationally guided design of electrocatalysts and systems for CO₂-to-fuels using renewable electricity. **Y. Li**, C. Dinh, Z. Wang, E.H. Sargent
- 9:05 157.** Next steps in electrochemical CO₂ reduction: From catalysts to devices to systems. **T. Burdyny**
- 9:35 158.** Nanoelectrocatalysts for selective CO₂ reduction. **G. Zheng**
- 10:00** Intermission.
- 10:15 159.** Cooperative catalysis for electrochemical carbon dioxide conversion and energy storage. **H. Wang**
- 10:45 160.** Dynamic electrocatalysis in three dimensions. **N. Kornienko**
- 11:10 161.** Catalytic materials for the making of renewable fuels and chemicals. **I. Chorkendorff**
- 11:40 162.** Unique star decahedron Cu nanocatalyst with highly active hydrocarbon production. **C. Choi**, T. Cheng, M. Espinosa, H. Fei, X. Duan, W.A. Goddard, Y. Huang

SECTION G

San Diego Convention Center
Room 25A

Hybrid Organic-Inorganic Semiconductors for Energy

Hybrid Perovskite Materials

M. C. Beard, Y. Yan, *Organizers*
J. Gu, Y. Zhao, *Presiding*

- 8:10** Introductory Remarks.
- 8:15 163.** Atomic-scale study of the degradation process on single-crystal perovskite surfaces: From ultra-high vacuum to ambient pressures. **J. Choi**, M.E. Khan, J. Hawash, H. Lee, L.K. Ono, Y. Qi, Y. Kim, J. Park
- 8:35 164.** Hybrid organic-inorganic perovskite photoelectrodes: Photocorrosion vs. solar fuel generation. G.F. Samu, A. Balog, P.V. Kamat, **C. Janaky**
- 8:55 165.** Metal-ligand catalytic site distortion induced by internal strain through vapor-phase infiltration. **J. Gu**, F. Yang
- 9:25 166.** Withdrawn
- 9:55** Intermission.
- 10:05 167.** Direct-bandgap 2D silver-bismuth iodide double perovskite: Structure-directing influence of an oligothiophene spacer cation. **M.K. Jana**, S.M. Janke, D.J. Dirkes, S. Dovletgeldi, C. Liu, X. Qin, K. Gundogdu, W. You, V. Blum, D.B. Mitzi
- 10:25 168.** Synchrotron-based, *in situ*, real-time study of the crystallization dynamics of metal halide perovskite. **K. Meng**, G. Chen
- 10:45 169.** Selective adsorption induced systematic relaxation of dimensional confinement: New mechanistic insight in gas induced band gap tuning of methylammonium lead iodide film. **S. Sasmal**, R. Pala, S. Sivakumar, S. Valiyaveettil
- 11:05 170.** Functions and interactions of hole transport layer components in perovskite solar cells. **S. Wang**, S. Meng
- 11:25 171.** Covalent attachment and characterization of perylene monolayers on Si(111) and TiO₂ for electron-selective carrier transport in tandem-junction PV. A. Carl, **R. Grimm**
- 11:45** Concluding Remarks.

SECTION H

San Diego Convention Center
Room 25B

Understanding of Energy Materials with Advanced Computation & Characterization

H. Zhao, *Organizer*
L. Cheng, T. Li, *Organizers, Presiding*

- 8:00** Introductory Remarks.
- 8:05 172.** Visualization of single grain evolution *in operando* cathode materials with the coherent hard X-ray diffraction. **L. Li**, Y. Xie, Z. Chen, R. Harder
- 8:35 173.** Understanding the degradation mechanisms of battery materials *via* synchrotron-based X-ray techniques. **L. Wang**, T. Li

- 8:55** **174.** Understanding electrolyte oxidation and reduction at electrode and SEI surfaces. **O. Borodin**, T.P. Pollard, J. Vatamanu
- 9:15** **175.** Resolving the anomalous interfacial stress generation during sodium intercalation/extraction in MoS₂ nanofilm anodes. **Z. Li**, K. Jiang, T. Thundat
- 9:35** Intermission.
- 9:50** **176.** Characterization of ion transport and functional polymers in next generation electrochemical energy storage devices. J. Liu, B. Park, H. Ford, **J.L. Schaefer**
- 10:10** **177.** Catalyzing active materials for energy storage and water technology by *in situ* and *operando* studies. **J. Wang**
- 10:40** **178.** Capacitance of electrode/electrolyte interfaces predicted by fixed-voltage, molecular dynamics with *ab initio* force fields. **J.G. McDaniel**
- 11:00** **179.** Exploring electrochemical reaction dynamics of Li⁺-solvation structures with large-scale quantum mechanical simulations. **B.M. Wong**, J. Guo, C. Fu, L. Xu, F. Aquino
- 11:20** Concluding Remarks.

Electrocatalysis for Energy Generation & Storage Fuel Cells

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Advances in Catalysis with Ceria & Other Reducible Oxides

Reactions of Ceria Catalysts

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Catalytic Conversion of Biomass-Derived Oxygenates

Biomass Conversion in Liquid Environments

Sponsored by CATL, Cosponsored by ENFL

MONDAY AFTERNOON – ENFL

SECTION A

San Diego Convention Center
Room 23A

2D Materials & Beyond: Innovative Materials, Assemblies & Devices for Energy & Fuel

L. Hu, Y. Lin, Y. Zhu, *Organizers*

V. Barone, M. Song, *Organizers, Presiding*

- 1:00** Introductory Remarks.

- 1:05** **180.** 2D materials as effective coating and additives for solid-state batteries. **Y. Yang**
- 1:30** **181.** Regulating the 2D materials for high-performance sodium metal batteries. **W. Li**, J. Luo, X. Hu, H. Wang
- 1:55** **182.** Role of morphology and nitrogen speciation on the reversible Li- and Na-capacity of Mg-reduced graphitic carbon nitride. **B.D. Fahlman**
- 2:20** **183.** 2D transition metal oxides for multivalent ion cathodes. **M. Smeu**
- 2:45** Intermission.
- 2:50** **184.** Understanding carbon catalysis with well-defined graphene nanostructures. **L. Li**
- 3:15** **185.** Electronic and mechanical properties of individual Ti₃C₂T_x MXene monolayer flakes. **A. Sinitskii**
- 3:40** **186.** Electrochemical behavior of functionalized transition metal dichalcogenide nanosheets. D. Soares, **G. Singh**
- 4:05** **187.** First-principles modeling of layered electrodes for water splitting and charge storage. Q. Campbell, **I. Dabo**
- 4:30** **188.** Tuning the properties of two-dimensional materials toward efficient photocatalysis. **K.L. Shuford**
- 4:45** **189.** Sequential-series multijunction dye-sensitized solar cells with 10.1% efficiency and 2.3 V output. **H. Cheema**, J.H. Delcamp

SECTION B

San Diego Convention Center
Room 23B

Advancing Innovative Battery Technologies

B. Liu, H. Pan, D. Wang, K. Xu, *Organizers*

C. Wang, W. Yang, *Presiding*

- 1:00** Introductory Remarks.
- 1:10** **190.** *In situ* and *ex situ* TEM diagnosis guided designing of electrode materials for better battery. **C. Wang**
- 1:40** **191.** Independent probe and quantification of cationic and anionic redox reactions in positive electrodes. **W. Yang**
- 2:10** **192.** Love affair with lithium metal anodes and sulfur cathodes: All that glitters is not gold. **J. Muldoon**, P. Bonnick
- 2:40** Intermission.
- 3:00** **193.** New innovations for *operando* diffraction studies of battery electrodes with spatial and temporal resolution. **P. Khalifah**
- 3:30** **194.** Poly-rotaxanes as novel solid polymer electrolytes for lithium-ion battery: Insight into Li⁺ dynamics from molecular dynamics simulations. **D. Dong**, **D. Bedrov**

SECTION C
San Diego Convention Center
Room 23C

Atomic-level Understanding & Design of Materials & Processes for Energy Applications

H. Zhuang, *Organizer*

Y. Liu, *Organizer, Presiding*

- 1:00** Introductory Remarks.
- 1:05** **195.** Modeling heterogeneous catalysis with molecular-level understanding. **L. Gagliardi**
- 1:35** **196.** Catalyst design for electrochemical hydrogenation of organic compounds. **R. Rousseau**, V. Glezakou, M. Lee, M. Nguyen, S. Akhade, J. Lopez Ruiz, E. Andrews, J. Holladay, A.B. Padmaperuma, O.Y. Gutierrez Tinoco, K. Koh, A.J. Karkamkar, U. Sanyal, S. Yuk
- 2:05** **197.** Tailoring charge storage and electrocatalytic performance of carbon-based nanomaterials via structural and chemical modifications. **G.S. Hwang**
- 2:35** Intermission.
- 2:50** **198.** Understanding the influence of cation doping on the surface chemistry of sodium tantalate. Z. Tang, **A. Selloni**
- 3:20** **199.** Designing 3-D active sites in MOFs for oxygen electrochemistry. **A. Kulkarni**
- 3:50** **200.** Atomistic understanding and design of metal/nitrogen co-doped carbon electrocatalysts for proton-exchange membrane fuel cells. **G. Wang**
- 4:20** **201.** First-principles approach to model electrochemical reactions at solid-liquid interfaces. S. Surendralal, M. Todorova, **J. Neugebauer**

SECTION D
San Diego Convention Center
Room 24A

Photocatalysis for Energy & Environment

Y. Lin, M. Long, *Organizers*

F. Wang, W. Wei, *Organizers, Presiding*

- 1:00** Introductory Remarks.
- 1:05** **202.** Efficient photocatalytic conversion of light hydrocarbons to highly valuable compounds. **Y.H. Hu**
- 1:45** **203.** Room-temperature reduction of carbon dioxide. **R. Sharma**, C. Wang, W. Yang, A. Bruma
- 2:15** **204.** Fabrication of cobalt complex-based catalysts/ photocatalysts for robust photocatalytic CO₂ reduction. **F. Wang**
- 2:35** Intermission.
- 2:50** **205.** Knitting porous polymer on TiO₂-graphene surface to enhance the CO₂ conversion efficiency under visible light. X. Hu, J. Yu, M. Xu, **J. Wang**

- 3:20** **206.** Synthesis and characterization of carbon quantum dots/TiLiAl layered double-hydroxide composite for photocatalytic reduction of CO₂ to hydrocarbon fuel. **A. Zhou**, G. Li, D. Lei, R. Li, X. Zhao
- 3:40** **207.** Photocatalytic carbon dioxide reduction with zinc dipyrin sensitizers. **S. Rasheed**, A. Day, C. McCusker
- 4:00** **208.** Artificial foliage with remarkable quantum efficiency in converting photons to formate. **H. Pan**, M.D. Heagy
- 4:20** Concluding Remarks.

SECTION E
San Diego Convention Center
Room 24B

Innovative Chemistry & Materials for Electrochemical Energy Storage

H. Chen, R. J. Clement, W. Kan, F. Lin, W. Xu, *Organizers*

B. Gallant, P. Liu, *Presiding*

- 1:00** Introductory Remarks.
- 1:05** **209.** Electrolytes and coatings for high-efficiency lithium-metal anodes. **P. Liu**
- 2:05** **210.** *In situ* fluoride modification of Li storage materials for advanced battery chemistries. **B. Gallant**
- 2:35** **211.** 3-D carbon materials as dendrite-free lithium metal anodes. **Y. Xu**, Y. Kang
- 2:55** **212.** Properties of thin lithium metal electrode in electrolytes based on carbonate solvents. **J. Zhang**, J. Guo
- 3:15** Intermission.
- 3:25** **213.** Oxygen redox activities in Li-rich layered oxides: Pushing the limit of intercalation. **S. Meng**
- 3:55** **214.** Monitoring capacity losses through *operando* X-ray diffraction of lithium metal anodes. **M. Toney**
- 4:25** **215.** Thermodynamic relationships between composition and defect concentration in NMC cathodes resolved using novel high-precision powder diffraction methods. **P. Khalifah**, L. Yin, Z. Li, G. Mattei, J. Zheng, W. Zhao, F. Omenya, C. Fang, W. Li, J. Li, Q. Xie, E. Erickson, J. Zhang, M.S. Whittingham, S. Meng, A. Manthiram
- 4:55** Concluding Remarks.

SECTION F
San Diego Convention Center
Room 24C

Sustainable Energy & Water via Innovative Electrocatalytic, Photocatalytic & Hybrid Catalytic Systems

Y. Cheng, Y. Shao, G. Wu, *Organizers*

F. Jiao, C. Liu, *Organizers, Presiding*

- 1:00** Introductory Remarks.
- 1:05** **216.** Hydrogen in catalysis and catalysts. **D. Jiang**
- 1:35** **217.** Computational study of metal/nitrogen doped carbon electrocatalysts for CO₂ reduction reaction. **G. Wang**
- 2:05** **218.** Tuning selectivity of ethylene and ethanol in CO₂RR using density functional theory and microkinetic modelling. **Z. Wang**, E.H. Sargent
- 2:35** **219.** Activities of single-atom Fe, Co, Ni embedded on nitrogen-doped graphene for CO₂ reduction: Theoretical study. **Q. Wu**
- 3:05** Intermission.
- 3:20** **220.** Electrocatalytic reduction of carbon dioxide over nanostructured catalysts. **G. Wang**
- 3:50** **221.** Electrocatalytic conversion of CO to acetate. X. Fu, W. Luc, Y. Liu, F. Jiao, **Y. Kang**
- 4:20** **222.** Facile synthesis of highly porous Bi electrocatalysts for high efficiency formate production from CO₂ in various electrolytes. **G. PIAO**, H. Park
- 4:40** **223.** Understanding vapor-fed carbon dioxide reduction at the gas diffusion electrode and electrolyte interface Using flow-electrolyte systems. **D. Lee**, D. Koshy, K. Abiose, D. Corral, L. Wang, D. Higgins, C. Hahn, T.F. Jaramillo

SECTION G

San Diego Convention Center
Room 25A

Hybrid Organic-Inorganic Semiconductors for Energy

Hybrid Perovskite Materials

M. C. Beard, Y. Yan, *Organizers*

J. Gu, X. Zhu, *Presiding*

- 1:00** Introductory Remarks.
- 1:05** **224.** 1,3,5-Triazine-based Pt(II) metallogel material: Synthesis, photophysical properties, and optical power limiting performance. **R. Liu**, H. Su, S. Zhu, H. Zhu
- 1:30** **225.** Functionalization of graphene oxide film with Au and MoO_x nanoparticles as efficient *p*-contact electrode for perovskite solar cells. **S.S. Bhosale**, E. Diau
- 1:45** **226.** Silicon for pharmaceutical molecule synthesis: Passivated Si quantum dots for 4 + 2 annulation of tertiary amine and N-Boc protected secondary amines. **Y. Sun**, J. San Martin, Y. Yan
- 2:00** **227.** Towards elusive hybrid perovskite carrier dynamics through ultrafast THz spectroscopy: Influence of quantum confinement and charge transport layers. **K. Virgil**, H. Atwater, G.A. Blake

- 2:15** **228.** Solvents-induced aggregation based on a heteroleptic Ir(III) complex via hydrogen bonds. **H. Zhu**, Z. Song, J. Wang, R. Liu
- 2:40** Intermission.
- 2:50** **229.** Interfacial engineering of metal oxides as electron-transport layers for efficient and stable perovskite solar cells. **D. Zheng**, G. Wang, W. Huang, T.J. Marks, A. Facchetti
- 3:05** **230.** Hydrogen evolution at a hybrid organometallic catalyst-silicon interface and the decomposition of the interface. **N.B. Williams**, J. Gu
- 3:20** **231.** Solar energy induced drug synthesis: Lead-halide perovskite nanocrystals as efficient photocatalysts for N-hetero cyclization reactions. **Y. Lin**, Y. Sun, J. San Martin, C. Manabat, D. Zhu, X. Zhu, Y. Yan
- 3:35** **232.** Interplay of magnetic coupling, structural dimensionality, and chirality in hybrid perovskite halide semiconductors. **A. Maughan**, M.C. Beard, J. Berry
- 3:55** **233.** Pd doping CsPbBr₃ hybrid perovskite: Photocatalytic asymmetric Suzuki-Miyaura cross-coupling reactions under visible light irradiation. **X. Zhu**, Y. Yan
- 4:15** **234.** Photoelectrochemical H₂ generation via zinc-doped 1T-MoS₂ on silicon nanowires. **S. Younan**
- 4:30** Concluding Remarks.

SECTION H

San Diego Convention Center
Room 25B

Understanding of Energy Materials with Advanced Computation & Characterization

H. Zhao, *Organizer*

L. Cheng, T. Li, *Organizers, Presiding*

- 1:00** Introductory Remarks.
- 1:05** **235.** Simple descriptors on the geometric, energetic, and electronic properties of proton inside cubic perovskites. **L. Xu**, D. Jiang
- 1:25** **236.** Atomically dispersed metal species on mixed metal support for highly efficient catalysis. **Q. Zhang**
- 1:45** **237.** Modeling copper-based dyes and hole-transporting materials for dye-sensitized solar cells. **S. Fantacci**
- 2:05** **238.** Electrochemical study on the corrosion of structural materials for DCFC. **H. Zhao**, E. Engmann, M. Shi, D. Ding, T. He
- 2:25** Intermission.
- 2:40** **239.** Structural and electronic properties of Co nanoparticles supported on reducible CeO₂(111) thin films. **L. Du**, **J. Zhou**

- 3:10 240.** Investigating the effect of solvatochromism in thermally activated delayed fluorescence emitters exhibiting circularly polarized luminescence. **J. Scher, A. Chakraborty**
- 3:40 241.** Raman spectroscopy for energy materials. **A. Falcone, M. Ben Yahia, M. Doublet**
- 4:00 242.** Facile fabrication of RuCo single-atom alloyed catalysts for levulinic acid hydrogenation to -valerolactone. **Y. Yang, S. Shao, Y. Ke**
- 4:20 243.** Optimization of Donors and Acceptors for Organic Photovoltaics Guided by Molecular Simulations. **M. Matta, T.J. Marks, G.C. Schatz**
- 4:40** Concluding Remarks.

Identification & Design of Catalytic Sites in Electrochemical Reactions

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Electrocatalysis for Energy Generation & Storage

Sponsored by CATL, Cosponsored by ENFL

Advances in Catalysis with Ceria & Other Reducible Oxides

Reactions and Other Metal Oxides

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Catalytic Conversion of Biomass-Derived Oxygenates

Theoretical & Mechanistic Studies of Biomass-Derived Oxygenates

Sponsored by CATL, Cosponsored by ENFL

Charge & Substrate Transport in 3D Electrocatalytic Materials

Sponsored by INOR, Cosponsored by CATL and ENFL

MONDAY EVENING – ENFL

SECTION A

San Diego Convention Center
TBD

Sci-Mix

H. Lin, *Organizer*

8:00 - 10:00

9, 15, 16, 21, 58, 63, 96, 108, 112, 133, 148, 151, 160, 162, 166, 172, 205, 223, 225, 227, 229, 232, 238. See Previous Listings.

253, 267, 282, 289, 303, 309, 321, 342, 346, 397, 402, 422, 438, 452, 456, 471, 481, 487, 503, 504, 521, 524, 528, 548, 571, 572, 586, 595, 610, 616, 618, 621, 629, 633. See Subsequent Listings.

TUESDAY MORNING – ENFL

SECTION A

San Diego Convention Center
Room 23A

Accelerating Scientific Breakthroughs at the Energy-Water Nexus in Engineered & Natural Environment

Cosponsored by WCC

G. Gadikota, A. E. Gordon, A. A. Park, L. Tribe, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 244. Interfacial dynamics in radioactive environments and materials (IDREAM): Energy frontier research center focused on accelerating innovation for radioactive waste processing. **S.B. Clark**

8:35 245. Managing high salinity brines from geological carbon sequestration. **M.S. Mauter**

9:05 246. *Ab initio* simulations of energy conversion processes at water-solid interfaces. **G.A. Galli**

9:35 247. Molecular modules for photochemical and catalytic function in artificial photosynthesis. **K.L. Mulfort, L.X. Chen, O. Poluektov, L.M. Utschig-Johnson, D.M. Tiede**

10:05 Intermission.

10:15 Panel Discussion.

SECTION B

San Diego Convention Center
Room 23B

Advancing Innovative Battery Technologies

B. Liu, H. Pan, D. Wang, K. Xu, *Organizers*

V. Murugesan, L. Suo, *Presiding*

8:00 248. Advanced aqueous Li/Na ion batteries for electric energy storage application. **L. Suo, O. Borodin, Y. Hu, C. Wang, K. Xu**

8:30 249. Application of magnesiothermic reduction of silica to produce porous silicon for lithium-ion batteries. **S.V. Patwardhan, J. Entwistle**

8:50 250. Intentional surface oxidation of silicon nanoparticles for improved Li-ion battery composite anodes. **M. Carroll**

9:10 Intermission.

- 9:30 251. Facile chemical route to prelithiation in silicon monoxide powders for lithium-ion batteries. **D. Ito**
- 9:50 252. Withdrawn
- 10:10 253. Development of thick cathodes for high-energy lithium-ion batteries. **L. Rao, J. Sayre, J. Kim**

SECTION C

San Diego Convention Center
Room 23C

Atomic-level Understanding & Design of Materials & Processes for Energy Applications

H. Zhuang, *Organizer*

Y. Liu, *Organizer, Presiding*

- 8:00 Introductory Remarks.
- 8:05 254. Car–Parrinello monitor method for circumventing self-consistent field convergence failure in reactive Born–Oppenheimer molecular dynamics. **L. Wang, C. Song**
- 8:35 255. Descriptors and atomic level understanding for post-Li battery technologies. **A. Gross**
- 9:05 256. Theoretical insights into activity-stability relationships of transition metal based electrocatalysts. **V. Alexandrov**
- 9:35 257. Well-defined nanographene-based systems for catalytic applications. **R. Schauggaard, L. Li, K. Raghavachari**
- 10:05 Intermission.
- 10:20 258. Catalysis on atomically precise ligand-protected nanoclusters. **G. Mpourmpakis**
- 10:50 259. Computational screening and design principles of COF materials as high-performance catalysts for clean energy conversion. **C. Lin, D. Zhang, L. Gong, L. Zhang, Z. Xia**
- 11:20 260. Bayesian chemisorption model for adsorbate-specific tuning of electrocatalysis. **S. Wang, H. Xin**

SECTION D

San Diego Convention Center
Room 24A

Photocatalysis for Energy & Environment

Y. Lin, F. Wang, *Organizers*

M. Long, W. Wei, *Organizers, Presiding*

- 8:00 Introductory Remarks.
- 8:05 261. Anti-photocorrosion 2-D layer over CdS for hydrogen generation. **G. Lu**
- 8:45 262. Optically resonant dielectric nanostructures for efficient conversion of solar to chemical energy. **F. Mohammadparast, S. Bhardwaj Ramakrishnan, A. Ravi Teja, M. Andiappan**
- 9:15 263. Pyrene-based organic frameworks for photocatalytic hydrogen evolution. **X. Chen, X. Wang**

- 9:35 Intermission.
- 9:50 264. Recent development of BiOX for artificial photosynthesis of ammonia from water and nitrogen. **J. Bao, M. Mohebinia, C. Wu, Z. Wang**
- 10:20 265. Interfacial engineering of hematite photoanodes through layer-by-layer assembly for solar water splitting. **D. Jeon, J. Ryu**
- 10:40 266. Theoretical limits of multiple exciton generation and singlet fission tandem devices for solar water splitting. **M. Martinez, A. Nozik, M.C. Beard**
- 11:00 267. Emulsion polymerization derived organic photocatalysts for improved light-driven hydrogen evolution. **C.M. Aitchison, R.S. Sprick, A.I. Cooper**
- 11:20 C oncluding Remarks.

SECTION E

San Diego Convention Center
Room 24B

Innovative Chemistry & Materials for Electrochemical Energy Storage

H. Chen, R. J. Clement, W. Kan, F. Lin, *Organizers*

W. Xu, *Organizer, Presiding*

B. McCloskey, S. Meng, *Presiding*

- 8:00 Introductory Remarks.
- 8:05 268. Quantifying outgassing, surface oxygen depletion, and solid carbonate evolution in Li(Ni, Co, Mn)O₂ Li-ion cathodes. **B.D. McCloskey**
- 8:35 269. Interfacial speciation determines interfacial chemistry: X-ray-induced lithium fluoride formation from “water-in-salt” electrolytes on solid surfaces. **H. Steinrueck, C. Cao, M.R. Lukatskaya, G. Wan, C.J. Takacs, J.F. Wishart, M. Toney**
- 8:50 270. Identifying active sites for parasitic reactions at cathode electrolyte interface. **Z. Chen**
- 9:20 271. Understanding performance degradation in Li-rich cation-disordered rocksalt cathodes. **G. Chen, D. Chen**
- 9:50 Intermission.
- 10:05 272. Neutron scattering in promoting the development for lithium-ion batteries. **F. Wang**
- 10:35 273. Understanding electrode-electrolyte interface in Li-ion batteries by *in situ* Fourier transform infrared spectroscopy (FTIR). **Y. Zhang, Y. Katayama, Y. Shao-Horn**
- 11:05 274. Applications of *operando* neutron scattering for battery study. **B. Song**
- 11:35 275. Improving stability in high volume change alloy anodes through the use of nanoporous electrodes and *operando* TXM imaging. **S.H. Tolbert**
- 11:50 Concluding Remarks.

SECTION F
San Diego Convention Center
Room 24C

Sustainable Energy & Water via Innovative Electrocatalytic, Photocatalytic & Hybrid Catalytic Systems

F. Jiao, C. Liu, Y. Shao, *Organizers*
Y. Cheng, G. Wu, *Organizers, Presiding*

- 8:00** Introductory Remarks.
- 8:05** **276.** Understanding electrode design and degradation in fuel cells. **D.A. Cullen**, K. More
- 8:35** **277.** Understanding the role of interfaces for water management in PGM-free electrodes in polymer electrolyte fuel cells. **I. Zenyuk**
- 9:05** **278.** Advanced atomically dispersed metal catalysts for fuel cells. **G. Wu**
- 9:35** **279.** Scale up of advanced fuel cell catalysts in batch and flow reactors. **R. Wang**, K. Puppek, T. Dzwiniel, H. Lv, N. Becknell, P. Papa Lopes, P. Farinazzo Bergamo, N. Markovic, V. Stamenkovic
- 10:05** Intermission.
- 10:10** **280.** Atomic arrangement engineering of metallic nanostructures for electrocatalysis revealed by transmission electron microscopy. **D. Su**
- 10:40** **281.** Heterostructure-promoted oxygen electrocatalysis enables rechargeable zinc–air battery. **S. Zhang**, Z. Zhang, C. Liu, G. Johnson, Y. Zhang
- 11:10** **282.** Oxygen reduction reaction promoted by manganese porphyrins. **D. Dogutan Kiper**, M. Qui, G. Passard, C. Costentin, D.G. Nocera
- 11:35** **283.** Manipulating active sites using molten salts for synthesizing highly efficient electrocatalysts. K. Lu, **Y. Cheng**

SECTION G
San Diego Convention Center
Room 25A

Sustainable Biofuels & Bio-Based Products

J. Fu, A. B. Padmaperuma, Y. Yang, *Organizers*
H. Lin, H. Wang, *Organizers, Presiding*

- 8:00** Introductory Remarks.
- 8:05** **284.** Catalyst-solvent interactions in selective hydrogenolysis and hydrogenation of lignin-based compounds. A. Chamas, L. Qi, **S.L. Scott**
- 8:45** **285.** Biphasic catalytic process: Generic platform technology for biomass conversion. **H. Lin**
- 9:15** **286.** Selective production of phase-separable product from a mixture of biomass-derived aqueous oxygenates. Y. Wang, **F. Wang**

- 9:45** **287.** Carbohydrate stabilization by acetal formation prevents degradation and leads to new reactivity during biomass depolymerization. **J. Luterbacher**
- 10:15** Intermission.
- 10:30** **288.** Identification and structural characterization of oligomers formed from the pyrolysis of different kinds of biomass. **C. Hu**
- 11:10** **289.** Promoting deoxygenation in lignocellulosic biomass: Co-pyrolysis with clay minerals as *in situ* catalysts. **A. Hubble**, L. Gao, F. Wang, J.L. Goldfarb
- 11:30** **290.** Isolation of bio-oil phenol and cresols through a continuous extraction process. **Y. Elkasabi**, C.A. Mullen, A.A. Boateng
- 11:50** Concluding Remarks.

SECTION H
San Diego Convention Center
Room 25B

Materials for Energy & Environmental Sustainability

L. Fan, L. Qin, *Organizers, Presiding*

- 8:00** Introductory Remarks.
- 8:05** **291.** Withdrawn
- 8:25** **292.** Silanated cellulose acetate membranes with enhanced gas permeabilities and plasticization resistance in pure and mixed gas feeds. **B.J. Sundell**, D. Harrigan, S.C. Hayden, J.A. Lawrence III, M.L. Ostraat
- 8:45** **293.** Harnessing multi-dimensional metal-organic frameworks in mixed-matrix membranes for energy-efficient separations and enhanced plasticization resistance. **W. Chi**, B.J. Sundell, K. Zhang, D. Harrigan, S.C. Hayden, Z. Smith
- 9:05** **294.** Self-assembly of tri-peptides to design a novel proton transfer membrane for fuel cell applications. **S. Pollozi**, D.M. McGregor, G.E. Lopez, H. Elshendidi, G. Reyes
- 9:25** **295.** Fouling phenomena and fouling mitigation of ion exchange membranes in reverse electrodialysis for salinity power generation. S. Han, **J. Park**
- 9:45** Intermission.
- 10:00** **296.** Robust CNTs/Al₂O₃ composite membrane for effective fouling mitigation via coupling electric field. **H. Mao**, M. Qiu, X. Chen, Y. Fan
- 10:20** **297.** Self-healing solid polymer electrolyte formed via quadruple hydrogen bonding for lithium-ion batteries. **Z. Xue**
- 10:40** **298.** Transient metals in micromotor design. **E. Karshalev**, C. Chen, J. Wang
- 11:00** **299.** Withdrawn

SECTION A

San Diego Convention Center

Room 23A

7th International Symposium on Mesoporous Zeolites

K. Li, *Organizer*J. Garcia Martinez, *Organizer, Presiding*F. Thenayan, *Presiding*

1:00 Introductory Remarks.

1:10 **302.** What makes mesoporous zeolites unique: Abundant external acid sites and fast molecular transport. **M. Choi**1:50 **303.** Interactions between surface species and confined solvent structures within Lewis acid zeolites: (De)stabilization of catalytically-relevant intermediates. **D. Bregante**, J.Z. Tan, R.L. Schultz, A.Y. Patel, C. Torres, E.Z. Ayla, D. Flaherty

2:20 Intermission.

2:40 **304.** Revisiting the old dealumination and desilication of synthetic zeolites: Way forward. **X. Fan**3:20 **305.** Nanostructural evolution of hierarchically-structured single-unit-cell-thick siliceous MFI zeolite nanosheets under steaming. **Y. Guefrachi**, M. Tsapatsis3:50 **306.** Small molecule soft-templates for the design and synthesis of mesoporous beta zeolites for crude to chemical applications. **S. Fernandez**, S. Kobaslija, J.A. Lawrence III, J.T. O'Brien, T.J. Kucharski, B.S. Hanna, E. Converse, M.L. Ostraat

SECTION B

San Diego Convention Center

Room 23B

Advancing Innovative Battery Technologies

B. Liu, H. Pan, D. Wang, K. Xu, *Organizers*B. Adams, G. Li, *Presiding*1:00 **307.** Zinc-based flow battery for large-scale energy storage. **X. Li**1:30 **308.** Practical aspects of developing the zinc-ion battery. **B. Adams**2:00 **309.** Long cycle life self-healing zinc-iodine flow battery with high power density. **C. Xie**

2:20 Intermission.

2:40 **310.** Advanced Na beta-alumina batteries (NBBs) for energy storage systems applications. **G. Li**3:10 **311.** High-performance porous membranes for vanadium flow battery. **W. Lu, X. Li**11:20 **300.** Synthesis and characterization of thick transparent nanoparticle-based mesoporous silica monolithic slabs by template-free sol-gel synthesis on omniphobic liquid substrates. **M. Marszewski**, S. King, Y. Yan, T. Galy, M. Li, A. Dashti, D. Butts, J.S. Kang, P. McNeil, E. Lan, B. Dunn, Y. Hu, S.H. Tolbert, L. Pilon11:40 **301.** Powder-river-basin coal based carbon fiber. **T. Wang**, H. Xin, W. Lu, K. Sun, M. Fan

11:55 Concluding Remarks.

Gerry Meyer: The First 100 Years

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- 3:30 **312.** Factors impacting zinc cation intercalation into manganese dioxide. S. Jin, M. Cuisinier, **B. Adams**
- 3:50 Concluding Remarks.

SECTION C

San Diego Convention Center Room 23C

Atomic-level Understanding & Design of Materials & Processes for Energy Applications

Y. Liu, *Organizer*

H. Zhuang, *Organizer, Presiding*

- 1:00 Introductory Remarks.
- 1:05 **313.** First-principles materials design for energy conversion. **K. Yang**, Y. Li
- 1:35 **314.** Atomic-scale understanding and control over planar defects in cesium lead-halide perovskite nanocrystals for optoelectronic applications. **R. Mishra**, A.S. Thind, G. Luo, M.V. Morrell, J. Hachtel, A.Y. Borisevich, J. Idrobo, Y. Xing
- 2:05 **315.** Energy material design based on electric dipole simulations. **J. Jiang**
- 2:35 Intermission.
- 2:50 **316.** Automatic structure search versus chemical rules in 2D materials study. **M. Miao**
- 3:20 **317.** Electronic function by atomic design of heteroanionic materials. **J. Rondinelli**
- 3:50 **318.** Searching for materials with exceptional opto-electronic properties using *ab initio* high-throughput computing. **G. Hautier**
- 4:20 **319.** *Ab initio* nonadiabatic molecular dynamics investigations on the excited carriers in condensed matter systems. Q. Zheng, W. Chu, C. Zhao, L. Zhang, Y. Wang, H. Guo, X. Jiang, **J. Zhao**

SECTION D

San Diego Convention Center Room 24A

Photocatalysis for Energy & Environment

F. Wang, W. Wei, *Organizers*

Y. Lin, M. Long, *Organizers, Presiding*

- 1:00 Introductory Remarks.
- 1:05 **320.** “Cocktail” approach for effective passivation of metal halide perovskite magic sized clusters and quantum dots involving planar molecular ligands based on metal coordination compounds. **J.Z. Zhang**
- 1:45 **321.** Influence of graphene and copper on the photocatalytic response of titanium oxide nanotubes. E. Zghab, M. Hamandi, F. Dappozze, H. Kochkar, M. Saïd Zina, C. Guillard, **G. Berhault**

- 2:15 **322.** Enhanced photoelectrochemical CO₂ reduction activity of metal-organic framework via gas phase infiltration method. **F. Yang**, J. Gu
- 2:35 Intermission.
- 2:50 **323.** Visible light photocatalytic degradation of tetracycline over TiO₂. **Y. Lin**, S. Wu, Y.H. Hu
- 3:20 **324.** Polyelectrolyte/molecular catalyst multilayers for efficient solar water oxidation through catalyst loading and surface-state passivation of BiVO₄ photoanodes. **S. Bae**, J. Ryu
- 3:40 **325.** Plasmonic metal nanocatalysts for photohydrogenation of CO₂ to CO or CH₄ with unrivaled high photon to product efficiency. **P. Buskens**, F. Sastre, C. Versluis, N. Meulendijks, J. Rodríguez-Fernández, J. Sweelssen, K. Elen, M.K. Van Bael, T. Den Hartog, M. Verheijen
- 4:00 **326.** Highly efficient thermo-photo catalytic water splitting on a low-cost Ni@NiO-loaded TiO₂ catalyst. **S. Fang**, Z. Sun, Y.H. Hu
- 4:20 Concluding Remarks.

SECTION E

San Diego Convention Center Room 24B

Innovative Chemistry & Materials for Electrochemical Energy Storage

H. Chen, W. Kan, F. Lin, W. Xu, *Organizers*

R. J. Clement, *Organizer, Presiding*

K. A. See, Y. Yao, *Presiding*

- 1:00 Introductory Remarks.
- 1:05 **327.** High conductivity, chemically stable, hydroxide conducting block copolymer poly(norbornene) membranes for alkaline electrolyzers and fuel cells. M. Mandal, G. Huang, **P. Kohl**
- 1:35 **328.** Electrolyte dictated organic electrode materials design for beyond lithium-ion batteries. **Y. Yao**
- 2:05 **329.** Control of galvanic replacement reactions on electrodeposited cuprous oxide thin-films for rationally structured electrocatalytic interfaces. J. Lowe, **R. Coridan**
- 2:20 **330.** Fused hybrid linkers for metal-organic frameworks-derived bifunctional oxygen electrocatalysts. **M. Alam**, K. Ping, R. Bhadoria, P. Starkov
- 2:35 **331.** Development of high-performance Na-ion battery cathodes. **X. Li**, J. Song, B. Xiao, D. Reed, V. Sprenkle
- 3:05 Intermission.
- 3:20 **332.** Multi-electron redox in alkali-rich sulfides. **K.A. See**

- 3:50 333. Improving cell resistance and cycle life with solvate/thiophosphate hybrid electrolytes in lithium-metal and lithium-sulfur batteries. **A.A. Gewirth**, M. Philip, M. Shin
- 4:20 334. High-rate electrode materials for sodium-ion batteries. **S. Chen**
- 4:50 Concluding Remarks.

SECTION F

San Diego Convention Center
Room 24C

Sustainable Energy & Water via Innovative Electrocatalytic, Photocatalytic & Hybrid Catalytic Systems

Y. Cheng, F. Jiao, C. Liu, Y. Shao, G. Wu, *Organizers*
O. Y. Gutierrez Tinoco, U. Sanyal, *Presiding*

- 1:00 Introductory Remarks.
- 1:05 335. Electrochemical epoxidation of olefins using water as oxygen-atom source. **K. Manthiram**, K. Jin, J. Maalouf, N. Lazouski, N. Corbin, D. Yang
- 1:35 336. Electrocatalysis of alkene functionalizations. **S. Lin**
- 2:05 337. Enabling electrocatalytic routes for aldehyde hydrogenation with proton-donating chemical species. **O.Y. Gutierrez Tinoco**
- 2:30 338. Photocatalytic organic transformations on two-dimensional semiconductor systems. **Y. Sun**
- 3:00 Intermission.
- 3:15 339. Electrocatalytic hydrogenation of oxygenates exhibits particle size effects and they are metal specific. **U. Sanyal**, K. Koh, N. Singh, J. Fulton, A.J. Karkamkar, O.Y. Gutierrez Tinoco, J.A. Lercher
- 3:45 340. Electrochemically controlled redox switchable copolymerization reactions. Z.C. Hern, R. Dai, C. Liu, **P. Diaconescu**
- 4:10 341. E switchable polymerization catalysis. **J.A. Byers**, M. Qi, Q. Dong, D. Wang
- 4:35 342. Finding harmony among incompatibility in the selective oxidation of CH₄ to CH₃OH with atmospheric O₂. **B.S. Natinsky**, S. Lu, E.D. Copeland, J.C. Quintana

SECTION G

San Diego Convention Center
Room 25A

Sustainable Biofuels & Bio-Based Products

H. Lin, H. Wang, Y. Yang, *Organizers*
J. Fu, A. B. Padmaperuma, *Organizers, Presiding*

- 1:00 Introductory Remarks.
- 1:05 343. Co-processing of biomass thermochemical liquefaction liquids with gas oil in hydrocracking. **H. Wang**, D. Santosa, I. Kutnyakov, M. Flake, S. Lee

- 1:35 344. Conversion of low-grade biomass lipids to long-chain alkanes. **J. Fu**
- 2:05 345. Application of a combined wet *in situ* transesterification and hydrothermal liquefaction (iTHL) for the catalyst-free production of fuels from non-dried biomass. **B. Kim**, J. Park, J. Son, J.W. Lee
- 2:25 346. Effect of reaction conditions on hydrothermal treatment of food waste. **B. Motavaf**, P.E. Savage
- 2:45 347. Strategy and mechanism on hydrothermal catalysis to valorize biomass into add-value chemicals. **L. Kong**, Y. Sun
- 3:15 Intermission.
- 3:30 348. Bimetallic alkaline thermal treatment catalysts for enhanced H₂ production with suppressed CO₂ formation from unconventional biomass. **W. Li**, J. Chen, A.A. Park
- 3:50 349. Waste-to-energy conversion of biomass using a new two-stage sorption-enhanced thermochemical technology. **X. Yang**, Y. Jiang
- 4:10 350. Enhanced biofuel production through microbial electroreduction using novel cathode. A.H. Anwer, **M.Z. Khan**
- 4:30 351. Mechanistic investigation on biomass oxidation using nickel oxide nanoparticles in CO₂-saturated electrolyte for paired electrolysis. **S. Choi**, K. Nam
- 4:50 Concluding Remarks.

SECTION H

San Diego Convention Center
Room 25B

Materials for Energy & Environmental Sustainability

L. Fan, L. Qin, *Organizers, Presiding*

- 1:00 Introductory Remarks.
- 1:05 352. Heterojunction of reduced graphene oxide and graphitic-carbon nitride as a bi-functional photoelectrochemical catalyst for water splitting reaction. **Y. Sim**, H. Choi, U. Sim
- 1:25 353. Highly conductive 3D mesoporous graphene for highly efficient new generation solar cells. **W. Wei**, Y.H. Hu
- 1:45 354. Engineering technology of fractal dimension of graphene-based materials for energy applications. **J. Shin**, F. Moghadam, H. Yoo, H. Kim
- 2:05 355. Aluminosilicates catalysts for low and medium matured shale oil *in situ* upgrading. **J. Bian**, X. Meng, C. Li
- 2:25 356. Withdrawn
- 2:45 Intermission.
- 3:00 357. Dopant-mediated exsolved metal catalysts and catalytic behaviour in steam reforming of Glycerol. **A. Umar**

ENFL General Posters

Posters

H. Lin, L. Yang, *Organizers*

6:00 - 8:00

- 3:20 358.** Electrocatalytic oxidation of ethanol using modified copper nanoparticles/polypyrrole and multi-walled carbon nanotubes paste electrode in alkaline media. **A. El Attar, M. El Rhazi**
- 3:40 359.** Kinetic studies of electrocatalytic alcohol oxidation using cobalt oxide catalysts. **S.E. Michaud, C.C. McCrory**
- 4:00 360.** Dictating Pt-based electrocatalyst performance in PEFCs: From formulation to application. **T. Van Cleve, S. Khandavalli, S. Medina, K. More, D. Myers, N. Kariuki, M. Ulsh, S. Pylypenko, S. Mauger, K. Neyerlin**
- 4:20 361.** Electronically switchable windows using reversible metal electrodeposition for energy-efficient buildings and automobiles. **C. Barile, S.M. Islam, D. Miller, J. Jeanetta**
- 4:40** Concluding Remarks.

Gerry Meyer: The First 100 Years

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- 362.** Food waste valorization for the production of chemical: Study of ethyl levulinate production from citrus peels through an *in situ* hydrothermal reaction. **B. Kim, J. Yang, J. Park, J. Son, J.W. Lee**
- 363.** 3D nanosheet arrays structure oxygen vacancies modulated lithium manganese oxide on Ni foam for high performance lithium ion capacitor. **D. Yao, X. Xia, W. Lei, Q. Hao**
- 364.** Modeling nonaqueous proton wires built from helical peptide. **J. Bian**
- 365.** Technoeconomic analysis of photoelectrochemical hydrogen production from waste brine. **M. Contreras, S. Mubeen, C.O. Stanier**
- 366.** Infiltration of solution processable solid electrolytes for sheet-type all-solid-state lithium-ion batteries. **D. Klm, Y. Song, Y. Jung**
- 367.** Decarboxylation studies of activated carbon of oleic acid and other renewable feedstocks in subcritical water. **S.J. Fraser**
- 368.** Sustainable wastewater treatment via algal lipid accumulation. **Y. Li, I. Adame, J. Bouchard, r. kang, A. Mine, K. Maitra**
- 369.** Carbon/wrinkled graphene sheet double-coated nano-silicon composite as high-performance anode materials for lithium-ion batteries. **K. Lam, X. Hou, H. Chen**
- 370.** Facile synthesis of silicon/nanocrystalline cellulose film as anode material for lithium-ion batteries. **X. Li, Y. Shang**
- 371.** Facile synthesis of yolk-shell Cu-Sb-O nanospheres constituting a stable anode for lithium-ion storage. **T. Nguyen, I. Kim**
- 372.** Revealing superior electrochemical kinetics of $\text{Na}_3\text{V}_2(\text{PO}_4)_3/\text{rGO}$ for the cathode of Na-ion storage system. **K. Shin, H. Park**
- 373.** Radially assembled open-porous micro graphene-ball with immobilized sulfur nanorods for lithium-sulfur batteries. **H. Park, Y. Jeongseok, J. Park**
- 374.** Efficient *in situ* cross-linked binder for silicon anodes in lithium-ion batteries. **J. Lee, S. Bolloju, C. Chiou**

- 375.** Development of advanced multifunctional polymer binders for lithium-ion battery cathodes. **L. Rao**, A. Schmidt, C. O'Meara, J. Sayre, J. Kim
- 376.** Facile and versatile strategy towards high-performance Si anodes for practical Li-ion capacitors: Concomitant conductive network construction and dual-interfacial engineering. **R. Shao**, J. Niu, F. Zhu, M. Dou, Z. Zhang, F. Wang
- 377.** Porous carbons with tailored heteroatom doping and well-defined porosity as high-performance electrodes for robust Na-ion capacitors. M. Liu, J. Niu, **F. Wang**
- 378.** Calcium ion rechargeable battery comprising highly conductive and thermally stable ionic liquid gel electrolyte. **S. Biria**
- 379.** First row transition metal complexes as charge carriers in non-aqueous redox flow battery applications. **S. Sharma**, N.C. Smythe, G. Andrade, B.L. Davis, S. Maurya, R. Mukundan, J.C. Gordon
- 380.** Electrocatalytic effects of N and O dual doping on graphite felt electrodes for vanadium redox flow battery. H. Lim, S. Kim, **D. Lee**
- 381.** Effects of effluent and surrounding run-off from a lead battery industry on the water of River Ele in Nnewi, Anambra State Nigeria. **A.S. Ogbuagu**
- 382.** Stable, dual redox unit organic cathodes. **S. An**, T. Schon, D.S. Seferos
- 383.** Reversible and sustainable electrochemical Li-CO₂ reactions catalyzed by blood protein. J. Lee, J. Lee, H. Kim, **W. Ryu**
- 384.** From cathode to anode: An adventure of the elemental studies with X-ray fluorescence microscopy. **L. Li**, t. liu, X. Liu, G. Xu, F. Lin, Z. Chen
- 385.** Direct ascorbate fuel cell utilizing only carbon materials for anode and cathode. **K. Hendrix**, I. Chino, A. Keramati, J. Haan
- 386.** Potential electrolytes for Al-ion batteries. **Z. Slim**, E.J. Menke
- 387.** Renewable flexible supercapacitor based on lignin electrode and electrolyte. **J. Park**, H. Rana, H. Park
- 388.** Novel Fe₂O₃@N-doped porous carbon shell as an efficient electrocatalyst for the oxygen reduction reaction. **D. Kim**, E. Choi, M. Kim, C. Kim
- 389.** Facile and versatile wettability tuning of hydrocarbon reservoirs to mitigate liquid banking using omniphobic nano-texturing. **M. Sayed**, R. Saini, H. Ow, Z. Wang
- 390.** Cobalt nanoparticles packaged into nitrogen-doped porous carbon derived from metal-organic framework nanocrystals as efficient hydrogen evolution catalysts. P. Liu, K. Zhang, **N. Zhao**
- 391.** Facile preparation of multi-heteroatom doped three-dimensional hierarchically porous carbon from earth-abundant cattle bones as an efficient metal-free oxygen reduction electrocatalyst. **Y. Zan**, Z. Zhang, M. Dou, F. Wang
- 392.** Construction of the mixing entropy batteries driving the salinity difference by the phase state control of zwitterion/salt solution systems. **R. Sato**, H. Shibata, H. Ohno, N. Nakamura
- 393.** Synthesizing a novel Janus carbon nano-onions modified as a support for electrocatalytic nanoparticles. **A. Del Valle-Perez**, K. Gonzalez-Aponte, J. Reyes-Morales, Y.N. Escalera-Torres, L. Cunci
- 394.** Pore controlled heteroatom-doped carbon as oxygen reduction catalysts. **M. Kim**, J. Park, S. Kim, Y. Cho, Y. Sung
- 395.** Synthesis of activated carbon@MOF composites for biogas filtration. **C. Manquian**, F. Herrera, S. Dinesh
- 396.** Carbon nano onions used as support for electrocatalyst by applying the rotating disc electrode technique. **J. Ortiz**, H. Delgado, L. Cunci
- 397.** Identifying the role of pore modalities in oxygen reduction for optimizing Fe-N-C electrocatalyst. **J. Kim**, T. Hyeon
- 398.** Two-dimensional conjugated aromatic networks as high-site-density and single-atom electrocatalysts towards oxygen reduction reaction. **S. Yang**, Y. Yu, M. Dou, Z. Zhang, F. Wang
- 399.** Highly dispersed and crystalline Ta₂O₅ anchored Pt electrocatalyst with improved activity and durability toward oxygen reduction: Promotion by atomic-scale Pt-Ta₂O₅ interactions. **W. Gao**, Z. Zhang, M. Dou, F. Wang
- 400.** Copolymer-induced intermolecular charge transfer: Enhancing activity of metal-free catalysts for oxygen reduction. **Y. Yu**, Z. Zhang, L. Dai, F. Wang
- 401.** Importance of interfacial band structure between substrate and Mn₃O₄ nanocatalysts during electrochemical water oxidation. **H. Ha**, M. Lee, K. Nam
- 402.** Microwave metal discharge synthesis of graphite carbon-coated metal (M@C) nanoparticles. **J. Sun**, W. Wang
- 403.** Highly conductive N,P-co-doped porous carbon nanotubes for efficient electrocatalysis in rechargeable Zn-air batteries. **E. Choi**, M. Kim, D. Kim, C. Kim
- 404.** Self-assembly of NiFe-based ultrathin nanosheets on nickel foam as highly active and efficient electrocatalyst for water oxidation. **J. Wang**, Z. Chen
- 405.** Self-growing Ni-based hybrid nanosheet arrays on nanowires for overall water splitting. **X. Teng**, Z. Chen

- 406.** Polarization ferroelectric lithium-doped zinc oxide nanowires photoanodes for electrical water splitting. **J. Nah**
- 407.** Synthesis and application of novel low cost $\text{Cu}_{0.5}\text{Mn}_{0.5}\text{Fe}_2\text{O}_4$ spinel as cathode catalyst in microbial fuel cell. I. Das, **S. Das**, A. Agrawal, M.M. Ghangrekar
- 408.** Synthesis and application of Zr-metal–organic framework as cathode catalyst in the microbial fuel cell. **I. Das**, M.M. Ghangrekar
- 409.** New self-humidifying dual exchange membrane fuel cell (DEMFC) for non-humidified conditions. **S. Lee**, J. Chae, H. Kim
- 410.** Fuel-flexible split pH direct liquid fuel cell for alcohols. **I. Chino**, K. Hendrix, A. Keramati, O. Muneeb, **J. Haan**
- 411.** Effect of microstructure of porous flow field on performance of polymer electrolyte membrane fuel cell. **W. Hwang**, J. Park, Y. Sung
- 412.** Development of microbial fuel cell to produce electricity from cellulosic biomass using bovine rumen bacteria. **S. Chung**, E. Kang, Y. Shin, P. Park, C. Han, S. Moon, J. Park
- 413.** M-doped (M=Mn, Co, Zn) ferrites as electrocatalytic cathode materials for alkaline membrane fuel cells (AMFC). **J. Del Pilar**
- 414.** Simultaneous production of electricity and hydroxide by a cation exchange membrane direct formate fuel cell. **V. Galvan**, S. Kar, S.G. Prakash
- 415.** Influence of hydrocarbon polymer-based electrode ionomer conditions on polymer electrolyte fuel cell performance. **J. Chae**, S. Lee, H. Kim
- 416.** Synthesis of CeO_2 - ZrO_2 solid solutions for thermochemical CO_2 splitting. H. Shi, F. Wang, **N. Zhao**, F. Xiao
- 417.** Preparation of amino-functionalized metal–organic frameworks $\text{Cu}_3(\text{BTC})_2$ for CO_2 adsorption. X. Lu, F. Wang, **F. Xiao**, L. Li, N. Zhao
- 418.** Nanostructured tin electrode for high-performance electrochemical CO_2 reduction. **J. Jeong**, J. Kang, H. Shin, Y. Sung
- 419.** Withdrawn
- 420.** Electrochemical conversion of carbon dioxide into formate on tin surfaces. **S. Xiong**, R. Clark, C. Franco, J. Haan
- 421.** Electrocatalytic reduction of carbon dioxide using self-assembled metal porphyrins. **J. Mennel**, S. Supakul, C. Barile
- 422.** Exploring the spatial distribution of triplet states in perfluoroalkyl zinc porphyrins for solar energy conversion. **E. Viere**
- 423.** Imidazole-containing small molecule-based hole-transporting materials for efficient perovskite solar cells: Management of transition dipole moments and bifacial passivation of organic hole-transport interlayer for p-i-n type devices. **S. Park**
- 424.** First-principles investigation on the photovoltaic properties of Sn and Sr mixed organic perovskites. **L. Meng**, Y. Jia, H. Liu
- 425.** Amplified hot electron flow on perovskite modified plasmonic Au-TiO₂ nanodiode. **Y. Park**, J. Choi, C. Lee, A. Cho, N. Park, H. Ihee, J. Park
- 426.** Cation engineering for its application to perovskite solar cells. **B. Kim**
- 427.** Fine-controlling nanostructured silicon interfaces using core-shell magnetic nanoparticles for efficient solar energy conversion. **M. Patrick**
- 428.** Chemical reduction and characterization of Pt nanoparticles for an ammonia oxidation electrocatalyst. **N.A. Huertas**, A.D. Rivera-Ruiz, I. Gonzalez-Gonzalez
- 429.** Electrochemical oxidation of dimethyl carbonate on Pt and Pt-Ru supported catalysts. **A. Baxter**, V. Galvan, S.G. Prakash
- 430.** Electrocatalytic methane oxidation with transition metal catalyst. **J. Iniguez**, C. Liu
- 431.** Hydrogenation of selected heavy oil model systems using iron-based dispersed catalyst. **B. Antwi Peprah**
- 432.** In-depth study on the effect of oxygen-containing functional groups in pyrolysis oil by P-31 NMR. **Z. Wu**, H. Ben, G. Han, W. Jiang, A.J. Ragauskas
- 433.** Exergy analysis of hydro-desulfurization (HDS) unit of linear-alkyl benzene plant using aspen HYSYS: Case study of Kaduna refining and petrochemical company. **O. Isaac**
- 434.** Promising technology potentially fueled with mixtures of gasoline and biodiesel to meet future engine efficiency and emission targets with gasoline compression ignition. **O. Lim**
- 435.** Sandwich bed CuZnOx-Cu/mordenite-CuZnOx coupling catalysis to produce ethanol from syngas. **K. Zhang**, P. Liu, N. Zhao
- 436.** Ionic liquid pretreatment for sustainable biofuels from low-temperature biomass pyrolysis. **L. Ma**, G. Dou, D. Wang, J.L. Goldfarb
- 437.** Insights into the chemical structure-fuel property relationship of myrcene derived bio-fuels. **T. Rajale**, C.M. Moore, A.D. Sutton
- 438.** Hydrothermal liquefaction of clay-biomass mixtures for simultaneous production of heterogeneous hydrochars and upgraded biofuels. **Q. Ma**, K. Wang, F. Wang, J.W. Tester, G. Huang, L. Han, J.L. Goldfarb
- 439.** Biological production of isopropanol through propane oxidation using *Methylobacterium*

alcaliphilum 20Z. **J. Na**, H. Ko, E. Lee, S. Park, H. Kim, J. Lee

440. Efficient glycerolysis process of high free fatty acid feedstock for the production of fatty acid methyl ester. **R. Kundu**

441. Selective hydrotreating and hydrocracking of light cycle oil into benzene, toluene, and xylene over Ni₂P/β catalyst. **Y. Kim**, Y. Lee

442. Evaluating fuel properties of *Pongamia pinnata*. **S. Summers**, J. Fu, S.Q. Turn

443. Study of wet *in situ* transesterification of spent coffee grounds with supercritical methanol for the production of biodiesel. **B. Kim**, J. Son, J. Park, J. Yang, J.W. Lee

444. Comparisons of properties of asphaltenes from Brazilian offshore fields. **E. Chrisman**, R. Santana, M. Queiroz, R. Gonçalves, P.R. Seidl, F. Barbosa Silva, M. Guimarães, A. Magalhães, S. Menezes

445. Regeneration of spent denitration catalyst of coal fired power plant. **T. Kato**, K. Sakusabe, Y. Mochizuki, H. Okawa, K. Sugawara

446. Sequential extraction of small molecular substances in coal and its effect on coal adsorption of methane. **Y. Zhiyuan**

447. New catalytic two-stage coal processing technology for optimal uses of C and H and production of desired gases. **W. Lu**, Q. Cao, B. Xu, M. Fan

448. Enumeration of the model for optimal design of fired heaters. **I. Intararit**, U. Suriyaphadilok, M. Bagajewicz, A. Costa

449. M–Al spinel oxides (M=Mg, Ni, Mn, Co) doped ordered mesoporous alumina supported cobalt-based catalysts for Fischer–Tropsch synthesis. J. Wang, J. Wang, B. Hou, **L. Jia**

450. Theoretically predicted structure and morphology of Ru_n clusters on Co surfaces. L. Liu, Q. Wang, L. Jia, B. Hou, **D. Li**

451. Mercury forms in FGD gypsum produced from different FGD systems. **K. Sakusabe**, T. Kato, H. Okawa, K. Sugawara

452. Enzyme-mimetic heterogeneous catalysis: Reversible and cooperative photoactivation between titanium dioxide and isolated copper atom. **B. Lee**, T. Hyeon

453. Determination of alkanolamines in scrubbing amines samples with improved separation technology and suppressed conductivity detection. **T.T. Christison**, J.S. Rohrer

454. High-resolution quadrupole mass spectrometry analysis for fusion reactor and plasma facing materials. **G. Thier**, L. Kephart

455. Microemulsion formation by the hydrophilic-

lipophilic deviation concept using carboxylate based extended surfactants: Effect of ethylene oxide group. **S. Kumkhuntod**, A. Charoensaeng, U. Suriyaphadilok

456. Color neutral smart windows using nickel oxide electrochromism and ion intercalation with reversible metal electrodeposition. **S.M. Islam**, T.S. Hernandez, M.D. McGehee, C. Barile

457. Synthesis and low temperature thermoelectric properties of Cu₂Te included Bi–Sb–Te p-type materials. **D. Roh**, W. Shin, J. Song, H. Jeh

458. Modification of catalyst-ionomer interface and pore structure by controlling anion-exchange ionomer dispersion. **S. Kim**, M. Her, Y. Sung

459. Non-catalytic and catalytic pyrolysis of low density polyethylene (LDPE) into liquid fuel using local clay composites. **A.I. Inyangudoh**, O. Edem, E. Inam

460. Synthesis of 2-hydroxy-6-naphthoic acid (2,6-HNPA) over alkali metal carbonates. **D. Kim**, Y. Lee

461. Mo-incorporated nickel oxides improves the alkaline hydrogen evolution reaction of crystalline Ni: Accelerated Volmer reaction. **J. Huang**, S. Jin, B. Song

462. Understanding degradation of Ni-Rich LiNi_xMn_yCo_{1-x-y}O₂ (NMC): Moisture impact and chemical composition relationship. **J. Choi**, L. Dong, C. Yu, C. O'Meara, E. Lee, J. Kim

WEDNESDAY MORNING – ENFL

SECTION A

San Diego Convention Center

Room 23A

7th International Symposium on Mesoporous Zeolites

K. Li, *Organizer*

J. Garcia Martinez, *Organizer, Presiding*

X. Fan, *Presiding*

8:00 **463.** Mesoporous zeolites in crude oil valorization: Potentials, challenges, and research essentials. **F. Althenayan**

8:40 **464.** Selective conversion from methanol into propene over mesoporous high silica beta zeolite. **F. Xiao**, C. Zhang

9:10 Intermission.

9:30 **465.** Catalyst performance trends and correlations between real-world and surrogate test conditions. **T.J. Kucharski**, E. Converse, J.T. O'Brien, S. Fernandez, S. Kobaslija, B.S. Hanna, K. Zhang, T. Pilyugina, M.L. Ostraat

- 10:00** **466.** Preparation of micro-mesoporous composite sieves catalyst and its catalytic cracking performance of coal tar. **Y. Zhiyuan**
- 10:30** Concluding Remarks.

SECTION B
San Diego Convention Center
Room 23B

Energy Conversion Technologies Based on Solid Oxide Electrolyte Electrochemical Cells

Solid Oxide Electrolysis Cell

K. Zhao, *Organizer*
S. Ha, *Organizer, Presiding*

- 8:20** Introductory Remarks.
- 8:25** **467.** Carbon dioxide reduction via molybdenum doped strontium ferrite cathode in solid oxide electrolysis cell. **C. Xia**, Y. Li, Y. Jiang
- 8:55** **468.** High-temperature steam electrolysis for renewable hydrogen production. **O. Marina**, J. Holladay, J. Stevenson, K. Meinhardt, G. Whyatt, C. Coyle, D. Edwards, K. Recknagle, J. Bao
- 9:25** **469.** Performance characteristics of flat-tubular solid oxide co-electrolysis cells for syngas production by electrochemical conversion of H₂O/CO₂. **T. Lim**, H. Kim, J. Hong, S. Lee, S. Park, R. Song
- 9:55** Intermission.
- 10:15** **470.** Performance and degradation of metal-supported solid oxide electrolysis cells with infiltrated catalysts. **F. Shen**, E. Dogdibegovic, R. Wang, G. Lau, M.C. Tucker
- 10:45** **471.** Nano-/micro- honeycomb solid oxide electrolysis cell anodes for rapid oxygen generation, diffusion, and exhalation. **W. Tong**, W. Zhang, Y. Li, Y. Zheng, B. Yu, J. Chen, X. Sun
- 11:15** **472.** Solid oxide fuel cell reactors for CO₂-emission free co-generation of power and ethylene from ethane. **X. Fu**

SECTION C
San Diego Convention Center
Room 23C

Atomic-level Understanding & Design of Materials & Processes for Energy Applications

H. Zhuang, *Organizer*
Y. Liu, *Organizer, Presiding*

- 8:00** Introductory Remarks.
- 8:05** **473.** Excited state resonating Hartree-Fock models of excited state processes in methane activation applications. **L.M. Thompson**

- 8:35** **474.** Computational design of oxides and nitrides in the presence of defects and disorder. **S. Lany**
- 9:05** **475.** Selective solvent induced stabilization of polar oxide surfaces in electrochemical environment. **M. Todorova**, S. Yoo, J. Neugebauer
- 9:35** **476.** Modeling organic solar cells. **G.C. Schatz**
- 10:05** Intermission.
- 10:20** **477.** Atomic prediction of energy landscape of the charge transfer reaction at the complex Li/SEI/electrolyte interface. **Y. Qi**, Y. Li
- 10:50** **478.** Excited electronic states and ultrafast dynamics: Pushing towards design of materials. **A. Schleife**
- 11:20** **479.** Structure inference from X-ray absorption spectroscopy for *operando* experimentation. **M.S. Hybertsen**

SECTION D
San Diego Convention Center
Room 24A

Photocatalysis for Energy & Environment

Y. Lin, M. Long, *Organizers*
F. Wang, W. Wei, *Organizers, Presiding*

- 8:00** Introductory Remarks.
- 8:05** **480.** Heterogeneous catalysts for highly efficient electrochemical reduction of CO₂. **M. Wang**, X. Jiang, X. Wang, Y. Shen
- 8:45** **481.** Semi-metallic tungsten trioxide with improved conductivity for infrared light photoelectrochemical water splitting. **F. Wang**
- 9:15** **482.** Enzyme-based photoelectrochemical systems for photo-biocatalytic processes. **O. Yehezkeili**
- 9:35** Intermission.
- 9:50** **483.** Multi-modal optimization of bismuth vanadate photoanodes *via* combinatorial alloying and hydrogen processing. **P. Newhouse**, D. Guevarra, M. Umehara, D. Boyd, L. Zhou, J. Cooper, J. Haber, J.M. Gregoire
- 10:20** **484.** Improving performance of water oxidation photoanodes with nanoparticle-polymer hybrid films: Enhanced light-harvesting and catalytic efficiency. **H. Kim**, J. Ryu
- 10:40** **485.** Optoelectronic properties of copper-based P-type semiconductor: Combined experimental and theoretical approach. **Z. Zhang**, J. Cooper
- 11:00** **486.** Unraveling interface energetics and operating principle in ultrathin metal film/Si photoelectrodes. **J. Jung**, J. Lee
- 11:20** Concluding Remarks.

SECTION E
San Diego Convention Center
Room 24B

Innovative Chemistry & Materials for Electrochemical Energy Storage

H. Chen, R. J. Clement, F. Lin, W. Xu, *Organizers*

W. Kan, *Organizer, Presiding*

G. He, S. Oh, *Presiding*

- 8:00** Introductory Remarks.
- 8:05** **487.** Fabrication of dendrite-free anodes with liquid metal for highly stable sodium metal batteries. **G. He**, Q. Zhang, Y. Ding
- 8:35** **488.** Designing a novel all-solid-state sodium-carbon dioxide battery. **W. Li**, X. Hu
- 9:05** **489.** Various types of air cathode materials for metal air battery and all solid-state rechargeable Al air battery. **R. Mori**
- 9:25** Intermission.
- 9:40** **490.** S₈ reduction processes and Mg reactivity in a Mg-S₈ battery. **S.C. Bevilacqua**, K.A. See
- 10:00** **491.** Reaction mechanisms for long-life rechargeable Zn/MnO₂ batteries. Y. Li, S. Wang, J.R. Salvador, J. Wu, B. Liu, W. Yang, J. Yang, W. Zhang, J. Liu, **J. Yang**
- 10:30** **492.** Non-aqueous zinc-ion batteries based on an open framework cathode. **Y. Liao**, W. Kaveevivitchai
- 11:20** **493.** Electrode/electrolyte compatibility in rechargeable aluminum batteries: Chemical reactions and electrochemical properties between chloroaluminate ionic liquids and vanadium pentoxide. **X. Wen**, J. Guo
- 11:40** Concluding Remarks.

SECTION F
San Diego Convention Center
Room 24C

Sustainable Energy & Water via Innovative Electrocatalytic, Photocatalytic & Hybrid Catalytic Systems

F. Jiao, C. Liu, Y. Shao, *Organizers*

Y. Cheng, G. Wu, *Organizers, Presiding*

- 8:00** Introductory Remarks.
- 8:05** **494.** Molecularly precise single atom catalysts for energy conversion. M. Jackson, C.J. Kaminsky, S. Oh, M. Pegis, J. Rosenberg, P. Smith, **Y. Surendranath**
- 8:35** **495.** Challenges in development of electrocatalysts for water splitting. D. Jung, P. Papa Lopes, D. Strmcnik, N. Markovic, **V. Stamenkovic**

- 9:05** **496.** Designing earth-abundant catalysts for electrocatalytic and photoelectrochemical conversion of energy. **S. Jin**
- 9:35** **497.** Carbon-rich organic semiconductors for photoelectrochemical water splitting. **X. Feng**
- 10:05** Intermission.
- 10:10** **498.** Molecular-level design for high-density catalytic active sites towards high-performance nonprecious metal electrocatalysts. **J. Hu**
- 10:40** **499.** B2-phase intermetallic palladium copper nanowires enable enhanced electrocatalysis. **M.M. Flores Espinosa**, M. Xu, T. Cheng, C. Choi, W.A. Goddard, Y. Huang
- 11:10** **500.** Uniform, assembled sub-5 nm Mn₃O₄ nanoparticles as water oxidation electrocatalysts at neutral pH. **K. Cho**, S. Park, H. Seo, Y. Lee, M. Lee, K. Nam
- 11:35** **501.** [2Fe-2S]-Based catalytic metallopolymers for hydrogen generation from aqueous feedstocks. **M. Karayilan**, K.C. McCleary-Petersen, K. Clary, R.S. Glass, D.L. Lichtenberger, J. Pyun

SECTION G
San Diego Convention Center
Room 25A

Sustainable Biofuels & Bio-Based Products

H. Lin, A. B. Padmaperuma, H. Wang, *Organizers*

J. Fu, Y. Yang, *Organizers, Presiding*

- 8:00** Introductory Remarks.
- 8:05** **502.** Synthesis of renewable high density jet fuel with lignocellulose. **N. Li**, G. Li, Y. Liu, X. Sheng, F. Chen, J. Xu, J. Yang, Y. Cong, T. Zhang
- 8:45** **503.** Predicting physical properties of bio-renewable molecules in a search for a drop-in Jet-A fuel. **A. Landera**, R.P. Bambha, A. George
- 9:05** **504.** Biorefining impacts of novel octane hyperboosting phenomenon in prenil/gasoline blends. **E. Monroe**, R.W. Davis, A. Geoge
- 9:25** Intermission.
- 9:40** **505.** Tuning the structure of Pt-carbon complex catalysts for aerobic base-free oxidation of glycerol. **X. Duan**, G. Qian, X. Zhou
- 10:40** **506.** Structural engineering of Mo₂C catalysts for lignin depolymerization. **R. Ma**, X. Lu, W. Zhu
- 11:00** **507.** Computational studies on the efficient conversion of model biomass compounds into platform chemicals. **S. Li**
- 11:20** Concluding Remarks.

SECTION H
San Diego Convention Center
Room 25B

Materials for Energy & Environmental Sustainability

L. Fan, L. Qin, *Organizers, Presiding*

- 8:00** Introductory Remarks.
- 8:05** **508.** Development, integration and real environment investigation of off-grid solar thermal water and space heating system using phase-change materials. **D. Roan**, J. Prakash, A.M. Kannan
- 8:25** **509.** Multipronged approach to tackle luminophore losses in luminescent solar concentrators. G. Lyu, J. Kendall, **R.C. Evans**
- 8:45** **510.** Highly porous phase change materials based on Candelilla wax as renewable source for solar-to-thermal energy conversion and storage. A. Morales-Rosales, **C. Espinoza-González**, L. Arizmendi-Galaviz, S. Fernández-Tavizón, O. Rodríguez-Fernández
- 9:25** **511.** Biofuel cells for personalized biosensors and bioelectronics. **I. Jeerapan**
- 9:45** **512.** Algal biofuel: Culture and optimization of *Scenedesmus obliquus* in untreated energetic-laden wastewater streams. **J. Abraham**, A. RoyChowdhury, T. Abimbola, Y. Lin, C. Christodoulatos, A. Lawal, P. Arrienti, B. Smolinsky, W. Braida
- 10:00** Intermission.
- 10:15** **513.** Chemical looping partial oxidation of methane: Size effect of hematite on syngas selectivity. **Y. Liu**, L. Qin, Z. Cheng, M. Guo
- 10:35** **514.** Novel synthesis of high-stable Ca-based sorbent for CO₂ capture: Stabilizing effect of vanadium slag. **X. Zhao**, Y. Jiang, F. Yan, Z. Zhang
- 10:55** **515.** New type of CO₂ fixation process via mineral carbonation with electrodialysis. **A. Yamasaki**, M. Noguchi, t. Inagaki, M. Abe
- 11:15** **516.** Materials for CO₂-capture solvent storage: a computational and experimental assessment of steel vs. plastics. **M. Nguyen**, K. Grubel, D. Heldebrant, R. Rousseau, V. Glezakou
- 11:35** **517.** Nanostructuring of pseudocapacitive MnFe₂O₄/porous rGO electrodes in capacitive deionization. **H. Younes**, L. Zuo
- 11:55** Concluding Remarks.

Fundamentals of Catalysis in Nanoporous Materials

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WEDNESDAY AFTERNOON – ENFL

SECTION A
San Diego Convention Center
Room 23A

Advances in Fundamental Research for Energy Storage Beyond Lithium-Ion

R. Assary, L. Cheng, B. Narayanan, *Organizers, Presiding*

- 1:00** Introductory Remarks.
- 1:05** **518.** Next generation batteries. **G. Crabtree**
- 1:35** **519.** Multivalent battery chemistries: Anodes, cathodes, and electrolytes. **A.A. Gewirth**
- 2:05** **520.** Hexagonal boron nitride gel electrolytes for solid-state batteries. **M. Hersam**
- 2:35** **521.** Non-aqueous redox flow batteries: Challenges and opportunities. **J. Nanda**
- 3:00** Intermission.
- 3:05** **522.** Molecular simulation studies of the bulk electrolytes and interfaces for beyond Li-ion. **O. Borodin**, T.P. Pollard, J. Vatamanu
- 3:35** **523.** Atomically-informed phase-field modeling of Li and Mg electrodeposition morphologies. Z. Liu, Y. Li, L. Chen, **Y. Qi**
- 4:05** **524.** Dendrite formation in Li-metal anodes: Atomistic machine learned molecular dynamics study. **J.M. Seminario**, L.A. Selis, D.E. Galvez-Aranda
- 4:35** **525.** First-principles studies of electrochemical reactions at interfaces. **P. Zapol**

SECTION B
San Diego Convention Center
Room 23B

Energy Conversion Technologies Based on Solid Oxide Electrolyte Electrochemical Cells

Solid Oxide Fuel Cell

S. Ha, *Organizer*

K. Zhao, *Organizer, Presiding*

- 1:00** Introductory Remarks.
- 1:05** **526.** Requirements of SOFC technology for electric vehicles. **M. Abdul Jabbar**, F. Yosuke, N. Dale
- 1:35** **527.** Solid oxide fuel cell technology: Outlook and innovations. **N. Minh**, Y. Lee, T. Tran
- 2:05** **528.** Progress in metal-supported solid oxide fuel cells: Performance and durability. **E. Dogdibegovic**, R. Wang, G. Lau, M.C. Tucker
- 2:35** Intermission.
- 2:55** **529.** Vanadium doped intermediate temperature solid oxide fuel cell (IT-SOFC) cathodes. **O. Demircan**
- 3:25** **530.** Effect of coal properties on the performance of solid oxide direct carbon fuel cells. **A. Zhou**, G. Liu, Y. Zhang, J. Qiu
- 3:55** **531.** Enhancing the performance of partial oxidation of gasoline over Ni catalysts with Mo addition for SOFCs application: Experimental and DFT studies. **S. Ha**, Q. Bkour, F. Che, K. Lee, C. Zhou, J. Boscoboinik, K. Zhao, J.T. Gray, J. McEwen, S.R. Saunders, M. Norton, T. Kim

SECTION C
San Diego Convention Center
Room 23C

Atomic-level Understanding & Design of Materials & Processes for Energy Applications

Y. Liu, *Organizer*

H. Zhuang, *Organizer, Presiding*

- 1:00** Introductory Remarks.
- 1:05** **532.** Simulating direct images of the covalent bond from atomic force microscopy. **J.R. Chelikowsky**
- 1:35** **533.** Effects of abstractor strengths, C-H bond strengths and radical-surface interactions on reactivity and selectivity in reactions limited by C-H activation on metal oxides. **P. Deshlahra**, E. Iglesias
- 2:05** **534.** Materials design for plasma catalytic transformations. **W.F. Schneider**, P. Mehta
- 2:35** Intermission.

- 2:50** **535.** Theoretical study of acetic acid decomposition and the role of co-adsorbates. **L. Arnadottir**, K.C. Chukwu
- 3:20** **536.** Computer modeling of water-mediated proton conduction in metal-organic frameworks. **F. Paesani**
- 3:50** **537.** Dehydrogenation mechanisms of methylcyclohexane on γ -Al₂O₃ supported Pt₁₃; Impact of cluster ductility. **P. Sautet**, W. Zhao, C. Chizallet, P. Raybaud
- 4:20** **538.** Computational studies of Rh-containing isolated sites in bimetallic metal-organic frameworks for hydrogenation reactions. R. Thayalan, N.B. Shustova, D.A. Chen, **K.D. Vogiatzis**

SECTION D
San Diego Convention Center
Room 24A

Photocatalysis for Energy & Environment

M. Long, W. Wei, *Organizers*

Y. Lin, F. Wang, *Organizers, Presiding*

- 1:00** Introductory Remarks.
- 1:05** **539.** Development of photoactive TiO₂⁻, Bi₂WO₆⁻, and Fe₂O₄-based catalysts for the treatment of contaminants of emerging concern in water. **D.D. Dionysiou**
- 1:45** **540.** Surface defect chemistry modulation in photocatalytic NO conversion: Reactivity and mechanism. **C. Wang**
- 2:15** **541.** Photocatalysis-assistant extraction of uranium in water. **Y. Lu**, S. Liu
- 2:35** Intermission.
- 2:50** **542.** Critical roles of alcohols for sustainable photocatalytic production of H₂O₂ on TiO₂ at neutral pHs. **M. Long**, J. Zhang, L. Zheng
- 3:20** **543.** Photoelectrocatalytic degradation of phenol to promote hydrogen production. **z. zhou**, **G. Zhao**
- 3:40** **544.** Advanced graphene nanomembranes approaches to highly efficient solar thermal generation of clean water. **B. Hassan**, H. Javed, W. Que, A. Mahmood
- 4:00** **545.** Energy-resolved distribution of electron traps study for ZnTi mixed metal oxides as photocatalysts to degrade phenol. **C. Chuaicham**, K. Sasaki
- 4:20** Concluding Remarks.

SECTION E
San Diego Convention Center
Room 24B

Hybrid Functional Porous Materials: MOFs, Silica & Conductive Polymers

J. L. Lutkenhaus, S. V. Patwardhan, *Organizers*
S. K. Nune, *Organizer, Presiding*

- 1:00** Introductory Remarks.
- 1:05** **546.** MOF chemistry: Deliberate pore system control for gas separations and storage. **M. Eddaoudi**
- 1:45** **547.** Hybrid and functionalized MOFs for fuel production, transport, and storage. **M. Allendorf**, A. Schneeman, V. Stavila, T. Wang
- 2:15** **548.** Porous framework materials for sound attenuation applications. **S.K. Nune**, Q.R. Miller, H.T. Schaef, K. Jung, K.M. Denslow, M. Prowant, P. Martin, B. McGrail
- 2:35** **549.** Redox-active coordination polymers as electrode materials for rechargeable batteries. A. Li, Y. Liao, **W. Kaveevivitchai**
- 2:50** Intermission.
- 3:05** **550.** All-nanoporous hybrid membranes: Redefining upper limits on membrane separation performance. **S. Nair**
- 3:35** **551.** Engineered porous materials: Growth and separation of noble gases and critical materials. **M.A. Sinnwell**, P.K. Thallapally
- 3:55** **552.** Withdrawn
- 4:15** **553.** Metal-organic frameworks and the degradation of chemical warfare agent simulants. **M. Kalaj**, M.R. Momeni, M.S. Denny, K.C. Bentz, J. Palomba, F. Paesani, S. Cohen
- 4:35** Concluding Remarks.

SECTION F
San Diego Convention Center
Room 24C

Sustainable Energy & Water via Innovative Electrocatalytic, Photocatalytic & Hybrid Catalytic Systems

F. Jiao, C. Liu, Y. Shao, *Organizers*
Y. Cheng, G. Wu, *Organizers, Presiding*

- 1:00** Introductory Remarks.
- 1:05** **554.** Maximizing efficiencies of photocatalytic water splitting by engineering interfaces in multi-component photocatalysts. **S. Linic**
- 1:35** **555.** Nanoscale probing of carrier-selective catalyst-semiconductor contacts in water-splitting photoelectrodes. **S.W. Boettcher**, F. Laskowski, M. Nellist

- 2:05** **556.** *In situ* and *operando* spectroelectrochemical techniques for evaluating interfacial carrier behavior in emerging photoelectrodes for solar fuel production. **Y. Liu**, K.A. Sivula, N. Guijarro Carratala
- 2:30** **557.** Photocatalytic water disinfection by rationally doped titania nanostructures and electrocatalytic synthesis of value-added fuels from CO₂. **T. Xu**
- 2:55** Intermission.
- 3:10** **558.** Plasmonic catalysis: Heating vs. hot electrons. **J. Liu**
- 3:40** **559.** Electrochemical investigation of the effect of graphitic carbon nitride addition in BiVO₄ to improve photoelectrochemical water oxidation performance. **U. Prasad**, J. Prakash, B. Azeredo, A.M. Kannan
- 4:10** **560.** Sensing the potential at the semiconductor-liquid interface: Route to uncover the electronic dynamics during photoelectrosynthetic reactions. **N. Guijarro Carratala**
- 4:35** **561.** Close space sublimation synthesis and photoelectrochemical efficiency of vertical tin disulfide nanoflake photoanodes. **B. Giri**, M. Masroor, K. Kushnir, A. Carl, H. Zhang, A.A. McClelland, G. Tompsett, M.T. Timko, D. Wang, R.L. Grimm, L.V. Titova, P. Rao

SECTION G
San Diego Convention Center
Room 25A

Sustainable Biofuels & Bio-Based Products

J. Fu, H. Lin, A. B. Padmaperuma, *Organizers*
H. Wang, Y. Yang, *Organizers, Presiding*

- 1:00** Introductory Remarks.
- 1:05** **562.** Nitrogen-containing chemicals from biomass. **N. Yan**
- 1:45** **563.** *De novo* stereospecific biosynthesis of 1,2-propanediol from renewable feedstocks through lactic acid. **W. Niu**, L.D. Kramer, J. Mueller, J. Guo
- 2:05** **564.** Activity-tunable biocatalyst for algal cell wall degradation and lipids extraction. **C. Wu**, D. Liu, Q. Chen, I.D. Gates
- 2:25** **565.** Bioaccumulation of inorganic nitrogen and phosphorus for soil fertilization and remediation. **D. Loh**, P. Silver, D.G. Nocera
- 2:45** Intermission.
- 3:00** **566.** Efficient depolymerization of organosolv lignin in ethanol/iso-propanol media without catalyst. **C. Cheng**, J. Truong, J. Barrett, D. Shen, M.M. Abu-Omar, P.C. Ford

- 3:20 **567.** Characterization of lignin depolymerisation products by UV fluorescence spectroscopy. **E. Bartolomei**, Y. Le Brech, A. Dufour, E. Terrell, M. Garcia Perez, F. Aubriet, V. Carre, P. Arnoux
- 3:40 Concluding Remarks.

SECTION H

San Diego Convention Center
Room 25B

Cross-Scale Science for Energy & Resource Recovery

D. P. Butt, G. Gadikota, *Organizers, Presiding*

- 1:00 **568.** Towards multiscale characterisation of asphaltene intermolecular structure: Combined simulation and scattering approach. **T. Headen**, E. Muller, G. Jimenez-Serratos, M. Hoepfner, R. Rahman
- 1:25 **569.** Influence of self-assembly of polyaromatic macromolecules on the dynamic wettability alteration of calcite, silica, and illite surfaces. S. Mohammed, **G. Gadikota**
- 1:45 **570.** Reactive molecular dynamics approach to understand the chemistry-driven structural transformations in heat-treated clay minerals. **M. Muraleedharan**, A.C. Van Duin
- 2:05 **571.** GPU-accelerated simulations of fluid flow in nanoporous source rocks with many-body dissipative particle dynamics. **Y. Xia**, A. Blumers, J. Goral, Z. Li, L. Luo, Y. Tang, J. Kane, H. Huang, M. Andrew, M.D. Deo
- 2:25 Intermission.
- 2:35 **572.** Origin of reactivity thresholds and mechanisms in nanoconfined water films. **Q.R. Miller**, S.N. Kerisit, J.P. Kaszuba, H.T. Schaef, M.E. Bowden, B. McGrail, K. Rosso
- 3:00 **573.** Nanoscale analysis of chemo-mechanical effects on fracture tip propagation in synthetic geoarchitectures. **W. Nguyen**, T. Tran, C. Shaskey, P. Newell, K. Park, J. McLennan
- 3:20 **574.** Pore scale reduced order model describing the Darcy scale fracture-matrix interactions. S. Ashraf, **J. Phirani**
- 3:45 **575.** Gas hydrate slurry viscosity model towards hydrate plugging risk assessment. **A. Abdul Majid**, D. Wu, C.A. Koh
- 4:05 **576.** Withdrawn

Fundamentals of Catalysis in Nanoporous Materials

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In Situ & Operando Spectroscopy

Sponsored by CATL, Cosponsored by ENFL and PHYS

Understanding the Role of Water in Solid Acid-Base Catalysis

Sponsored by CATL, Cosponsored by ENFL, INOR and PHYS

Amorphous Materials: Challenges & Opportunities

Sponsored by CATL, Cosponsored by ENFL

Catalytic Conversion of Biomass-Derived Oxygenates

Sponsored by CATL, Cosponsored by ENFL

THURSDAY MORNING – ENFL

SECTION A

San Diego Convention Center
Room 23A

Advances in Fundamental Research for Energy Storage Beyond Lithium-Ion

R. Assary, L. Cheng, B. Narayanan, *Organizers, Presiding*

- 8:00 Introductory Remarks.
- 8:05 **577.** Lithium-sulfur batteries with practically necessary parameters. **A. Manthiram**
- 8:35 **578.** Reactivity and solvation at solid/liquid interfaces of Li-metal based batteries. **P.B. Balbuena**
- 9:05 **579.** Atomic scale simulations of performance-limiting phenomena in lithium-sulfur battery cathodes. **D. Siegel**
- 9:35 **580.** Metal-air batteries: O₂ electrochemistry in alkali metal ion-bearing nonaqueous electrolytes. **B.D. McCloskey**
- 10:05 Intermission.
- 10:20 **581.** Lithium air batteries: Challenges and opportunities. **A. Salehi-Khojin**
- 10:50 **582.** Superoxide batteries based on one-electron reduction of oxygen. **Y. Wu**
- 11:20 **583.** Insights into Li-O₂ electrochemistry for energy storage from computational studies. **L.A. Curtiss**
- 11:50 Concluding Remarks.

SECTION B
San Diego Convention Center
Room 23B

Energy Conversion Technologies Based on Solid Oxide Electrolyte Electrochemical Cells

New Materials & Characterizations

K. Zhao, *Organizer*

S. Ha, *Organizer, Presiding*

- 8:00** Introductory Remarks.
- 8:05** **584.** High performing and durable reversible proton-conducting solid oxide cells promoted by innovative materials and structure of electrode developed at INL. **D. Ding**, H. Ding, W. Wu
- 8:35** **585.** Studying the effects of secondary phases on high temperature electrochemical energy conversion with *operando* optical spectroscopy. **R.A. Walker**, M.M. Welander, H. Smith
- 9:05** Intermission.
- 9:25** **586.** “Extrinsic decoration” against “intrinsic segregation” to enhance electrocatalytic activity for perovskite oxides. **Y. Li**, B. Yu
- 9:55** **587.** Ni-free double perovskites as alternative solid oxide fuel cell anode materials: *In situ* structural and performance characterization. **S. Witt**
- 10:25** **588.** Nano-structured electrode design for reversible solid oxide cells (RSOCs). **H. Jeong**, J. Myung
- 10:55** Concluding Remarks.

SECTION C
San Diego Convention Center
Room 23C

Atomic-level Understanding & Design of Materials & Processes for Energy Applications

H. Zhuang, *Organizer*

Y. Liu, *Organizer, Presiding*

- 8:00** Introductory Remarks.
- 8:05** **589.** *Ab initio* modeling of transition metals dissolution from $\text{LiNi}_{0.5}\text{Mn}_{1.5}\text{O}_4$. **N.N. Intan**, K. Klyukin, V. Alexandrov
- 8:20** **590.** Correlating atomic and nanoscale structure of PEDOT:PSS polymers blends to thermoelectric behavior. **L. Heroux**, M.D. Dadmun
- 8:35** **591.** Melamine-doped carbon fiber texture as efficient electrocatalyst for seawater battery. **T.D. NGUYEN**, S. Kang, K. Baek
- 9:05** **592.** Unravelling the enhanced capacitive performance of hybrid C_{60} /graphene electrodes with first-principles simulations. **C. Zhan**, T. Pham, M. Ceron, P. Campbell, V. Vedharathinam, M. Otani, D. Jiang, J. Biener, B. Wood, M. Biener

- 9:35** Intermission.
- 9:50** **593.** Selective removal of hydrogen sulfide from simulated biogas streams using sterically hindered amines. **C. Okonkwo**, C.W. Jones, J. Lee, A. DeVlylder
- 10:05** **594.** Two-dimensional materials as high-pass filter of van der Waals interactions. **T. Tian**, F. Naef, E. Santos, C. Shih
- 10:20** **595.** Chemo-morphological coupling in CO_2 -responsive tunable nano-scale fluids for subsurface energy recovery. **H. Asgar**, **G. Gadikota**

SECTION D
San Diego Convention Center
Room 24A

Eco-Friendly, Derived Nanostructured Materials & Characterization for Renewable Energy Applications

S. Ravula, *Organizer*

F. M. Yurtsever, *Organizer, Presiding*

- 8:00** Introductory Remarks.
- 8:05** **596.** Nanolayers from earth-abundant elements for renewable energy applications. **F. Geiger**, T.F. Miller, M. Boamah, E. Lozier
- 8:30** **597.** Green synthesis of stable nano- SiO_2/CaO composites for fast CO_2 capture. **Y. Jiang**, X. Zhao, F. Yan, Z. Zhang
- 8:50** **598.** Aqueous synthesis of ultrathin PdCuP nanowires for improved electrocatalytic ethanol-oxidation performance. **H. Lv**, L. Sun, D. Xu, B. Liu
- 9:30** **599.** New PtMg alloy with enhanced electrocatalytic performance for oxygen reduction reaction. **E. Tetteh**, **J. Yu**
- 9:50** Intermission.
- 10:00** **600.** Synthesis of nitrogen-doped carbon dots as charge transport materials for photosystem I-based biohybrid photovoltaics. **C.D. Stachurski**, G. Jennings, D.E. Cliffl
- 10:20** **601.** Storage capacity improvement and intercalation mechanism studies of AlCl_4^- anion in graphite materials for rechargeable Al-ion battery. **T. Lee**, Y. Lai, **D. Wang**
- 10:45** **602.** Influence of interface layer on perovskite solar cell performance. **C. Chen**, O. Sharifi, **Q. Dai**
- 11:10** **603.** Atomically dispersed platinum by photodeposition: Application in electro- and photocatalytic hydrogen evolution. **J. Ji**, Z. Li, C. Chenchen Hu, M. Ling
- 11:30** Concluding Remarks.

SECTION E

San Diego Convention Center
Room 24B

Hybrid Functional Porous Materials: MOFs, Silica & Conductive Polymers

J. L. Lutkenhaus, S. V. Patwardhan, *Organizers*
S. K. Nune, *Organizer, Presiding*

- 8:00 Introductory Remarks.
- 8:05 **604.** MOFs for deactivation of nerve agents and their simulants. **J.T. Hupp**
- 8:45 **605.** Metal–organic frameworks for catalysis and energy. **Q. Xu**
- 9:15 Intermission.
- 9:30 **606.** Application of bioinspired green chemistry to design sustainable and scalable high value nanosilica. **S.V. Patwardhan**, J. Manning, M. Chiacchia
- 9:50 **607.** Polymer/MOF composite structure for gas separation membranes: Dimensional design. **K. Xie**, Q. Fu, P. Webley, G. Qiao
- 10:10 **608.** New vehicle for aqueous phase photon upconversion: Hollow/yolk-shell mesoporous silica microcapsules. **H. Lee**, J. Kim, H. Choe
- 10:30 Concluding Remarks.

SECTION F

San Diego Convention Center
Room 24C

Sustainable Energy & Water via Innovative Electrocatalytic, Photocatalytic & Hybrid Catalytic Systems

F. Jiao, C. Liu, Y. Shao, *Organizers*
Y. Cheng, G. Wu, *Organizers, Presiding*

- 8:00 Introductory Remarks.
- 8:05 **609.** Supramolecular assemblies of Cu(I) photosensitizers and Co(II) hydrogen evolving catalysts for photocatalytic hydrogen production. **A.M. Potocny**, K.L. Mulfort
- 8:35 **610.** Iridate perovskites as highly active catalysts for the oxygen evolution reaction in acidic conditions. **L.C. Seitz**
- 9:05 **611.** Photocatalytic and electrocatalytic hydrogen production from water. **Y.H. Hu**
- 9:30 **612.** Bifunctional electrocatalysts for overall water splitting. **S. Chen**
- 9:55 **613.** Vertically MoS₂ nanoarray grown on conducting MoO₂ films as self-supported electrodes for hydrogen evolution reactions. **H. Zhao**, X. Dai, Y. Wang
- 10:15 Intermission.

- 10:20 **614.** Highly efficient clean energy production and refractory organics degradation by a novel self-sustaining photoelectrocatalytic/photovoltaic system. **Q. Zeng**, S. Chang, A. Beyhaqi, M. Wang
- 10:40 **615.** Size effect of Ru as active auxiliary on Pt-based nanocrystals with enhanced ethylene glycol oxidation. **Y. Wang**, H. Zhao, X. Zhang
- 11:00 **616.** Single-atom tailoring of platinum nanowires for high-performance electrocatalysis. **C. Wan**, X. Duan, Y. Huang
- 11:20 **617.** NEW (nutrient-energy-water) synergy in an anammox bioelectrochemical system for resource-efficient wastewater treatment. **U. Ghimire**, V. Gude
- 11:40 **618.** *In situ* scanning tunneling microscopy investigation of molecular electrocatalytic reactions at the electrode/electrolyte interface. **W. Dong**

SECTION G

San Diego Convention Center
Room 25A

Remediation of Wastewater from Energy Usage

Cosponsored by PRES

Y. Li, J. L. Liu, J. J. Ren, Q. Zhen, *Organizers*
S. Raghuvver Chava, R. S. Weber, *Presiding*

- 9:00 Introductory Remarks.
- 9:05 **619.** Electrochemical remediation of wastewater from the production of renewable fuels. J.D. Egbert, E. Andrews, **R. Weber**
- 9:35 **620.** Modularized solutions applied to produced water treatment for reuse in the hydraulic fracturing process to improve shale gas and liquids development. **M.A. Reynolds**
- 10:05 **621.** Strategic design of highly-efficient solar water purification system with rGO-modified plasmonic nanocomposite. **A. Mahmood**, H. Javed, W. Que, B. Hassan
- 10:25 **622.** Nanotechnology based remediation of contaminated water from energy use: metal removal using porous materials. **Y. Olaseni**, **J.L. Liu**
- 10:45 **623.** Designing an engineered protein model to evaluate protein affinity probe for nitrogen. D. Guzman, **S. Raghuvver Chava**, S. Bashir
- 11:05 Intermission.
- 11:15 **624.** Synthesis, characterization and environmental application of nanometal and nanometal composites derived from natural products. **P. Merugu**, **S. Bashir**, J.L. Liu
- 11:35 **625.** Responses of surface water microbial communities exposed to spills of flowback and produced water. **C. Zhong**, C. Nesbø, B. Lanoil, D.S. Alessi

- 11:55 626.** Effects of salinity on the leachability of ionic species from the Duvernay formation, a Canadian hydraulic fracturing play. **K.N. Snihur**, J. Banks, K. von Gunten, N.B. Harris, M.K. Gingras, K. Konhauser, D.S. Alessi
- 12:15 627.** Remediating produced water in Kansas. **K. Shafer-Peltier**, M. Chen, S. Randtke, E.F. Peltier
- 12:35 628.** Physicochemical and microbiological characterization of digestate from swine manure biogas systems for its application as organic fertilizer. F.M. Jiménez-Arias, V. Chaves-Villarreal, D. Zambrano-Piamba, H.S. Martínez-Avila, J.L. Leon Salazar, R.A. Arias-Carrillo, A. Reyes-Martinez, **C.C. Villarreal**
- 12:55** Concluding Remarks.

SECTION H

San Diego Convention Center
Room 25B

Cross-Scale Science for Energy & Resource Recovery

D. P. Butt, G. Gadikota, *Organizers, Presiding*

- 8:00 629.** Design, development and synthesis of water-lean amine-based solvents as carbon dioxide capture materials. **D. Malhotra**, P.K. Koech, D.J. Heldebrant, M. Nguyen, V. Glezakou, R. Rousseau, F. Zheng
- 8:25 630.** Carbonation of steel slags: Combining two waste streams to create value. **A. Suresh**, R. Ragipani, S. Bhattacharya

- 8:50 631.** Direct capture, conversion and storage of CO₂ as calcium and magnesium carbonates using an innovative aqueous alkaline amine looping (A³L) process. M. Liu, **G. Gadikota**
- 9:10 632.** Improved recovery of high value-added metals from spent lithium-ion batteries by efficient reduction roasting and facile acid leaching. **Y. Zhang**, S. Xu
- 9:30** Intermission.
- 9:40 633.** Status: High-temperature, high-pressure viscosity standard search. **I. Gamwo**, H. Baled, M.A. McHugh, R.M. Enick
- 10:00 634.** Advanced characterization of fission products in nuclear fuels. **L. He**, M. Bachhav, C. Jiang, D. Sprouster, D.K. Shuh, B. Miller, I. Ecker, J. Gan
- 10:25 635.** Phosphate recovery by electrochemical precipitation of struvite in acidic environment: Pure magnesium vs. AZ31 alloy anode. **L. Kekedy-Nagy**, A. Teymouri, A.M. Herring, L.F. Greenlee
- 10:45 636.** Energy-efficient wastewater treatment schemes for urban communities: Quantitative mass and energy balance approach. G. Sarpong, **V. Gude**

In Situ & Operando Spectroscopy

Sponsored by CATL, Cosponsored by ENFL and PHYS

SUNDAY MORNING – ENVR

SECTION A

San Diego Convention Center
Room 28A

Catalysis for Environmental & Energy Applications

Treatment of Gas & Water Pollutants

Cosponsored by CATL

A. Orlov, A. Savara, Y. Wang, *Organizers, Presiding*

- 8:10** Introductory Remarks.
- 8:15** **1.** Revisiting effects of alkali and alkaline earth co-cation additives to Cu/SSZ-13 standard selective catalytic reduction catalysts. **F. Gao**, Y. Cui, Y. Wang, E.D. Walter, D. Mei, J. Szanyi, Y. Wang
- 8:35** **2.** Proof of concept study in experimental data-based combinatorial kinetic simulations for predictions of synergistic catalyst mixtures. **A. Savara**, H. Vuong, J.E. Sutton, A.J. Binder, T. Toops
- 8:55** **3.** Heterogeneous UV/Fenton for efficient VOCs oxidation over Fe/ZSM-5 catalyst in wet scrubber process. **R. Xie**, Y. Gao
- 9:15** **4.** Efficient photocatalytic oxidation of gaseous toluene in a bubbling reactor of water. **B. Liu**, Y. Zhan, H. Huang
- 9:35** **5.** Sonochemical and sonocatalytic degradation of PPCPs: Case study with methylparaben and salicylic acid. **N.H. Ince**, B. Savun-Hekimoğlu
- 9:55** Intermission .
- 10:15** **6.** Iron catalysts for dye containing wastewater treatment. B. McGhee, D. Henninger, R. Stefan, **S.A. Maicaneanu**
- 10:35** **7.** Bimetallic PdAg nanoparticles for sustainable nitrite reduction in drinking water. **J. Troutman**, S.M. Humphrey, C.J. Werth
- 10:55** **8.** Catalytic reduction of aqueous chlorate with vanadium/palladium bimetallic catalyst. **J. Gao**, C. Ren, J. Liu
- 11:15** **9.** Bimetal treatment of insensitive munitions 2,4-dinitroanisole (DNAN) and nitroguanidine (NQ). **A. Mai**, E. Hadnagy, A. Koutsospyros, W. Braida

- 11:35** **10.** Fabrication of fungal biochar supported silver nanoparticles for catalytic reduction of 4-nitrophenol. **Y. Zhang**, B. Chen
- 11:55** Concluding Remarks.

SECTION B

San Diego Convention Center
Room 28B

Emerging Contaminants in Wastewater

Financially supported by Association of Environmental Engineering & Science Professors (AEESP)

A. S. Adeleye, P. Cervantes, Y. Huang, *Organizers, Presiding*

- 8:30** Introductory Remarks.
- 8:35** **11.** Fate of pharmaceuticals in wastewater: Roles of environmental factors and toxicological implications. **G. Rubasinghege**
- 9:15** **12.** Antibiotic resistance genes, microbiomes, and *Salmonella* survival in lettuce exposed to antibiotics via soil surface irrigation. **Y. Shen**, W. Zhang, H. Li, E. Ryser
- 9:35** **13.** Deleterious effects of urban watersheds on HT29 colon cells. **D.A. Abdullah-Smoot**
- 9:55** **14.** Antibiotic resistance genes and heavy metal co-selection dynamics in reclaimed water for irrigation in northwest Mexico. **V.A. Whitener**, W. Hung
- 10:15** Intermission.
- 10:30** **15.** Fate of emerging contaminants in aerobic and anaerobic wastewater treatment: Non-targeted approach. **L.A. Steinberg**, W. Richardot, E. Hoh, N. Dodder, N. Mladenov, B.S. Martincigh, S. Chao, C. Graves
- 10:55** **16.** Ultrahigh resolution mass spectral characterization of carbon and nitrogen in a landfill leachate pretreated by a submerged anaerobic bioreactor. **A.M. McKenna**, H. Chen, L. Li, R. Li, Y. Tang
- 11:15** **17.** Nitrosamines analysis in drinking water using GC/MS/MS for performance equivalent to EPA Method 521. **D. Wong**, R. Honnold, T. Anumol

- 11:35** 18. Does a contaminant prefer soil or groundwater? Determination of adsorption isotherms *via* quantum chemistry. **G. Jenness**, S. Giles, M.K. Shukla
- 11:55** Concluding Remarks.

SECTION C

San Diego Convention Center
Room 28C

Water in the Solid State: Reactions & Interactions with Impurities

Nucleation & Growth

Cosponsored by PHYS

Financially supported by Korean Polar Research Institute (KOPRI)

W. Choi, K. Kim, *Organizers*

E. Asenath Smith, *Organizer, Presiding*

V. Molinero, *Presiding*

- 8:00** Introductory Remarks.
- 8:05** 19. Many faces of ice: Molecular view of growth and interactions. **M.J. Shultz**, P.J. Bisson, A.N. Carey, J.M. Marmolejos
- 8:35** 20. Understanding heterogeneous ice nucleation through synergistic simulations and experimental studies. **S. Sarupria**
- 9:05** 21. Surface features that promote heterogeneous ice nucleation. **M. Freedman**
- 9:35** 22. Modeling elementary heterogeneous atmospheric (photo)chemical processes on ice and their dynamics using amorphous solid water. **P. Ayotte**
- 9:55** 23. Acceleration of amorphous solid water crystallization by acidic impurities. **D. Lee**, H. Kang
- 10:15** Intermission.
- 10:25** 24. Icephobic surfaces: Definition and figures of merit. **H. Ghasemi**, P. Irajizad, S. Nazifi
- 10:55** 25. Antifreeze proteins: Nature's cryoprotectants. **K. Varga**, K.W. Elliott, K. Jovic, J. Sreter, E. Asenath Smith, P.W. Baures, J. Tsavalas
- 11:15** 26. Polymer bioconjugates and polyol based polymers for ice recrystallization inhibition and thermal hysteresis activity in anti-icing coatings. **J. Tsavalas**, M. Mousazadeh, M. Ishak, Y. Lin, A. Huebner, A. Pandey, A. Massie, R. Marquis, I. Lehner, P.W. Baures, J. Sreter, K. Jovic, K. Varga, E. Asenath Smith
- 11:35** 27. Physics of condensation frosting. **f. ahmadi**, S. Nath, C. Bisbano, G. Illiff, P. Yue, J. Boreyko
- 11:55** Closing Remarks.

SECTION D

San Diego Convention Center
Room 28D

Chemistry of Water Reuse Processes Toward Water Sustainability

Cosponsored by AGRO and PRES

Financially supported by Association of Environmental Engineering & Science Professors (AEESP)

R. Doong, W. Hou, C. Huang, Z. Qiang, V. K. Sharma, *Organizers*

H. Kim, T. Lin, T. Wang, *Presiding*

- 8:25** Introductory Remarks.
- 8:30** 28. Sustainable bimetallic catalyst supported by red mud for enhanced nitrate reduction. S. Hamid, S. Bae, E. Ramazanov, **W. Lee**
- 9:00** 29. Elucidation of phosphodiesterase Type V (PDE-5) inhibitors ozonation: Degradation pathway and kinetics. **I. Lee**, Y. Hong, S. Pan, L. Valentino, H. Kim
- 9:20** 30. Degradation of ketoprofen, ibuprofen, and atrazine by catalytic ozonation with graphene oxides (GOs): Determination of GOs kinetic behaviors and simulations of pollutant removal. **K. Chen**, Y. Lin
- 9:40** 31. Recovery of sulfuric acid from piranha solution over a dimensionally stable anode (DSA) Ti-RuO₂ electrode and beyond. **D. Sanchez Carretero**, C. Huang, C. Huang
- 10:00** Intermission.
- 10:15** 32. Effect of adding graphene oxide composite on the performance of anammox for nitrogen removal. **T. Huang**, F. Tung, J. Lin, W. Chen
- 10:35** 33. Ferrate oxidation of pharmaceuticals in hydrolyzed urine: Impacts of organic constituents. **C. Luo**, V.K. Sharma, C. Huang
- 10:55** 34. Performance of ferrate as a disinfectant under varying conditions of water reclamation: Physiological and chemical assessments. **S. Daer**, K. Ikuma
- 11:15** 35. Leaching of lithium and cobalt from spent lithium-ion batteries using subcritical water. **J. Liu**, J. lie, S. Tanda
- 11:35** 36. Withdrawn
- 11:55** Concluding Remarks.

SECTION E

San Diego Convention Center
Room 28E

Water, Health, & Environmental Justice in Marginalized Communities

(A) Toxic Chemicals in Water; & (B) Sanitation & Wastewater Resource Recovery Technologies

Cosponsored by CMA and PRES
F. de los Reyes, A. Harris, *Organizers*
J. Kearns, *Organizer, Presiding*

- 8:00** Introductory Remarks.
- 8:10** **37.** Is it time to move beyond the trihalomethane paradigm in developing countries? Lessons learned from wastewater-impacted drinking waters in South Asia. **K. Furst**, R. Coyte, D. Smith, J. Davis, A. Vengosh, W. Mitch
- 8:35** **38.** Meta-analysis of nationwide loadings of pharmaceuticals to Indian aquatic and terrestrial environments from human excreta. **V. Kelkar**, J. Steele, R.U. Halden
- 9:00** **39.** Field testing and deploying a low-cost groundwater defluoridation technology using locally sourced bauxite in resource-constrained regions. **K. Cherukumilli**
- 9:25** **40.** Developing biosensors for detecting pesticide traces in water for human use by marginalized communities. **D. Bahamon-Pinzon**, **D. Vanegas**, D.M. Hurtado-Chaves, A.M. Torres-Gonzalez, I. Velez-Torrez, E.S. McLamore
- 9:50** Intermission.
- 10:05** **41.** On-site sanitation, energy, and food nexus for climate justice. **B. Hunter**, M. Deshusses
- 10:30** **42.** Going viral: Emerging opportunities for phage-based bacterial control in water treatment and reuse. **P. Yu**, J. Mathieu, P. Zuo, P.J. Alvarez
- 10:55** **43.** Life cycle economic and environmental assessment of resource recovery from an agricultural waste system in Costa Rica. **K. Orner**, M. Alvarez, X. Ramirez, **P.K. Cornejo**
- 11:20** **44.** Light conducting photocatalytic membrane for low maintenance provision of safe water to marginalized communities. L.T. Nyamutswa, B. Zhu, D. Navaratna, S. Collins, K. Linden, **M. Duke**
- 11:45** Discussion.

SECTION F

San Diego Convention Center
Room 29A

Showcasing emerging investigators & future perspectives: A symposium by the RSC Environmental Science Journals

Financially supported by Royal Society of Chemistry; Association of Environmental Engineering & Science Professors (AEESP)
D. M. Cwiertny, *Organizer*
K. P. McNeill, S. Neil, P. Novak, P. J. Vikesland, *Organizers, Presiding*

- 8:15** Introductory Remarks.
- 8:20** **45.** Interactions of nanomaterials with the cell plasma membrane: Can model membranes predict nanoparticle-induced membrane damage in cells?. **A. Farnoud**
- 8:45** **46.** Quantitative analysis for the environmental fate of carbon nanotubes in soil-plant systems for their environmental implication and application. **Y. Yang**
- 9:10** **47.** Designing sustainably at the nanoscale. **L.M. Gilbertson**
- 9:35** **48.** Promoted heterogeneous reaction of SO₂ in atmosphere by CO₂ and flue gas SO₂ utilization. **L. Zhang**
- 10:00** Intermission.
- 10:15** **49.** Sunlight photolysis of anthropogenic chemicals on simulated environmental surfaces. **N. Dai**, L. Su
- 10:40** **50.** Using aerosol optical tweezers to learn and predict the chemical evolution of the composition, pH, and phase separated morphology of complex atmospheric particles. **R.C. Sullivan**, H. Boyer, K. Gorkowski, N.M. Donahue, L. Jahl, L. Monroe
- 11:05** **51.** Exploring the surface properties of aqueous organic aerosol. S. Li, S. Cheng, **L. Du**
- 11:30** **52.** Disentangling the contributions of metabolism, light, and flocculation to removing dissolved organic carbon from vertically stratified aquatic environments. **R.M. Couture**, J. Guerrero, T. Moore, H.A. DeWit, E. Jennings, D. Pierson
- 11:55** Concluding Remarks.

Novel Polymeric Materials & Polymer-Based Processes for Energy-Efficient Treatment of Water & Resource Recovery

Membrane Formation

Sponsored by PMSE, Cosponsored by ENVR

Geogenic & Anthropogenic Sources of Trace Elements within Surface & Groundwater Systems & their Effects on Water Quality

Sponsored by GEOC, Cosponsored by ENVR

Chemists Without Borders: Celebrating 15 Years of Scientific/Humanitarian Collaboration

Sponsored by MPPG, Cosponsored by CEI and ENVR

Future Insights into Syngas Conversion Catalysis: Symposium in honor of Burtron H. Davis

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

Advances in Catalysis with Ceria & Other Reducible Oxides

Model Ceria Catalyst

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

Characterization of Plastics in Aquatic Environments

Sponsored by POLY, Cosponsored by ANYL, BIOL, CEI, ENVR, I&EC, PMSE and PRES

Creative Thinking in Designing E fate Studies & Data Analysis to Meet Agrochemical Regulatory Challenges

Sponsored by AGRO, Cosponsored by ENVR

SUNDAY AFTERNOON – ENVR

SECTION A

San Diego Convention Center
Room 28A

Catalysis for Environmental & Energy Applications

Oxidative Process for Water Treatment

Cosponsored by CATL

A. Orlov, A. Savara, Y. Wang, *Organizers, Presiding*

- 1:30** Introductory Remarks.
- 1:35** **53.** Rapid photocatalytic degradation of glyphosate by palladium-decorated $m\text{-BiVO}_4/\text{BiOBr}$ nanosheets. **E.M. Zahran**, N. Ensinger
- 1:55** **54.** Novel bismuth oxyhalides-based hybrid materials with improved photocatalytic performance. L. Wang, X. Min, **Y. Wang**
- 2:15** **55.** Enhanced performance for catalytic ozonation of methyl mercaptan on single-atom ag deposited mesoporous MnO_2 . **C. He**, L. Hu, Y. Huang
- 2:35** **56.** Synthesis and photocatalytic degradation of pollutants using dual metal ferrite ($\text{Zn}_{0.5}\text{Mn}_{0.5}\text{Fe}_2\text{O}_4$) and its graphene oxide composite. **M. Zahid**, R. Asif, N. Nadeem, I.A. Bhatti, H.N. Bhatti
- 2:55** **57.** Activation of peroxymonosulfate by $\alpha\text{-Fe}_2\text{O}_3$ for oxidation of organic compounds through nonradical mechanism. **H. Kang**, H. Kim, K. Lee, J. Seong, S. Kim, C. Lee
- 3:15** Intermission .
- 3:35** **58.** Electro-catalytic degradation of antibiotic tetracycline in aqueous system by a novel CNTs/AG/ITO electrode. **H. Liu**, J. Qu, Y. Zhang

- 3:55** **59.** Electrocatalytic generation of reactive chlorine species and simultaneous conversion of CO_2 into formate. **W. Choi**, H. Park
- 4:15** **60.** Solar hydrogen peroxide production and As(III) oxidation using carbon nanotubes wired to titania nanorods arrays. **s. choi**, H. Park
- 4:35** **61.** Electodesalination-driven electrocatalytic water treatment and CO_2 conversion. **B. Kim**, H. Park
- 4:55** Concluding Remarks.

SECTION B

San Diego Convention Center
Room 28B

Emerging Contaminants in Wastewater

Financially supported by Association of Environmental Engineering & Science Professors (AEESP)

A. S. Adeleye, P. Cervantes, Y. Huang, *Organizers, Presiding*

- 1:30** Introductory Remarks.
- 1:35** **62.** Emerging contaminants: Occurrence and removal of PPCPs and steroids in wastewater treatment plants. **V. Phonsiri**, L. Sanchez
- 2:20** **63.** Spatial and temporal variability of pharmaceutical mixtures and potential impacts to a wastewater effluent-dominated stream in Iowa, September 2017 to August 2018. **G.H. LeFevre**, H. Zhi, D.W. Kolpin, R. Klaper, L.R. Iwanowicz, E.B. Meade, M.T. Meyer, R.F. Lane, S.M. Meppelink, M.M. Powers, J. Quin
- 2:45** **64.** Fate of pharmaceuticals and personal care products in wastewater treatment plants. **V. Desgens-Martin**, A.A. Keller
- 3:10** **65.** Fate and transport of extracellular DNA found in wastewater discharge and its role in antibiotic resistance propagation in rivers. **M. Legg**, K. Ikuma, C. Rehmann
- 3:35** Intermission.
- 3:50** **66.** Alternatives for removal of imidazolium ionic liquids in wastewater. A.F. Mohedano, E. Diaz, **I. Moreno-Andrade**
- 4:10** **67.** Extraction of dyes from water using an amino acid-based hydrophobic ionic liquid. D. Bwambok, **S. Smith**, **V. Marta**, M. Angon
- 4:30** **68.** Electrochemically-mediated redox-systems for the controlled remediation of emerging contaminants. **X. Su**
- 4:50** **69.** Ampicillin (AMP) degradation and AMP resistant *E.coli* and its gene removal by UV-LED/ chlorine process. **K. Zoh**, T. Kim
- 5:10** Concluding Remarks.

SECTION C
San Diego Convention Center
Room 28C

Water in the Solid State: Reactions & Interactions with Impurities

Microstructural & Mechanical Aspects of Ice

Cosponsored by PHYS

Financially supported by Korean Polar Research Institute (KOPRI)

E. Asenath Smith, W. Choi, K. Kim, *Organizers, Presiding*

- 1:30** Introductory Remarks.
- 1:35** **70.** Ion exclusion at the ice water interface: Surprising results and insight. **P. Wilson**, T. Haymet
- 2:05** **71.** Salty ice surfaces: Microscopy and reactivity. **T.F. Kahan**, S. Chakraborty, P. Malley, A. Stathis, A. Stubbs
- 2:25** **72.** Distributions and structures of ions in polycrystalline and monocrystalline ice. **T. Okada**, M. Harada, Y. Okada
- 2:55** Intermission.
- 3:15** **73.** Microstructures and mechanical response of ice mixtures, with application to terrestrial glaciers and icy satellites. **C. McCarthy**
- 3:45** **74.** How sulfuric acid affects the mechanical behavior and microstructural properties of polycrystalline ice. **K. Hammonds**, C. Donahue, I. Baker
- 4:15** **75.** Interaction of colloidal particles with propagating cracks in loaded ice. **E. Asenath Smith**, R. Lieb-Lappen, S. Taylor, R.D. Moser, R. Haehnel
- 4:35** Discussion.
- 4:50** Closing Remarks.

SECTION D
San Diego Convention Center
Room 28D

Chemistry of Water Reuse Processes Toward Water Sustainability

Cosponsored by AGRO and PRES

Financially supported by Association of Environmental Engineering & Science Professors (AEESP)

R. Doong, W. Hou, C. Huang, Z. Qiang, *Organizers*

V. K. Sharma, *Organizer, Presiding*

J. Liu, Y. Shih, *Presiding*

- 1:30** Introductory Remarks.
- 1:35** **76.** Inactivation of *E. tarda* and *V. harveyi* by free chlorine. **J. CHO**, T. Kim, C. Lee
- 1:55** **77.** Strengths of correlations between concentrations of chlorination disinfection byproducts and aquatic descriptors: What is important?. **B. Manivannan**

- 2:15** **78.** Reactivity of free chlorine with organic matter under wastewater treatment conditions. R.N. Tran, **S.P. Mezyk**
- 2:35** **79.** Performance and photo-disinfection mechanism of visible-light-responsive TiO_2 composites for removal of water pathogen. **K. Iamsaard**, C. Chang, C. Weng, J. Tzeng, L. Yen, Y. Lin
- 2:55** **80.** Interplay between manganese oxide and microporous carbonaceous support in capacitive deionization. S. Li, S. Xu, **T. Wang**, C. Wang
- 3:15** Intermission.
- 3:30** **81.** Controlling micro/mesoporosity of activated carbon fiber with electrospinning for membrane capacitive deionization. **N. Liu**, C. Hou
- 3:50** **82.** Polarization alleviation in flow-electrode CDI enables extremely high water recovery rate in desalination and reclamation. **J. Ma**, J. Ma, C. Zhang, R. Collins, D. Waite
- 4:10** **83.** Fit-for purpose water technology of selective desalination. **Y.J. Lin**
- 4:30** **84.** Removal of scale-forming constituents from desalination concentrate via photochemical oxidation of phosphonate-containing antiscalants. **T. Jain**, H. Liu
- 5:10** Concluding Remarks.

SECTION E
San Diego Convention Center
Room 28E

Water, Health, & Environmental Justice in Marginalized Communities

Socio-Cultural & Economic Dimensions of Water & Health

Cosponsored by CMA and PRES

F. de los Reyes, J. Kearns, *Organizers*

A. Harris, *Organizer, Presiding*

- 1:30** Introductory Remarks.
- 1:35** **85.** Water, sanitation, and hygiene for people experiencing homelessness: Transdisciplinary approach for developing sustainable solutions for unhoused individuals. **M. Welsh**, S. Flanagan, M. Garcia, N. Mladenov, M.E. Verbyla
- 2:00** **86.** Wastewater management issues in the rural Alabama Black Belt and a proposed path forward. **K. White**, M. Elliott, M.O. Barnett
- 2:25** **87.** Engineering justice in the sanitation value chain: Socio-technical responses to WASH insecurity in Placencia, Belize. **C. Wells**, C. Prouty, C. Haberstroh, W. Webb, M.A. Trotz
- 2:50** **88.** Systems-based, community-engaged insights that safeguard health and wastewater management in vulnerable communities and

- coastlines. **C. Prouty**, M. Trotz, Q. Zhang, D.A. Delgado, J.R. Mihelcic
- 3:15 Intermission.
- 3:30 **89.** Environmental justice and stormwater management: Tampa case study towards multi-functional stormwater infrastructure in coastal communities of color. **M.E. Carrasquillo**, E. Ortiz Carabantes, M. Trotz
- 3:55 **90.** Elemental contamination of Navajo unregulated water sources. J.M. Credo, L.M. Jones, **J.C. Ingram**
- 4:20 **91.** Water, health, and environmental justice in California's Central Valley: Geospatial analysis of water contamination and health disparities. **C. Naughton**
- 4:45 **92.** Baseline study evaluating water quality and microbial ecology in seven Alaskan native communities. **N.B. Saleh**, L. Rowles, M. Kirisits
- 5:10 Discussion.
- 5:25 Closing Remarks.

SECTION F

San Diego Convention Center
Room 29A

Showcasing emerging investigators & future perspectives: A symposium by the RSC Environmental Science Journals

Financially supported by Royal Society of Chemistry; Association of Environmental Engineering & Science Professors (AEESP)

D. M. Cwiertny, *Organizer*

K. P. McNeill, S. Neil, P. Novak, P. J. Vikesland, *Organizers, Presiding*

- 1:30 Introductory Remarks.
- 1:35 **93.** Organic contaminants of emerging concerns: Environmental fate and impacts. **Y. Men**, Y. Xing, Y. Yu, K. Zhang
- 2:00 **94.** Biomimetic and bioinspired membranes: Challenges and opportunities. **M. Kumar**
- 2:25 **95.** Next generation graphene-based membranes for water treatment: Evolving from 2D to 3D materials. **J. Fortner**
- 2:50 **96.** Chemistry of wildfire smoke: Measuring emissions and evolution of submicron particles. **D. Farmer**, L.A. Garofalo, E. Levin, M. Pothier, S. Kreidenweis
- 3:15 Intermission.
- 3:30 **97.** Characterizing urban stormwater impacts on water quality. **E.P. Kolodziej**, K.T. Peter, Z. Tian, J. McIntyre
- 3:55 **98.** Nucleic acid reactivity with UV radiation and HOCl and the impact of virus capsids. **K. Wigginton**, Z. Qiao

- 4:20 **99.** Development of low-cost colorimetric sensor for the detection of aqueous nitrite ion. **L. Philip**
- 4:45 **100.** Achieving low levels of lead at the tap through a multi-faceted corrosion control program. B. Trueman, **G. Gagnon**
- 5:10 Concluding Remarks.

Novel Polymeric Materials & Polymer-Based Processes for Energy-Efficient Treatment of Water & Resource Recovery

Membrane Processes

Sponsored by PMSE, Cosponsored by ENVR

Future Insights into Syngas Conversion Catalysis: Symposium in honor of Burtron H. Davis

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

Chemistry & Water: Opening Session

Sponsored by MPPG, Cosponsored by CEI, ENVR and PRES

Advances in Catalysis with Ceria & Other Reducible Oxides

Theory of Ceria Catalysts

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

Characterization of Plastics in Aquatic Environments

Sponsored by POLY, Cosponsored by ANYL, BIOL, CEI, ENVR, I&EC, PMSE and PRES

SUNDAY EVENING – ENVR

Surfaces & Interfaces in the Environment: Symposium in Honor of Vicki Grassian

Posters

Sponsored by COLL, Cosponsored by ENVR

Surfaces & Interfaces in the Environment: Symposium in Honor of Vicki Grassian

Posters

Sponsored by COLL, Cosponsored by ENVR

MONDAY MORNING

SECTION A

San Diego Convention Center

Room 28A

Current Advances in Water Analysis: From Citizen Scientists to Laboratory Breakthroughs

Cosponsored by AGRO and CEI

J. L. Goldfarb, *Organizer*

M. E. Verbyla, *Organizer, Presiding*

- 8:15 Introductory Remarks.
- 8:20 **101.** Optimum condition for formation of monochloramines during reagent addition to a pipeline for water disinfection. **F. Samadi**
- 8:45 **102.** Citizen science and water analysis. **S. Simoliunas**
- 9:35 **103.** Monitoring water quality in arctic rivers: Citizen science approach. **C. Gueguen**
- 10:00 Intermission.
- 10:15 **104.** How to make dioxin analysis in water simpler. **H. Lin, J. Betz, D. Wong, T. Anumol, M. Greg**
- 10:40 **105.** Imaging the coffee ring effect for tap water fingerprinting. **R. Lahr, X. Li**
- 11:05 **106.** Drinking water and citizen science: Between perceived concerns and actual microbiological quality. **X. Li, T. Yan**
- 11:30 **107.** Nontargeted screening of wastewater for water reuse using mass spectrometry. **J. Zweigenbaum, A.J. Williams**
- 11:55 Closing Remarks.

SECTION B

San Diego Convention Center

Room 28B

Emerging Contaminants in Wastewater

Financially supported by Association of Environmental Engineering & Science Professors (AEESP)

A. S. Adeleye, P. Cervantes, Y. Huang, *Organizers, Presiding*

- 8:15 Introductory Remarks.
- 8:20 **108.** Effects of man-made nanoparticles on aerobic denitrification by strain *Pseudomonas stutzeri* PCN-1. **Q. Chen**
- 8:45 **109.** Transformation of N-methylamine stimulant drugs to (halo)nitromethanes during wastewater reuse. **D. McCurry, J. Shi**
- 9:05 **110.** Assessment of the biodegradability of trace organic contaminants during biological treatment in water resource recovery facilities. **W. Khunjar**

- 9:25 **111.** Monochloramine reactivity with amino acids in wastewater: Kinetic and temperature dependence. **R. Shinh, J. Gleason, S.P. Mezyk**
- 9:45 Intermission.
- 10:00 **112.** Withdrawn
- 10:40 **113.** Fast multi-element quantification of nanoparticles in wastewater sludge using single particle ICP-MS. **Y. Huang, J. Nelson, P. Cervantes, A.A. Keller**
- 11:05 **114.** Multi-technique approach to study the stability of silver nanoparticles at environmental realistic concentrations in aqueous media. **P. Cervantes, Y. Huang, A.A. Keller**
- 11:30 **115.** Rapid screening technique for emerging contaminants utilizing spICP-MS/MS and MassHunter 4.5. **J. Nelson, M. Yamanda**
- 11:55 Concluding Remarks.

SECTION C

San Diego Convention Center

Room 28C

Water in the Solid State: Reactions & Interactions with Impurities

Ice in Earth & Environmental Systems

Cosponsored by PHYS

Financially supported by Korean Polar Research Institute (KOPRI)

E. Asenath Smith, W. Choi, K. Kim, *Organizers, Presiding*

- 8:00 Introductory Remarks.
- 8:05 **116.** Raman mapping of ice surface with organic constituents. **S. Chakraborty, T. Kahan**
- 8:35 **117.** Natural organic matter in snow and ice: Chemistry and characterization. **A.M. Grannas, V. Boschi, R. Tiu, M. Barr**
- 9:05 **118.** Interactions of acetone with ice monitored with IR spectroscopy and mass spectrometry. **R.R. Michelsen, J. Charney**
- 9:25 **119.** Enhanced fluorescence detection on ferrous ion by freezing. **Y. Lee, K. Kim**
- 9:45 Intermission.
- 10:05 **120.** Freezing-enhanced redox chemical reactions and their application for water treatment. **J. Kim, K. Kim, J. Ju, Y. Choi**
- 10:35 **121.** Application of biochar for removal of hexavalent chromium during freezing process. **T. Han, K. Kim**
- 10:55 **122.** Thermal imaging: Novel approach to study evaporation kinetics in porous media. **J. Maurais, É. Beaumont, J. Bourret, E. Dauphinais, C. Larivière-Loiselle, É. Morin, A. Royer, N. Bouchard, P. Ayotte**
- 11:15 **123.** New abiotic pathway of humification in frozen solutions. **D. Min, K. Kim, K. Lui, B. Kim, S. Kim, J. Cho, W. Choi**

- 11:35 124.** Marine surfactants as chemical herders for maritime oil spill remediation. H. Zhou, **G. John**, C. Maldarelli
- 11:55** Concluding Remarks.

SECTION D
San Diego Convention Center
Room 28D

Chemistry of Water Reuse Processes Toward Water Sustainability

Cosponsored by AGRO and PRES

Financially supported by Association of Environmental Engineering & Science Professors (AEESP)

R. Doong, C. Huang, Z. Qiang, V. K. Sharma, *Organizers*

W. Hou, *Organizer, Presiding*

W. Lee, Y. Peng, *Presiding*

- 8:00** Introductory Remarks.
- 8:05 125.** Mesoporous carbon nitride as a green multifunctional material for water purification. T. Nguyen, L. Paragas, M.G. de Luna, **R. Doong**
- 8:35 126.** Stability and phosphate adsorption study of a magnetic LDH composite as a function of pH. **C. Lu**, T. Kim, U. Gro Nielsen, H. Christian Bruun Hansen
- 8:55 127.** Heterogeneous activation of peroxymonosulfate by CoO-doped ordered mesoporous carbon nitride for removal of sulfamethoxazole from aqueous solution. **T. Nguyen**, C. Chen, C. Dong
- 9:15 128.** Simultaneous adsorption and biodegradation of soil washing solution containing PAHs with high concentrations by degrading bacteria immobilized in PVA-SA hydrogel beads. **W. Chen**, X. Wang
- 9:35 129.** Synergy of graphene oxide-iron oxide composite and hydrogen peroxide for adsorption and degradation of diclofenac and chlorphenamine in water. **W. Chen**, Y. Huang, J. Huang, S. Lin, C. Li
- 9:55** Intermission.
- 10:10 130.** Advanced oxidation of recycled water with UV/H₂O₂: Comparison of treatment efficiencies with UVC-LED and LPUV. H. Chen, D. Leong, T. Ou, **G. Wang**
- 10:35 131.** Impact of physical and chemical pretreatment to RO fouling during the water reuse. **H. Kim**, D. Park, A. Jang, S. Kang
- 10:55 132.** Novel hybrid ion exchange process for municipal wastewater reclamation and nutrient recovery driven by waste carbon dioxide. **H. Dong**, C. Shepsko, A. SenGupta
- 11:15 133.** Membrane bioreactor/reverse osmosis system for gray water treatment and reuse. **C.S. Griggs**
- 11:35 134.** Pore wetting in membrane distillation treatment of wastewater reverse osmosis concentrate: Causes and prevention. **F. Perreault**
- 11:55** Concluding Remarks.

SECTION E
San Diego Convention Center
Room 28E

Wastewater-Based Epidemiology: Opportunities, Challenges & Applications to Public Health & Safety

Financially supported by Biobot Analytics; Association of Environmental Engineering & Science Professors (AEESP)
D. A. Burgard, M. Matus, B. Subedi, *Organizers, Presiding*

- 8:00** Introductory Remarks.
- 8:05 135.** Expanding wastewater-based epidemiology to inform on public health. **K. Thomas**, J. O'Brien, B. Tscharke, P. Choi, P. Thai, M. Mackie, R. Verhagen, K. Shimko, F. Ahmed, E. O'Malley, Q. Zheng, J. Mueller
- 8:50 136.** Biobot analytics: Novel platform to estimate opioid consumption in cities by analyzing opioid urinary metabolites in wastewater. **M. Matus**
- 9:15 137.** Implication of in-sewer stability testing of markers for wastewater-based epidemiology. **J. O'Brien**, G. Jiang, J. Gao, J. Li, A. Banks, J. Mueller, P. Choi, K. Thomas, C. Ort, B. Tscharke, P. Thai
- 9:40 138.** Measuring the scale of opioid consumption in Australia by wastewater analysis. **C. Gerber**, I. nguyen, R. Bade, J. White, B. Tscharke, J. O'Brien, J. Mueller, K. Thomas
- 10:05** Intermission.
- 10:20 139.** New methods in wastewater-based epidemiology: Plant-based dietary trends and *in situ* active sample collection. **E.M. Driver**, D.A. Bowes, A.J. Gushgari, R.U. Halden
- 10:45 140.** Monitoring opioid use through wastewater-based epidemiology: Case of methadone in Australia and China. **P. Thai**, J. O'Brien, B. Tscharke, P. Du, X. Li, R. Bruno, K. Thomas, J. Mueller
- 11:10 141.** Is 24-hour composite sampling enough?. **R.A. Huffines**, J.E. Mauk, B. Nelson, T.L. Croft, B. Subedi
- 11:35 142.** Wastewater sampling as input to national statistics on recreational drug use: Results of a Canadian pilot study and future directions. **T. Werschle**, **S. McLean**

SECTION F
San Diego Convention Center
Room 29A

Showcasing emerging investigators & future perspectives: A symposium by the RSC Environmental Science Journals

Financially supported by Royal Society of Chemistry; Association of Environmental Engineering & Science Professors (AEESP)

D. M. Cwiertny, *Organizer*
K. P. McNeill, S. Neil, P. Novak, P. J. Vikesland, *Organizers*,
Presiding

- 8:20** Introductory Remarks.
- 8:25** **143.** Biologically mediated chiral inversion of emerging contaminants: Role of wastewater treatment. **S.J. Khan**, A. Branch, J. McDonald, S.N. Berry, L. Nghiem, P. Neale, F. Leusch, K.A. Jolliffe
- 8:55** **144.** Putting the “bio” in bioretention: Microbial, plant, and fungal transformation processes in green stormwater infrastructure for sustained removal of emerging contaminants. **G.H. LeFevre**
- 9:25** **145.** Which photo-oxidant for potable reuse? Treatment efficiency and toxicity considerations. **H. Liu**, D. Schlenk
- 9:55** Intermission.
- 10:10** **146.** Modulation of nanoparticle-membrane interaction by proteins. **J.A. Pedersen**, E.E. Carlson, C.J. Murphy, R. Hernandez
- 10:40** **147.** Transformation-determined nanotoxicity. **S. Liu**
- 11:10** **148.** Toward predictive analysis of nanoparticle protein corona populations. **K. Wheeler**, M. Findlay, D. Freitas, M. Mobed-Miremadi, S. Eramo, K. Baumgartner
- 11:40** Discussion.
- 11:55** Concluding Remarks.

Novel Polymeric Materials & Polymer-Based Processes for Energy-Efficient Treatment of Water & Resource Recovery

Fundamentals of Water & Solute Transport in Membranes

Sponsored by PMSE, Cosponsored by ENVR

Analytical Methodologies for Process Chemistry & Formulation Research

Sponsored by AGRO, Cosponsored by ENVR

Ocean Science: Research Reflections at the Marina

Sponsored by SOCED, Cosponsored by ENVR

Surfaces & Interfaces in the Environment: Symposium in Honor of Vicki Grassian

Catalysis, Surfaces & Minerals

Sponsored by COLL, Cosponsored by ENVR and WCC

Agrochemicals & Water: Advances in Prevention, Monitoring, & Treatment

Sponsored by AGRO, Cosponsored by ENVR

Agrochemicals & Water: Advances in Prevention, Monitoring, & Treatment

Sponsored by AGRO, Cosponsored by ENVR

Advances in Catalysis with Ceria & Other Reducible Oxides

Reactions of Ceria Catalysts

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

Future of Biomacromolecules at a Crossroads of Polymer Science & Biology

Synthetic Cells

Sponsored by POLY, Cosponsored by BIOL, CARB, CELL, COLL, ENVR, MEDI, PHYS and PMSE

Off-Target Transport of Field Applied Agricultural Chemicals: Study Designs, Monitoring, Modelling, & Risk Assessment

Sponsored by AGRO, Cosponsored by ENVR

MONDAY AFTERNOON – ENVR

SECTION A

San Diego Convention Center
Room 28A

Sensors & Biosensors for Widespread Environmental Monitoring

Cosponsored by AGRO

T. Li, V. V. Rajasekharan, W. Zhang, *Organizers*
M. Romero-Gomez, P. L. Schorr, *Organizers, Presiding*

- 1:00** Introductory Remarks.
- 1:05** **149.** Biological and ecological strategy for biomimicry and its application. **J. Kim**, E. Lee, H. Bae, Y. Lee, E. Park
- 1:25** **150.** Simple yet sophisticated environmental sensors for citizen science and widespread use. **J. Hofstetter**
- 1:45** **151.** Autonomous detection of nutrients in marine and freshwaters using next generation environmental sensors. **M. McCaul**, A. Donohoe, P. McCluskey, C. Hazel, A. Shinde, D. Diamond
- 2:05** **152.** Rapid and simple assay to detect the presence of biocides that inhibit nitrification. **P. Morkus**, D. Montpetit, C. Filipe, D.R. Latulippe
- 2:25** **153.** Evaluation of biosensors for in-situ hydrocarbon detection in aquatic environments. **H. Nandimandalam**, V. Gude

Nanomaterials & Sustainability

Cosponsored by CEI

S. Ahuja, *Organizer*

- 1:00** 168. Nanomaterials: Friends or foes. **S. Ahuja**
- 1:20** 169. Self-propelled natural halloysite nanoclay nanomotors for heavy metal remediation. **T. Maric**, C.C. Mayorga-Martinez, B. Khezri, M.M. Mohamad Nasir, X. Chia, M. Pumera
- 1:40** 170. Reduction of nitrate by nanoscale palladized zero-valent iron@graphene composite: Synthesis, characterization, kinetics, and reduction mechanism. **F. Zhang**, X. Huang, S. Li
- 2:00** 171. Simultaneous removal and inactivation of *Legionella pneumophila* using electrically heatable carbon nanotube interfaces. Y. Oh, R. Noga, V. Shanov, H. Ryu, J. Yadav, **S. Chae**
- 2:20** 172. Formulation rules for integration of metal organic framework nanoparticles into mixed-matrix membranes for post-combustion carbon capture. **S.K. Elsaïdi**, S. Venna, M.H. Mohamed, A. Sekizkardes, D. Hopkinson
- 2:40** Intermission.
- 2:55** 173. Enhanced water disinfection using vertically aligned TiO₂ nanowires through physical puncture and photocatalytic action. **E. Kim**, M. Choi, W. Kim
- 3:15** 174. Water treatment sludge as reactive sorbent for sulfate removal. **N. Pimpha**, K. Sitthisuwannakul
- 3:35** 175. Role of stomata in foliar sorption of silver nanoparticles by *Arabidopsis thaliana*. **J. He**, L. Zhang, S. He, E. Ryser, H. Li, W. Zhang
- 3:55** 176. Structural controls on reactivity and long-term performance of sulfidized zerovalent iron. **D. Tobler**, M. Mangayayam, K. Dideriksen, M. Ceccato
- 4:15** 177. Linking sulfidation treatment and contaminant selectivity of sulfidized zero-valent iron. **M. Mangayayam**, V. Alonso de Linaje, R. Espinosa, K. Dideriksen, D. Tobler
- 4:35** 178. Efficient removal of hazardous fluoride from drinking water by using bionanomaterial derived from nitro-oxidized carboxynanocellulose. **S. Sharma**, P. Sharma, B.S. Hsiao

- 2:45** 154. Withdrawn
- 3:05** Intermission.
- 3:15** 155. Electrochemical determination of copper(II) ions in water using polyacrylic-graphene-thiourea modified electrode. **N.B. Abdul Razak**, S.B. Hasbullah, L. Tan, Y. Lee
- 3:35** 156. Uranium isolation and concentration using reactive membranes for quantitative analysis. **A.W. Darge**, T.A. Devol, S.M. Husson
- 3:55** 157. Sensing of penicillins and cephalosporins in neutral aqueous solution using a calcein-PAMAM complex. **Y. Xu**, M. Bonizzoni
- 4:15** 158. Carbon nanomaterials sensors for lead detection in drinking water. **N.T. Alvarez**, K. Ojo, A. Kile, W.R. Heineman, V. Shanov, K. Gazica, C. Rahm
- 4:35** 159. Can spectroscopy with 'real time' monitors provide data to suggest horizontal gene transfer during an algal bloom?. **P.L. Schorr**
- 4:55** Concluding Remarks.

SECTION B

San Diego Convention Center

Room 28B

Emerging Contaminants in Wastewater

A. S. Adeleye, P. Cervantes, Y. Huang, *Organizers, Presiding*

- 1:00** Introductory Remarks.
- 1:05** 160. Pharmaceuticals in wastewater treatment plants: Presence, abundance, and fate. **Y. Sun**, Z. Han, J. Xue, Y. Zhu, A.S. Adeleye
- 1:30** 161. Direct electron transfer based peroxymonosulfate activation by iron doped manganese oxide (Mn₃O₄): New approach for water treatment. **K. Huang**, H. Zhang
- 1:55** 162. Pollen solutions: Novel and green approach to water treatment. **A. Meichanetzoglou**, A. Boa
- 2:20** 163. Carbon metal-organic framework composite (CMOF) for the adsorption of contaminants of emerging concern from water. **J. Munoz**, S. Kim, Y. Yoon, A.J. Hernandez
- 2:45** Intermission.
- 3:00** 164. Evaluation of contaminant of emerging concern removal in wastewater by a hybrid forward osmosis-reverse osmosis system. **A. Szczuka**, W. Mitch
- 3:25** 165. Removal of multidrug-resistant *Salmonella*, antibiotics and antibiotics resistance genes in water by electrochemical oxidation. **B. Wang**, H. Shi, Q. Huang
- 3:50** 166. Removal of meropenem from environmental matrices by electrochemical oxidation. **A. Ahmadi**, T. Wu
- 4:15** 167. Degradation of selected hormones and antibiotics in subcritical water. N. Saha, **M. Reza**
- 4:40** Concluding Remarks.

SECTION D
San Diego Convention Center
Room 28D

Chemistry of Water Reuse Processes Toward Water Sustainability

Cosponsored by AGRO and PRES

Financially supported by Association of Environmental Engineering & Science Professors (AEESP)

W. Hou, C. Huang, Z. Qiang, V. K. Sharma, *Organizers*

R. Doong, *Organizer, Presiding*

C. Dong, G. Wang, *Presiding*

- 1:00** Introductory Remarks.
- 1:05** **179.** Oxidation treatment of new cyanoneurotoxins BMAA and two isomers. **T. Lin**, Y. Chen, M. Lee, W. Chen
- 1:35** **180.** Characterization and applications of green-synthesized Cu₂O/ TiO₂ nanotube arrays. **Y. Peng**, Y. Lin, K. Chen
- 1:55** **181.** Evanescent waves generated in TiO₂-coated quartz optical fibers coupled with UV-LEDs improve quantum yields of pollutant degradation. **Y. SONG**, L. Ling, C. Shang
- 2:15** **182.** Sunlight-driven formation of silver nanoparticles: Roles of natural organic matter and silver-chloride complex. **A. Singh**, W. Hou, T. Lin
- 2:35** Intermission.
- 2:55** **183.** Photo-disinfection processes over visible-light selective non-metallic/metallic -TiO₂ composites. **J. Tzeng**, C. Weng, L. Yen, G. Gaybullaev, Y. Lin, C. Huang
- 3:10** **184.** Equilibrium modeling of struvite recovery in wastewater processes. **A. Bowers**
- 3:30** **185.** Morphological effect of electroless copper substrate on catalytic efficiency of CuPd, CuSn, CuSnPd electrodes in electrochemical reduction of nitrate ion. **Y. Shih**, C. Huang
- 3:50** **186.** Nickel hexacyanoferrate electrodes for sodium intercalation. **C. Peng**, C. Lin, H. Tung
- 4:30** Closing Remarks.

SECTION E
San Diego Convention Center
Room 28E

Wastewater-Based Epidemiology: Opportunities, Challenges & Applications to Public Health & Safety

Financially supported by Biobot Analytics; Association of Environmental Engineering & Science Professors (AEESP)

D. A. Burgard, M. Matus, B. Subedi, *Organizers, Presiding*

- 1:00** Introductory Remarks.

- 1:05** **187.** Wastewater-based epidemiology (WBE) toolkit platform: Could WBE be a Spotify, Netflix or Twitter like-platform for population health?. **J. Baz Lomba**, K. Thomas, M. Reid
- 1:30** **188.** 24-hour multi-omics analysis of residential sewage reflects human activity and informs public health. **M.G. Matus**, **C. Duvallet**, M. Kido Soule, K. Longnecker, N. Endo, N. Ghaeli, S. Kearney, I. Brito, C. Ratti, E.B. Kujawinski, E. Alm
- 1:55** **189.** Using municipal wastewater to monitor community microbial infectious diseases: Antimicrobial resistance in *Salmonella*. **T. Yan**, S. Diemert
- 2:20** **190.** Assessing the human condition globally in near real-time using the human health observatory. **R.U. Halden**
- 2:45** Intermission.
- 3:00** **191.** Determining diversity of community salmonellosis cases using municipal wastewater surveillance. **S. Diemert**, T. Yan
- 3:25** **192.** Multi-site sampling and risk prioritization reveals the public health relevance of antibiotic resistance genes found in wastewater environments. **C. Dai**, C. Duvallet, A. Zhang, M.G. Matus, N. Ghaeli, S. Park, N. Endo, S. Isazadeh, K. Jamil, C. Ratti, E. Alm
- 3:50** **193.** Wastewater pharmacometabolomics: Feasibility study using liquid-chromatography mass spectrometry to estimate illicit drug consumption during college football games. **D.J. Lemas**, M. Loop, M. Duong, A. Schleffer, C. Collins, A. Ciesielski, Z.D. Ridge, J. Wagner, C. Delcher
- 4:15** **194.** Four-year illicit stimulant use trends in Seattle, WA USA. **D.A. Burgard**, R. Rushing
- 4:40** Closing Remarks.

SECTION F
San Diego Convention Center
Room 29A

Green Chemistry & the Environment

Cosponsored by CEI

R. Luque, S. O. Obare, *Organizers, Presiding*

- 1:00** Introductory Remarks.
- 1:05** **195.** Using green chemistry for REE recovery from coal fly ash: Hydrothermal extraction and ligand-associated media sorption. **T.M. Dittrich**, M. Dardona, J. Hovey, M.J. Allen, S.K. Mohanty, H. Boukhalfa
- 1:25** **196.** Ultrasonic particle detection: Filter backwash optimization, Part I. **C. Steary**
- 1:45** **197.** Environmental issues associated with herbicidal ionic liquids: From synthesis to advanced

- field studies. **L. Chrzanowski**, L. Lawniczak, T. Praczyk, J. Pernak
- 2:05 198.** Towards sustainable water treatment: Selective adsorption of arsenic over competing phosphate by transition metal cross-linked chitosan. **L.N. Pincus**, J.B. Zimmerman
- 2:25 199.** Detoxification of waste water of Pb²⁺ and Cd²⁺ using agricultural waste of boiled groundnut (*Arachis hypogaea*) shells. **T.A. Abii**
- 2:45** Intermission.
- 2:55 200.** Green chemistry in a successful science coaches collaboration: Making molecules for water remediation. **M.A. Benvenuto**, S.P. Kosmas
- 3:15 201.** Medical waste management in the Republic of Serbia. **L.B. Stojkovic**
- 3:35 202.** Distribution, sources and carcinogenic potentials of polycyclic aromatic hydrocarbons in farmland soils and crops around the vicinity of tobacco processing local industry, Oke-Aran, Igboho, Nigeria. **T.A. Adedosu**, J.O. Ajibade, H.O. Adedosu
- 3:55 203.** Tetracycline sorption by a tailor-made adsorbent in aqueous system. **A.O. Ruth**
- 4:15 204.** Sustainable production of polyhydroxybutyrate (PHB) by *Zobellella denitrificans* ZD1 grown with non-sterile salty waste streams. **F. Asiri**, C. Chen, M. Hwangbo, Y. Shao, K. Chu
- 4:35 205.** Bi-functionalized ionic liquid immobilized on MIL-53(Al) for efficient carbon dioxide capture and conversion. **L. Sun**, **S. Tang**
- 4:55** Closing Remarks.

SECTION G

San Diego Convention Center
Room 30A

Plastics in Aquatic Environments, Part II: Transport, Fate & Global Impacts

Cosponsored by POLY

Financially supported by Association of Environmental Engineering & Science Professors (AEESP)

K. Ikehata, R. T. Mathers, S. V. Orski, M. A. Pasquinnelli,
Organizers

J. A. Glaser, *Organizer, Presiding*

- 1:00** Introductory Remarks.
- 1:10 206.** Environmental biodegradation of plastics. **J.A. Glaser**
- 1:40 207.** Toxicological effects of microplastics and its attachment of metals as vector on the zooplankton *Moina monogolica* Daday. **Z. Wang**
- 2:00 208.** Synthetic microfibers: Incorporating particulate pollutants into water quality

- monitoring. **J.R. Peller**, C.R. Iceman, L. Eberhardt, E. Kostelnik
- 2:30 209.** Addressing nano/microplastics fouling on filtration membranes by surface plasma treatment. **M. Enfrin**, L.F. Dumee, J. Lee
- 2:50** Intermission.
- 3:05 210.** Development of an experimental approach to improve lab-scale assessments of the environmental behavior of microplastics. **F. Perreault**
- 3:35 211.** Municipal sewage sludge as a source of microplastics in the environment. **C. Rolsky**, V. Kelkar, R.U. Halden
- 3:55 212.** Release of microfibers during textile laundering and their behavior in aquatic environments: Effect of fabric finishes. **M. Zambrano**, R.A. Venditti, J. Pawlak, J. Cheng, J. Daystar, C. Goller, M. Ankeny
- 4:15 213.** Adsorption behavior of antibiotics by microplastics in water. **F. Yu**, G. Huang, Y. Li, J. Ma
- 4:35** Concluding Remarks.

Novel Polymeric Materials & Polymer-Based Processes for Energy-Efficient Treatment of Water & Resource Recovery

Energy-Efficient Water Purification & Resource Recovery

Sponsored by PMSE, Cosponsored by ENVR

Surfaces & Interfaces in the Environment: Symposium in Honor of Vicki Grassian

Aqueous Surfaces to Ocean & Organic-Surface Interactions

Sponsored by COLL, Cosponsored by ENVR and WCC

Water Scarcity: Challenges for Agriculture

Sponsored by AGRO, Cosponsored by ENVR and PRES

Advances in Catalysis with Ceria & Other Reducible Oxides

Reactions and Other Metal Oxides

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

Future of Biomacromolecules at a Crossroads of Polymer Science & Biology

Tissue Engineering

Sponsored by POLY, Cosponsored by BIOL, CARB, CELL, COLL, ENVR, MEDI, PHYS and PMSE

Off-Target Transport of Field Applied Agricultural Chemicals: Study Designs, Monitoring, Modelling, & Risk Assessment

Sponsored by AGRO, Cosponsored by ENVR

MONDAY EVENING – ENVR

SECTION A

San Diego Convention Center
TBD

Sci-Mix

J. L. Goldfarb, *Organizer*

8:00 - 10:00

25, 33, 65, 66, 73, 82, 106, 116, 135, 136, 153, 162, 171, 172, 190, 195, 196, 201, 207. See Previous Listings.

215, 218, 237, 245, 247, 258, 265, 266, 302, 320, 322, 352, 373, 375, 388, 389, 390, 391, 392, 393, 399, 403, 408, 410, 419, 421, 426, 432, 436, 449, 471, 475, 477, 493, 497, 503, 508, 533, 547, 548, 553, 561, 584, 587, 595, 630, 645, 649, 657, 660, 666, 669, 671, 678, 699, 711. See Subsequent Listings.

TUESDAY MORNING – ENVR

SECTION A

San Diego Convention Center
Room 28A

Chemistry & Applications of Free Radical-based Technologies for Water Treatment & Purification

UV-Based Free Radicals-Based Technologies & Application

Cosponsored by AGRO

Financially supported by Association of Environmental Engineering & Science Professors (AEESP)

D. Minakata, K. E. O'Shea, W. Song, *Organizers*

D. D. Dionysiou, G. Li Puma, *Organizers, Presiding*

A. Pisarenko, *Presiding*

8:00 214. Degradation of some insensitive munitions compounds in water through computational chemistry approach. **M.K. Shukla**

8:25 215. Toward predicting potentially hazardous transformation products in aqueous-phase advanced oxidation processes: Where are we standing by and where are we heading. **D. Minakata**

8:50 216. Aldehydes and organosulfates: Advanced oxidation byproducts of direct radical addition to aromatic contaminants. **J. Van Buren**, C. Prasse, E. Marron, D.L. Sedlak

9:15 217. Innovative groundwater treatment of 1,4-Dioxane and VOCs in Los Angeles. **N. Blute, C. Cotton**, J. Collins, K. Wells, T. Rother, A. Siyahian

9:40 218. Coupling of UV/H₂O₂ and biological treatment for the removal of the pharmaceuticals metoprolol and metoprolol acid from hospital wastewater. A. Jaen-Gil, G. Buttiglieri, A. Benito, J. Mir-Tutusaus, R. Gonzalez-Olmos, G. Caminal, M. Sarra, S. Rodriguez-Mozaz, **D. Barcelo**

10:05 Intermission.

10:20 219. Predicting the contribution of chloramines to contaminant decay during UV/hydrogen peroxide advanced oxidation process (AOP) treatment for potable reuse. **Z. Zhang**, W. Mitch

10:45 220. Chloramines in UV/advanced oxidation processes: Impacts and insights into water reuse. **S.D. Patton**, K. Mangalgi, L. Wu, W. Li, K.D. Couch, S.P. Mezyk, K.P. Ishida, H. Liu

11:10 221. Impact of groundwater quality parameters on 1,4-dioxane removal and associated byproducts formation during UV/hydrogen peroxide advanced oxidation process treatment. **C. Lee**, A. Venkatesan, H. Walker, C. Gobler

11:35 222. Investigation of 1,4-dioxane oxidation byproducts during UV advanced oxidation processes. **L. Wu**, K. Mangalgi, S.D. Patton, D. Schlenk, H. Liu

SECTION B

San Diego Convention Center
Room 28B

Legacy & Emerging Per- & Polyfluoroalkyl Substances: Identification, Fate, Transport, Exposure, & Removal

Financially supported by Association of Environmental Engineering & Science Professors (AEESP)

K. Chu, J. Liu, M. Sun, *Organizers*

F. Xiao, *Organizer, Presiding*

8:05 Introductory Remarks.

8:10 223. Defluorination of PFAS by *Acidimicrobiaceae* sp. A6 during Feammox incubations. **P.R. Jaffe**

8:40 224. Removing PFOA and PFOS from water by reductive processes. **S.P. Mezyk**, L. Twight

9:05 225. Degradation of PFAS in AFFF-contaminated water by oxidative BOHP/UV and reductive BiPO₄/UV photocatalytic processes within a commercial pilot-scale slurry reactor. D. Wang, M. Qanbarzadeh, **E.L. Cates**

- 9:30** **226.** UV assisted electrochemical oxidation of PFAS by degenerate semiconductor electrodes. **Y. Yang**, S. Yang
- 9:55** Intermission.
- 10:15** **227.** Relationship between perfluorooctanoate and perfluorooctane sulfonate blood concentrations in the general population and routine drinking water exposure. S. Zhang, Q. Kang, H. Peng, M. Ding, F. Zhao, Y. Zhou, Z. Dong, H. Zhang, M. Yang, S. Tao, **J. HU**
- 10:40** **228.** Per- and polyfluoroalkyl substances (PFASs): Percutaneous absorption and implications for total human exposure. **J.N. Rewerts**, J.C. Kissel, J.A. Field
- 11:05** **229.** PFAS binding affinity with liver fatty acid binding protein, intestinal fatty acid binding protein, and peroxisome proliferator-activated receptors alpha, delta, and gamma. M. Khazaei, E. **Christie**, M. Michalsen, J.A. Field, C. Ng
- 11:30** **230.** Screening of PFAS in aqueous film forming foam for binding to human serum albumin and characterization of mechanisms. **W. Li**, T.M. Young, H. Bischel
- 11:55** Concluding Remarks.

SECTION C

San Diego Convention Center
Room 28C

Nanomaterials & Sustainability

Cosponsored by CEI
S. Ahuja, *Organizer*

- 8:00** Introductory Remarks.
- 8:05** **231.** Effect of nano and bulk copper oxide particles on the development of two varieties of bok choy (*Brassica rapa*) plants. **C. Deng**, Y. Wang, J.A. Hernández-Viezcás, J. Peralta-Videa, J.L. Gardea-Torresdey
- 8:25** **232.** Effect of the presence of iron oxide nanoparticles on the transport of zinc oxide nanoparticles through water-saturated porous media under different condition. **D. Kumari**, T. Raychoudhury
- 8:45** **233.** Lithium extraction from hydraulic fracturing flowback water. **A. Seip**, S. SafariMohsenabad, D.S. Alessi
- 9:05** **234.** Inhibited dinitrogen fixation in soybeans grown with carbonaceous nanomaterials is compensated by enhanced soil nitrogen assimilation. **Y. Wang**, J.P. Schimel, R.M. Nisbet, J.L. Gardea-Torresdey, P. Holden
- 9:25** **235.** Radiation grafted microfibrillar and nanofibrillar amine-containing adsorbents for carbon dioxide capture. N. Mohamed, A. Abbasi, E.

- Abouzari, A. Ahmad, **M.M. Nasef**
- 9:45** Intermission.
- 10:00** **236.** Characterization of nanoparticle suspensions with microdeposition and microscopy. **L.C. Elliott**, R. Verkouteren, A. Pintar, S.M. Stavis
- 10:20** **237.** Process modification for organic solvent separation via carbon nanotube immobilized membrane using membrane distillation. **O. Gupta**, S. Roy, S. Mitra
- 10:40** **238.** Inactivation of *Legionella pneumophila* harbored by amoebae using a nano-enabled alternative technology. **N.B. Saleh**, C. Ayres, M. Kirisits
- 11:00** **239.** Passive sampling of pesticides in air and water using electrospun nanofiber mats. **M. Nagorzanski**, J. Qian, A. Martinez, R.F. Marek, D.M. Cwiertny
- 11:20** **240.** Membranes made of nitrogen-doped CNTs decorated with magnetite NPs for cleaning treated wastewater. **E. Contreras**, D. Dominguez, H. Tiznado, J. Guerrero-Sánchez, N. Takeuchi, G. Alonso-Nunez, O.E. Contreras, M.T. Oropeza, J. Romo-Herrera
- 11:40** **241.** Nanocellulose scaffold for water purification. **P. Sharma**, S.K. Sharma, B.S. Hsiao

SECTION D

San Diego Convention Center
Room 28D

Chemistry of Water Reuse Processes Toward Water Sustainability

Cosponsored by AGRO and PRES
Financially supported by Association of Environmental Engineering & Science Professors (AEESP)
R. Doong, W. Hou, C. Huang, Z. Qiang, V. K. Sharma, *Organizers*

- 8:15** Introductory Remarks.
- 8:20** **242.** Treatment and reuse of tunnel construction wastewater by coagulation-flocculation process. **J. Liu**
- 8:40** **243.** Reactions of dichloramine with amino acids in wastewaters: Kinetic study. **E.D. Walker**, K.P. Ishida, S.P. Mezyk
- 9:00** **244.** Development of energy-efficient electrokinetic separation for water reuse in agriculture. **S. Pan**, C. Fan, H. Kim, S.W. Snyder
- 9:20** **245.** Wastewater production footprints of hydraulic fracturing operations: Current pace and future impacts. **A. Zolfaghari**, J. Gehman, D.S. Alessi
- 9:40** **246.** Catalytic regeneration and surface reactivity of soot-laden diesel particulate filter. J. Chang, T. Yang, C. Chen, **C. Hsieh**
- 10:00** Intermission.

- 10:15 247.** Enhancing carbon capture and utilization for energy-positive wastewater treatment. **G. Sarpong, V. Gude**
- 10:35 248.** Overcoming the yuk factor: How public understanding, politics, and framing mediate support for recycled water policies. **D.L. Kriner, J.L. Goldfarb**
- 10:55 249.** Morphology and adsorption removal of ^{110m}Ag in the radioactive waste liquid of the pressurized water reactor nuclear power plant. **Q. Zhao**
- 11:15 250.** Fenton-like degradation of RB-5 dye using the magnetite recovered from iron-containing wastewater treated by fluidized-bed homogeneous crystallization (FBHC) process. **Y. Huang, N.N. Mahasti, Y. Shih**
- 11:35 251.** Efficient, energy-saving, and energy-recovering fuel cell type wastewater treatment system with activated carbon in anode and catalytic cathode. **L. Liu**
- 11:55** Concluding Remarks.

SECTION E

San Diego Convention Center
Room 28E

Non-targeted Analysis to Understand Fate & Effects of Pharmaceuticals & Emerging Contaminants in Agriculture & Natural Environments

Cosponsored by AGRO

Financially supported by Association of Environmental Engineering & Science Professors (AEESP)

D. S. Aga, J. B. Sallach, *Organizers, Presiding*

- 8:00** Introductory Remarks.
- 8:05 252.** Global reconnaissance of antimicrobials and other emerging contaminants in surface water by target and non-target LC/MS/MS analysis. **D.S. Aga, L. Angeles**
- 8:35 253.** Integrated cell culture-mass spectrometry method for monitoring infectious human viruses in environmental samples. **K. Wigginton, Y. Ye**
- 9:05 254.** Suspect screening to determining pharmaceutical fate in urine-derived fertilizers. **W.A. Tarpeh, D.S. Aga, N. Love, K. Wigginton, D.E. Helbling**
- 9:35 255.** Non-targeted analysis supported by data and cheminformatics delivered via the US EPA CompTox Chemicals Dashboard. **A.J. Williams, A. Chao, T. Cathey, T. Transue, E.M. Ulrich, J. Sobus**
- 10:00** Intermission.
- 10:15 256.** Structure/reaction directed analysis for environmental metabolites. **M. Yu, G. Dolios, L. Petrick**

- 10:40 257.** Suspect and non-target screening of organic pollutants in marine water and stormwater. **Z. Tian, K.T. Peter, C. Wu, D. Wark, H. Zhao, H. Mathews, A. Cortina, C. James, E.P. Kolodziej**
- 11:05 258.** Using suspect screening to determine Hurricane Florence's impact on chemicals of concern at a forested water reuse site. **M.L. Hedgespeth, D. Rashash, D. Shea, M. Strynar, J. Delborne, E.G. Nichols**
- 11:30 259.** Phototransformation of wastewater effluents organic matters: High resolution mass spectrometry characterization. **L. Lushi, S. Weihua**
- 11:55** Concluding Remarks.

SECTION F

San Diego Convention Center
Room 29A

Sensors for Water Quality Assessment in Resource Limited Environments

Cosponsored by AGRO

E. Brack, C. Gomes, *Organizers*

E. McLamore, M. S. Wiederoder, *Organizers, Presiding*

- 8:20** Introductory Remarks.
- 8:25 260.** SENSEE: Open source portfolio tool for sensor comparative studies and technology transfer. **E.S. McLamore**
- 8:45 261.** Rapid, label-free detection of *Escherichia coli spp* for on-farm water quality assessment based on temperature-sensitive nanobrush actuation. **C. Giacobassi, D. Oliveira, C. Pola, N. Cavallaro, E. McLamore, C.L. Gomes**
- 9:05 262.** Bacteriophage-based nanoprobe enable rapid and low-cost testing for *Escherichia coli* in drinking water. **M.M. Duong, H. Zurier, J.M. Goddard, S.R. Nugen**
- 9:25 263.** Simple impedance spectroscopy system for biofilm detection and monitoring. **P. Takhistov**
- 9:45 264.** Capillary flow dynamics-based sensing modality for direct environmental pathogen monitoring. **K.E. Klug, K.A. Reynolds, J. Yoon**
- 10:05** Intermission.
- 10:25 265.** Paper-based gene network detection of heavy metals for in-field water quality testing. **C. Bernhards, K. Turner, K. Beabout, J.L. Chavez, S. Walper, M. Lux**
- 10:45 266.** Disposable voltammetric sensors for onsite detection of arsenic, selenium, and cadmium. **C. Sullivan, D. Lu, E. Brack, C. Drew, P. Kurup**
- 11:05 267.** Inexpensive 2D and 3D printed sensors for rapid instrument-free detection of emerging contaminants in water. **K. Kirk, A. Finny, E. Andreescu**

- 11:25 268.** Characterization of PTE-nanoparticle bioconjugates for rapid and sensitive detection of organophosphates. **J. Breger**, J.C. Claussen, M. Ancona, S. Walper, K. Susumu, M. Stewart, J. Deschamps, E. Oh, I. Medintz
- 11:45 269.** Printed and laser induced graphene electrochemical sensors for in-field pesticide and fertilizer ion monitoring. J. Hondred, N. Garland, I. Kucherenko, R. Hjort, C.L. Gomes, **J. Claussen**
- 12:05** Concluding Remarks.

Advances in Analytical Technologies Supporting Environmental Fate, Metabolism, & Residue Analysis

Sponsored by AGRO, Cosponsored by ENVR

Novel Polymeric Materials & Polymer-Based Processes for Energy-Efficient Treatment of Water & Resource Recovery

Energy-Efficient Water Purification & Resource Recovery

Sponsored by PMSE, Cosponsored by ENVR

Future Insights into Syngas Conversion Catalysis: Symposium in honor of Burtron H. Davis

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

Advances in Catalysis with Ceria & Other Reducible Oxides

Reactions and Other Metal Oxides

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

TUESDAY AFTERNOON – ENVR

SECTION A

San Diego Convention Center
Room 28A

Chemistry & Applications of Free Radical-based Technologies for Water Treatment & Purification

Various Free Radicals-Based Technologies

Cosponsored by AGRO

Financially supported by Association of Environmental Engineering & Science Professors (AEESP)

D. D. Dionysiou, G. Li Puma, D. Minakata, K. E. O'Shea, *Organizers*

W. Song, *Organizer, Presiding*
N. Blute, D. Minakata, *Presiding*

- 1:00** Introductory Remarks.
- 1:05 270.** Performance of UV/free chlorine AOP for removal of 1,4-dioxane in potable reuse applications. **A.N. Pisarenko**, Y. Qu, E. Chen, D. Hokanson, R.R. Trussell, R.S. Trussell, J. Quicho
- 1:45 271.** Kinetics of chlorine atom reactions in advanced oxidation processes. **L. Ruiz Armenta**, L. Watts, K.P. Ishida, G. Ferraudi, S.P. Mezyk
- 2:10 272.** Using advanced oxidation processes as treatment barrier to eliminate cyanotoxins from drinking water. M. Kong, X. Duan, **D.D. Dionysiou**
- 2:35 273.** Algal toxins in drinking water: UV/Cl₂ and UV/H₂O₂ advanced oxidation processes as treatment method. **F. Brancheshme**, O. Keen
- 3:00** Intermission.
- 3:15 274.** Novel advanced oxidation process by peracetic acid and Fe(II). **J. Kim**, T. Zhang, C. Huang
- 3:40 275.** Pesticides and metal chelates in reverse osmosis concentrate: Removal by radicals formed during ozonation in a pilot-scale ozone-wetland system. **J. King**, W. Mitch
- 4:05 276.** Photo-assisted catalytic ozonation for the treatment of ozone-resistant water pollutants. W. Yang, X. Chen, M. Bunian, Y. Lei, **T. Wu**
- 4:30 277.** Efficient Fenton oxidation of atrazine at circumneutral pH mediated by a complexing agent, picolinic acid. **Z. Yang**, J.J. Pignatello, B. Pan
- 4:55** Closing Remarks.

SECTION B

San Diego Convention Center
Room 28B

Legacy & Emerging Per- & Polyfluoroalkyl Substances: Identification, Fate, Transport, Exposure, & Removal

Financially supported by Association of Environmental Engineering & Science Professors (AEESP)

K. Chu, M. Sun, F. Xiao, *Organizers*

J. Liu, *Organizer, Presiding*

- 1:00 278.** Adsorption behavior and mechanism of emerging perfluoro-2-propoxypropanoic acid (GenX) on activated carbons and resins. **S. Deng**, W. Wang, A. Maimaiti
- 1:25 279.** Removal of perfluoroalkyl substances (PFASs) in groundwater using activated carbon and ion exchange resin: Column test. **C. Zeng**, N. Sharma, A. Hjelmstad, K. Venkatesh, P.K. Westerhoff
- 1:50 280.** Removal of poly- and perfluoroalkyl substances (PFAS) in aqueous film-forming foam

- (AFFF) impacted water using ion exchange and nonionic resins. **Y. Fang**, A. Ellis, Y. Choi, T.H. Boyer, C.P. Higgins, C. Schaefer, T.J. Strathmann
- 2:15 281.** Biotransformation and persistence of polyfluoroalkyl zwitterionic betaines and amines in aerobic soils. **M. Liu**, G. Munoz, S. Vo Duy, S. Sauve, J. Liu
- 2:40 282.** Sorption and desorption mechanisms of cationic and zwitterionic per- and polyfluoroalkyl substances in natural soils. **F. Xiao**, B. Jin, S. Golovko, M. Golovko, B. Xing
- 3:05** Intermission.
- 3:20 283.** Quantitative measurements of emerging perfluoroether carboxylic acids in surface water using UHPLC-MS/MS. Y. Pan, J. Yao, **J. Dai**
- 3:45 284.** Ultrahigh-resolution Fourier-transform ion cyclotron resonance mass spectrometry for identification of per- and polyfluoroalkyl substances (PFASs). **A.M. McKenna**, N. Pica, H. Chen, J. Blotevogel
- 4:10 285.** Detection of PFOA by sensitive ToF-SIMS. J. Yao, C. Yang, **X. Yu**
- 4:35 286.** Occurrence and distribution of selected perfluoroalkyl substances in the surface soils of Vermont. **W. Zhu**, H. Roakes, S. Zemba, **A. Badireddy**

SECTION C

San Diego Convention Center
Room 28C

Nanomaterials & Sustainability

Cosponsored by CEI
S. Ahuja, *Organizer*

- 1:00** Introductory Remarks.
- 1:05 287.** Effect of rhamnolipid on aggregation and deposition of surface stabilized magnetite nanoparticles in environment. **A. Ghosh**, K. Parker, J. Fortner
- 1:25 288.** Solar thermal water purification enabled by photothermal conversion using the 1T/2H phases of MoS₂. **D. Ghim**, Q. Jiang, S. Cao, S. Singamaneni, Y. Jun
- 1:45 289.** SERS for characterizing nanosilver in textiles. **M.B. Hillyer**, S. Nam, B.D. Condon
- 2:05 290.** Reduction of inorganic fouling in microwave induced membrane distillation on carbon nanotube immobilized membrane. **M. Humoud**, S. Roy, S. Mitra
- 2:25 291.** Effect of surface coated TiO₂ NPs on carrot (*Daucus carota*) development. **Y. Wang**, C. Deng, J.A. Hernández.Viezcas, J. Peralta-Videa, J.L. Gardea-Torresdey

- 2:45** Intermission.
- 2:55 292.** Precise control of graphene oxide structure for electrically controllable membranes. **J. Shin**, J. Roh, J. Jang, I. Park, H. Park
- 3:15 293.** Molecular insight into the effects of Cu(II) on sulfamethoxazole and 17β-estradiol adsorption by carbon nanotubes/CoFe₂O₄ composites. **W. Sun**, S. Li, F. Wang
- 3:35 294.** Polymer-nano composite degradation, release, detection, and toxicity of nanomaterials during accelerated aging. **E. Sahle Demessie**, C. Han, E. Varughese
- 4:15 295.** Functionalized MOFs based mixed matrix membranes for CO₂ separation. **W. Zheng**
- 4:35 296.** Multifunctionalized superparamagnetic nanoparticles as an efficient material for removal of rhodamine B from wastewater by adsorption. **M.O. Ojemaye**, A. Okoh
- 4:55** Closing Remarks.

SECTION D

San Diego Convention Center
Room 28D

Biochar & Hydrochar for Energy, Environmental & Agricultural Applications

Cosponsored by AGRO

Financially supported by Frontiers in Energy Research; Association of Environmental Engineering & Science Professors (AEESP)

N. D. Berge, J. L. Goldfarb, A. Shah, *Organizers*
R. Volpe, *Organizer, Presiding*

- 1:00** Introductory Remarks.
- 1:05 297.** Effect of pyrolysis temperature on various acidic and basic functional groups on hydrochar. N. Saha, D. Xin, P. Chiu, **M. Reza**
- 1:30 298.** Biochar as a nanosilver support medium for water disinfection. **D. Xin**, S. Lobo, P. Chiu
- 1:55 299.** Study of char morphology during biomass pyrolysis and gasification via micro-computed tomography. **M. Barr**, Y. Zhang, R. Jervis, R. Volpe
- 2:20** Intermission.
- 2:35 300.** Designing activated biochars: Impacts of porosity and particle size on adsorption. **Z. Pollard**, Q. Ha, A. Roshandelpoor, P. Vakili, E. Ryan, J.L. Goldfarb
- 3:00 301.** Effects of air-oxidation induced changes in biomass chars on their adsorption of contaminants. **Y. Yang**, J.J. Pignatello
- 3:25 302.** Molecular design approach to understand the reactivity of pyrogenic carbonaceous materials using conjugated microporous polymers. **Z. Li**, J. Mao, W. Chu, W. Xu

- 3:50 303. Production of catalytically active activated biochar and the application to environment. **A.G. Karunanayake, R. Anderson**
- 4:15 Closing Remarks.

SECTION E

San Diego Convention Center
Room 28E

Fundamental Chemical Processes Common to Dissolved Organic Matter & Atmospheric Organic Aerosols

N. Borduas, S. A. Nizkorodov, *Organizers, Presiding*

- 1:00 Introductory Remarks.
- 1:05 304. Chemical aging of brown carbon aerosol material. **J.P. Abbatt**, R. Hems, E. Schnitzler, A. Trofimova, R. Zhao
- 1:35 305. Insights on photochemical degradation of dissolved organic matter from electrospray ionization Fourier transform ion cyclotron resonance mass spectrometry. **C. Gueguen**, S. Islam
- 2:05 306. Photochemical studies of atmospheric brown carbon using excitation-emission matrix spectroscopy. **A.W. Harrison**, W.J. De Bruyn
- 2:25 307. Aqueous phase reactivity of polyfunctional organic nitrates under atmospheric conditions. **J. Gonzalez Sanchez**, M. Julien, B. Temime-Roussel, S. Ravier, A. Durand, J. Clément, a. Monod
- 2:45 Intermission.
- 3:00 308. Aqueous aerosol chemistry and impacts: Sulfur oxidation, formation of organosulfur compounds and titration of aerosol pH. **V.H. Grassian**
- 3:30 309. Photosensitization in the air: Bridging fundamental bulk processes with secondary organic aerosol production. **C. George**, R. Gemayel, S. Dumas
- 4:00 310. Interfacial characterization of polysaccharide enrichment in sea surface microlayer proxy films. **K.A. Carter-Fenk**, M.E. Fiamingo, H.C. Allen
- 4:20 311. Oligomers formation from cross-reactions of carbonyl compounds in the atmosphere: Insight at a molecular level. **M. Mekic**, J. Liu, Y.G. Lazarou, M. Brigante, D. Vione, S. Gligorovski
- 4:40 312. Spatial determination of organic matter on sediment particles by scanning electron microscope analysis. **F.M. Dunnivant**, M. Clay

SECTION F

San Diego Convention Center
Room 29A

C. Ellen Gonter Environmental Graduate Student Award Symposium

D. D. Dionysiou, *Organizer*
K. E. O'Shea, *Organizer, Presiding*

- 1:00 Introductory Remarks.
- 1:05 313. Treatment of domestic wastewater by simulated solar-light mediated N- and B-codoped TiO₂ AOP for reuse: Mechanistic aspects and implications of inorganic species. **W.H. Abdelraheem**, M. Nadagouda, D.D. Dionysiou
- 1:30 314. Defluorination of per- and polyfluoroalkyl substances (PFASs) with hydrated electrons: Structural dependence and implications to PFAS remediation and management. **M.J. Bentel**, Y. Yu, L. Xu, Z. Li, B.M. Wong, Y. Men, J. Liu
- 1:55 315. Reductive defluorination of per- and polyfluoroalkyl substances by a dechlorinating microbial community. **Y. Yu**, K. Zhang, Z. Li, C. Ren, J. Liu, Y. Men
- 2:20 Intermission.
- 2:35 316. Iodinating agents of dimethenamid in chloraminated water. **M. Rose**, A. Roberts
- 3:00 317. Demonstration and evaluation of hybrid microalgae aqueous conversion systems for biofuel production. **Y. Li**, S. Leow, T. Dong, N.J. Nagle, E.P. Knoshaug, L.M. Laurens, P.T. Pienkos, J. Guest, T.J. Strathmann
- 3:25 318. Electrochemical cell lysis of gram-positive and gram-negative bacteria: DNA extraction from environmental water samples. **S. Wang**, Y. Zhu, Y. Yang, J. Li, M.R. Hoffmann
- 3:50 Closing Remarks.

Novel Polymeric Materials & Polymer-Based Processes for Energy-Efficient Treatment of Water & Resource Recovery

Energy-Efficient Water Purification & Resource Recovery

Sponsored by PMSE, Cosponsored by ENVR

Simulating Fumigant Transport & Emissions: The Evolving Role of Modeling in California Regulations

Sponsored by AGRO, Cosponsored by ENVR

Future Insights into Syngas Conversion Catalysis: Symposium in honor of Burtron H. Davis

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

Environmental Chemistry through the Transformative Power of Film: A Showcase of CEI-ENVR Environmental Film Competition Awardees

Sponsored by MPPG, Cosponsored by CEI and ENVR

Next Generation Watershed Modeling of Agrochemicals

Sponsored by AGRO, Cosponsored by ENVR

TUESDAY EVENING – ENVR

SECTION A

San Diego Convention Center
TBD

Artificial Water Channels for Water Purification & Desalination

Financially supported by Association of Environmental
Engineering & Science Professors (AEESP)
M. Barboiu, J. Hou, B. Mi, *Organizers*

5:00 - 7:00

- 319.** Nanofiber enhanced forward osmosis membrane. S. Langevin, J. Skerritt, M. Logan, **Z. Xia**
320. Insight into the importance of ionic strength and membrane type on biofouling of BSA and hemoglobin binary solutions. **N.T. Kilmer, Y. Zhang, E.M. Stennett**

SECTION A

San Diego Convention Center
TBD

Biochar & Hydrochar for Energy, Environmental & Agricultural Applications

Cosponsored by AGRO
N. D. Berge, J. L. Goldfarb, A. Shah, R. Volpe, *Organizers*

5:00 - 7:00

- 321.** Contaminant removal potential of charred and iron-oxide-charred composites produced from coffee waste. **M. Chehbouni, A. Lam, O. Harvey**
322. Heterogeneous adsorbents from clay-biomass pyrolysis and CO₂ activation for treatment of heavy

metal contaminated water. F. Wang, A. Hubble, L. Gao, **J.L. Goldfarb**

323. Functionalization of sewage sludge-derived biochar with humus sediment slurry and its use for treatment of crude-oil derived hydrocarbons in a simulated soil. **N.O. Offiong, E. Inam**

324. Preparation of high carbon content of hydrochar from biomass via hydrothermal carbonization. **S. Sattasathuchana, B. Kitiyanan, P. Rangsunvigit, P. Khemthong, S. Youngian, K. Faungnawakij**

325. Removal of pyrene by biochar immobilized cells of fusant bacterial strain F14. **J. Lu, B. Hou**

326. Adsorptive removal of pharmaceuticals from contaminated water by magnetized biochar. **S.D. Canada, A.S. Liyanage, T. Mlsna**

327. Adsorption of malachite green dye from aqueous solution using carbonized *Gliricidia sepium* leaves. **A.A. Giwa, D.O. Aderibigbe, M.O. Adesina**

SECTION A

San Diego Convention Center
TBD

Catalysis for Environmental & Energy Applications

Cosponsored by CATL
A. Orlov, A. Savara, Y. Wang, *Organizers*

5:00 - 7:00

- 328.** Promoting effect of K⁺ ions on HCHO degradation over MnO₂ catalysts studied with *in situ* DRIFTS. L. Ye, **H. Huang, R. Fang**
329. Facile synthesis of amorphous mesoporous manganese oxides for efficient catalytic decomposition of ozone. **H. Huang, J. Ji, S. Liu, Y. Yu, L. Ye**
330. Deep insights into the relationship between Fe-MOFs' coordination environment and catalytic ozonation performances. **D. Yu**
331. Reduction of nitrophenol using Fe-doped natural carbon dots. **B. Akhetova, Z. Salkenova, M.P. Balanay**
332. Electrocatalytic sulfur oxidation in anaerobic wastewater effluents. **X. Shao, W. Tarpeh**
333. Benzimidazole based ionic liquids coupled with ZnO nanoparticles for the capture of CO₂. **I.m. garcia, C.A. Huerta-Aguilar, T. Pandiyan**
334. Photocatalytic hydrogen production by strontium titanate-based perovskite doped europium (Sr_{0.97}Eu_{0.02}Zr_{0.1}Ti_{0.9}O₃). **A.F. Lopez Vasquez, P. Delgado, D. Salas**

- 335.** Nitrate reduction by catalytic hydrogenation: Controlling hydrogen delivery with nano-enabled polymeric hollow fibers. **J. Levi**, S. Guo, S. Kavadiyaa, Y. Yin, A. Atkinson, Z. Holman, C. Zhou, B. Rittmann, M.S. Wong, S. Garcia-Segura, P.K. Westerhoff
- 336.** Cobalt-iron layered double hydroxide on metal-organic-framework derived cobalt phosphide electrodes for efficient oxygen evolution reaction. **G. Choi**, J. Lim, S. Lim, J. Moon, U. Baek, J. Park
- 337.** Bioinspired catalyst for perchlorate reduction in water and brine. **E. Bi**, C. Ren, J. Liu

SECTION A

San Diego Convention Center
TBD

Chemistry & Applications of Free Radical-based Technologies for Water Treatment & Purification

Cosponsored by AGRO

D. S. Aga, D. D. Dionysiou, G. Li Puma, D. Minakata, K. E. O'Shea, W. Song, *Organizers*

5:00 - 7:00

- 338.** Biochar-mediated oxidation of phenol by persulfate activated with zero-valent iron. **T. Nguyen**, **S. Oh**
- 339.** Multiple pathways for sulfate radical production during electrolysis at boron-doped diamond electrode. **Y. Shin**, J. Lee
- 340.** Carbonate radical mediated degradation of bisphenol A in UV/sodium percarbonate system. **J. Gao**, X. Duan, D.D. Dionysiou
- 341.** Porous polylactide/kapok foams prepared by nonsolvent-induced phase separation method for effective oil sorbent. **R. Yu**, M. Chen, X. Sun
- 342.** Rapid removal of tetrabromobisphenol A by $-\text{Fe}_2\text{O}_{3-x}$ @Graphene@montmorillonite catalyst with oxygen vacancies in peroxymonosulfate-based systems: Role of halogen and alcohol radicals. **S. Yang**, P. Wu, D.D. Dionysiou
- 343.** Adsorption of molybdenum(VI) on solids derived from sludge of water treatment processes. **J. Lian**, B. Chen, M. Yang, F. Zhou
- 344.** Withdrawn
- 345.** Structure of iron oxides generated in air-cathode assisted iron-electrocoagulation for water treatment. **A. Kumar**, S. Bandaru, C. van Genutchen, M. Nahata, D. Hernandez, A. Gadgil
- 346.** TiO_2 coated magnetic particle for removal of organic pollutants from drinking water. **S. Sultana**, A. Amirbahman, C. Tripp

- 347.** Pulsed power plasma induced degradation of chloroform and chlorobenzene in aqueous solution and an insight into their degradation mechanism.

L. Philip

- 348.** Formation of nitrophenolic by-products in sulfate radical based oxidation processes in the presence of NOM and nitrite. **J. Lu**, P. Yang
- 349.** Wet scrubbing process coupled with UV/PMS: Novel and efficient gaseous VOCs degradation method. **R. Xie**
- 350.** *In situ* activation of peroxymonosulfate by natural ore for the remediation of acetaminophen-contaminated groundwater. **X. Fan**, H. Zhang
- 351.** Use of MOFs for the elimination and degradation of Naproxen in persulfate activated systems: Application to highly concentrated effluents. **A. Ghauch**, R. El Asmar, A. Baalbaki
- 352.** *In situ* EPR observation of radical electrogeneration, transformation at boron-doped diamond and sustainable degradation of plasticizer. **J. Cai**, **G. Zhao**
- 353.** Unveiling the important roles of coexisting contaminants on photochemical transformations of pharmaceuticals: Fibrate drugs as a case study. **Y. Zhang**
- 354.** Effect of chloride on the degradation efficiencies and products of bezafibrate and carbamazepine in UV/persulfate processes. **Y. Liu**, Y. Wu, L. Zhang, L. Feng
- 355.** Simple iron immobilization on graphene oxide for persulfate activation: Radicals and singlet oxygen mediated oxidation. **Y. Kang**, H. Vu, H. Yoon, D. Oh, Y. Chang, Y. Chang
- 356.** Activation of permanganate by UV irradiation for enhanced oxidation of micropollutants. **K. Guo**, J. Fang

SECTION A

San Diego Convention Center
TBD

Chemistry of Water Reuse Processes Toward Water Sustainability

Cosponsored by AGRO and PRES

R. Doong, W. Hou, C. Huang, Z. Qiang, V. K. Sharma, *Organizers*

5:00 - 7:00

- 357.** Study on COD degradation of high salt content radioactive wastewater. **Z. Shi**, H. Zhang, L. Jiang, S. Li, H. Huang
- 358.** Biological treatment of copper-containing NMF/MDG organic wastewater from the TFT-LCD industry. T. Pien, **L. Whang**, P. Liu

- 359.** Electrocoagulation for the wastewater treatment of chemical mechanical polishing: Kinetic study of particle removal. Y. Liu, S. Yen
- 360.** Reductive degradation of aqueous doxycycline by nZVI. A. Malikova, D. Kondratyuk, M. Babaa, W. Lee
- 361.** Preparation and characterization of hollow porous carbon nanofibers. Y. Chiang, S. Lee, Y. Chen
- 362.** Development of an ammonium-selective adsorbent for energy-efficient wastewater nutrient recovery. B.D. Clark, W. Tarpheh
- 363.** Novel disinfection system using recyclable magnetic nanoparticles. Q. Gao, A.A. Keller
- 364.** Assessment of greywater treatment systems for the removal of antibiotic resistant genes and bacteria. M. Henderson, S.J. Ergas, K. Ghebremichael, Z. Ronen
- 365.** Capacitive deionization and disinfection of salt water effected by (Cu-Ag)@C electrodes. H.P. Wang

SECTION A

San Diego Convention Center

TBD

Emerging Contaminants in Wastewater

A. S. Adeleye, P. Cervantes, Y. Huang, *Organizers*

5:00 - 7:00

- 366.** Review of the use of conventional and emerging technologies for removing pharmaceuticals from wastewater. Z. Han, Y. Zhu, Y. Sun, J. Xue, A.S. Adeleye
- 367.** Determination of benzotriazole and analog compounds by liquid chromatography-mass spectrometry in surface runoff water samples from Wilmington Air Park. J. Wiese, T. Luncan, A. McGowin
- 368.** Accumulation of *N*-nitrosodiethanolamine in spinach. D.I. Nielsen-Franco, D. Sanchez, J.A. Pedersen
- 369.** Fate of antibiotic resistance genes and intl1 in soil and fertilizer microcosms at varying levels of copper. C. Echeverria-Palencia, M. Hernandez-Cira, I. Callejas, K. Jimenez, R. Herrera, J.A. Jay
- 370.** Distributions and degradation of brominated flame retardants (PBDEs) in limed and THP-AD treated wastewater biosolids. T. Motley, S. Fischer, N.A. Andrade, B.V. Kjellerup, A. Torrents
- 371.** Toxicological study on photo-degradation products of environmental ibuprofen: Ecological and human health implications. E. Ellepola, T. Ogas, R. Gurung, D.N. Turner, S. Maldonado-Torres, R. Tello-Aburto, P. Patidar, M.E. Piyasena, G. Rubasinghege, S. Rogelj

Fundamental Chemical Processes Common to Dissolved Organic Matter & Atmospheric Organic Aerosols

N. Borduas, S. A. Nizkorodov, *Organizers*

5:00 - 7:00

- 372.** Carbon isotopic characterization of biological influences on sea spray aerosol chemical speciation. D.R. Crocker
- 373.** Natural organic matter characterization of composition and reactivity from permafrost soils in the sub-Arctic. K. Gagne, J.J. Guerard
- 374.** Characterization of secondary organic aerosol formation by aqueous reactions of iron (III) with biomass burning volatile organic compounds. H. Chin, S.A. Nizkorodov, L. Fleming, H.A. Al-Abadleh
- 375.** Determining the dependence of size fractionation and oxidative aging on hygroscopicity and phase state of sea spray aerosol. P.R. Tumminello, K. Mayer, V. Or, A.W. Cooper, V.H. Grassian, K.A. Prather, J.H. Slade
- 376.** Aqueous-phase oxidation kinetics of terpene-derived acids. T. Otto, T. Schaefer, H. Herrmann
- 377.** Brown carbon photolysis: Impacts of organic and inorganic components in cloud water proxies. L. Dolvin, R. O'Brien, M.L. Ambrose, W. Perrine
- 378.** Kinetics for the aqueous oxidation of atmospheric phenols with an organic triplet excited state. L. Ma, C. Guzman, C. Anastasio
- 379.** Effects of transition metal ions on the formation of aqueous organosulfur compounds from methacrolein and methyl vinyl ketone. L. Huang, E. Coddens, V.H. Grassian
- 380.** Decadal trends in organic carbon volatility fractions across the United States. A. Christiansen, J. Davis, A. Carlton
- 381.** Fog water chemical composition in Namibia during the AEROCLO-sA-2017 campaign. a. Monod, D. Napolitano, J. Gonzalez Sanchez, C. Giorio, R. Mushi, G. Maggs-Kölling, B. D'Anna, B. Coulomb, J. Boudenne, S. Piketh, A. namwoonde, F. Burnet, P. Formenti, P. Herckes
- 382.** Assimilating the effects of natural water compositions, ions, and humic acid on fate and transport of insensitive munition compounds. T. Schutt, M.K. Shukla
- 383.** Dynamic nature of the particle phase for select green leaf volatile derived secondary organic aerosols. K.B. Fischer, G. Petrucci

384. Formation of light absorbing compounds from reactions of carbonyl species under highly acidic aqueous aerosol conditions. **K. Mejia Escobar**, M. Dam, M. Li, T. Truong, R. Alnajjar, J. de Sousa, A. Sandoval, E. Ventura, M. Clemente, S. Somepalle, F. Hussain, A. Shen, R. Spangler, A.L. Van Wyngarden

385. Development of an incoherent broadband cavity enhanced absorption spectrometer (IBBCEAS) designed for the study of marine produced HONO. **S.L. Mora Garcia**, M.N. Sullivan, M. Alves, V.H. Grassian

SECTION A

San Diego Convention Center

TBD

General Poster Session

J. L. Goldfarb, *Organizer*

5:00 - 7:00

386. Geochemical profile of residential indoor dust from an industrial city. **I.N. Doyi**

387. How to write a great paper and get it accepted by a good environmental journal like Science of the Total Environment (Elsevier): Guide and recommendations. **D. Barcelo**

388. Sustainable land management enabled by ecosystem services mapping: Case study on agricultural water use in California's Central Valley. **E. Matios**, J. Burney

389. Communicating water quality data using the grammar of graphics. **B. Trueman**, D. Dunnington, G.A. Gagnon

390. Isolation of ligninolytic yeasts from sugar cane luggage for lignin degradation. **A. Bautista Guerrero**

391. Improvement velocity of sedimentation by biogranules in an aerobic batch reactor. **M. Gómez Gallegos**, J. Sanchez-Salas

392. Environmentally friendly waterless fracturing with supercritical CO₂ foam prepared in produced water: Mechanistic study. **H. Hosseini**, J. Syung Tsau, K. Shafer-Peltier, C. Marshall, Q. Ye, R. Barati

393. Evaluation and extrapolation of the solubility of CH₄ in CO₂ + H₂O using molecular simulation: CO₂ EOR and sequestration. **H. Lee**, M. Ostadhassan

394. Disinfection of water in swimming pools by combined action of UV-light and ozone. A. Semenov, **T. Sakhno**, I. Korotkova, N. Barashkov

395. Hydrothermal synthesis of fine stabilized superparamagnetic nano-particles manganese ferrite and their application in photocatalytic degradation of methylene blue. **S. Ata**, I. Mirza

396. Optical properties of chromophoric dissolved organic matter (CDOM) in Pacific Northwest lakes. **C.D. Clark**, K. Juetten, Z. Landram, W.J. De Bruyn

397. Influence of ultrasonic treatment on hydroxyl radicals formation during chloride-free electrolysis of water contaminated with *E.coli*. **N. Barashkov**, I. Irgibayeva, A. Mantel, T. Sakhno, A. Aldongarov

398. Increased conductive of PEDOT:PSS by ionic additive for direct-printable piezoresistive sensors on textile substrate. **I. Jin**, J. Jung

399. Release behavior of mercury during iron ore sintering process. **N. Tsubouchi**, J. Bud, Y. Mochizuki

400. Enhanced efficiency of green solvent-processed non-fullerene organic solar cells via morphology optimization. **S. Park**, J. Jung, I. Jin, K. Kim, Y. Noh

401. Additive engineering of low bandgap perovskite from hot-casting process for high efficiency perovskite solar cells. **Y. Noh**, J. Jung

402. Measuring dissolved-phase polychlorinated biphenyls (PCBs) in the Great Lakes by high-resolution mass spectrometry. **J.J. Pagano**, A.J. Garner, B.J. Crimmins, M. Milligan, P.K. Hopke, T.M. Holsen

403. Iron speciation and concentration in the Arabian Gulf. **D. Al Wahaib**

404. Effect of absorption liquid types on CO₂ capture efficiency of silane coated PP membrane contactor. **S. Kim**, Y. Seo

405. Identification of acid-lasting particles in sediment of the Yangjae stream flowing through the Seoul metropolitan, South Korea. **Y. Kim**, E. Chung, N.C. Woo

406. CO₂-philic surfactants for high salinity reservoir applications towards efficient CO₂ sequestration. **A. Gizzatov**, G. Jian, K. Mohammed, A.I. Abdel-Fattah, S.D. Allen

407. Diethyl(bromodifluoromethyl) phosphonate as a versatile reagent for the difluoromethylation of bisphenols for their detection and identification by gas chromatography-mass spectrometry. **C.A. Valdez**, R.N. Leif, S. Hok, K.E. Mason

408. Phosphorous chemistry affecting nutrient runoff in agriculture. **S.D. Fleischman**, S.M. Barrowcliff, L. Magana

409. Analysis of 16 bisphenol analogues in Canadian indoor house dust by gas chromatography-tandem mass spectrometry. **X. Fan**, C. Kubwabo, G. Katuri, A. Caza, P. Rasmussen

410. Physico-chemical assessment of ground and surface water within the vicinity of Atenda Abattoir Ogbomoso, Nigeria. O.O. Onawumi, P.I. Egwuatu,, **F.A. Amoo**, A.O. Ibrahim

- 411.** Organic–inorganic electron transport layer for enhancing efficiency and stability of 2-dimensional ruddlesden-popper perovskite solar cells. **K. Kim**, J. Jung, Y. Noh, S. Park, I. Jin
- 412.** Functionalized three-dimensionally ordered macroporous silica: Aldehyde compounds sensing material. P. Seesuwana, T. Leepasert, **S. Achiwawanich**
- 413.** New technology for controlling biofilm formation in water distribution system. Y. Li, **O.V. Ezeh**, W. Han, Q. Wu, K. Kwan, K. Yeung
- 414.** Analysis of chemical composition and odor of model thirdhand smoke (THS). **A. Yamasaki**, **M. Noguchi**
- 415.** Improvement of water quality based on nanotechnology methods. T. Chhetri, G. Cunningham, R. Kannan, A. Upendran, **Z. Afrasiabi**
- 416.** Spatiotemporal dynamics of metabolites in residential wastewater revealed through longitudinal sampling and untargeted metabolomics. **E. Evans**, C. Dai, S. Isazadeh, K. Longnecker, M. Kido Soule, S. Park, F. Ling, C. Ratti, E.B. Kujawinski, E. Alm
- 417.** Monitoring enzymatic activities of agricultural soil after exposure to silver nanoparticles of different sizes and coatings. Y. Xue, P. Mishra, **M. Fukada**, F. Eivazi, Z. Afrasiabi
- 418.** Application of anaerobic fluidized bed membrane bioreactor (AFMBR) to enrich nitrite/nitrate dependent anaerobic methane oxidation (N-DAMO) microorganism for simultaneous nitrogen and carbon removal. **Y. Wu**, Y. Chen, L. Whang
- 419.** Implication of nutrient concentrations related to a harmful algae bloom (HAB) and microcystin formation in Caesar Creek Lake, Wilmington, Ohio. **B.J. Foskuhl**, T. Lunan, R. Schaffer, A. McGowin
- 420.** Use of EPI Suite™ fugacity model in assessing environmental fate. **E. Wong**, M. Citra, M. Kawa, C. Coley
- 421.** Solar induced formation of emulsification in petroleum on water. **C. Brown**, A. Cluen-Brown, M. Giraudier, M.A. Tarr
- 422.** Measuring sediment black carbon contents using phenanthrene sorption. **Z. Lu**
- 423.** Evaluating acyl homoserine lactones removal efficiencies of isolated quorum quenching bacteria and their application for biofouling control in membrane bioreactors. **I. Chien**, C. Chu, Y. Ge, J. Chen
- 424.** Inhibition of microbially induced carbonate precipitation by soil solution Cu and its effect on the stabilization of soil Cu. **H. Chung**, S. Kim, K. Nam
- 425.** Assessment of polyaromatic hydrocarbons and heavy metals in the River Rwizi, Mbarara, Uganda. **M. Soanirina**, **J. Bolender**, L. Asia, S. Lebarillier, C. Kiwanuka, P. Doumenq
- 426.** Electrochemical studies of perfluoroacids (PFAs) and perfluorooctane sulfonate (PFOS). B. Kenney, **B. Workie**, E. Sahle-Demessie
- 427.** Disinfection of water using a reactive membrane system with activated carbon fiber cloth (ACFC). E. Huang, **H. Shi**, B. Wang, J. Liu
- 428.** Identification of water soluble oil photodegradation products containing N and O atoms. **S.L. Patil**, P.A. Zito, M.A. Tarr
- 429.** Fabrication of wood fiber-rubber composites with microwave-modified waste rubber powder. **D. Shao**, C. Xia, L. Cai, S.Q. Shi, D. Jiang, S. Rong, J. Wang
- 430.** Synthesis and characterization of imines and Schiff bases as organic sensors for the detection of cyanide and aluminum ions. **C.A. Arro**, Y.M. Hijji
- 431.** Efficiency enhancement of anaerobic digester in microbial fuel cell using bacteria. **S. Chung**, S. Chang, H. Kim, Y. Kim, D. Go, S. Kang, S. Lee, J. Cho, L. Kim
- 432.** Development and evaluation of consensus metamodel for estimating national concentrations of organic chemicals in surface water. **R.R. Sayre**, P. Saranjampour, K. Isaacs, J. Wambaugh
- 433.** Quantifying metal contaminants in rodents in Yuma, AZ. **C.J. Chęcinski**, J.M. Credo, J.C. Ingram, F.A. von Hippel
- 434.** Removal of phenolic compounds from superficial water and wastewater using a viscous organic phase retained in porous polyethylene. **E.P. Beiguel**, E.A. Hughes, A. Zalts, J. Montserrat
- 435.** Development of engineered soil surrogates for predicting natural soil behavior. **G. Abdalla**, A. Pandey, B.J. Haywood, S.P. Smith, R.L. Cook, D. Spivak
- 436.** Concentrations and loadings of anthropogenic contaminants during storm events in the San Diego River and its tributary. **F. Pinongcos**, J. Calderon, N. Mladenov, M.E. Verbyla, A.M. Kinoshita, R. Gersberg, J. Monroe, M. Gil, **E. Mikita**, **A. Kinney**, S. Chao
- 437.** Photosensitization and production of nitrous acid using marine chromophoric dissolved organic matter. **D. Dang**, M. Alves, V.H. Grassian
- 438.** Presence and risk assessment of antidepressants in tidal freshwater Potomac River water, sediments, and fish. **L. McNulty**, T.B. Huff, G.D. Foster
- 439.** LC-MS/MS analysis of UV-filter and paraben micropollutants in Potomac River sediments. **T. Haji**, T.B. Huff, G.D. Foster

440. Polycyclic aromatic hydrocarbons among childcare centers in Tampa Bay. N. Vijayakumar, A. Tumpudi, R. Park, M. Badru, **M. Bourgeois**, M. Acheampong, T. Mason, M. Bourgeois, J. Marshall, F.M. Jaward

441. Improved light-harvesting properties of quasi-solid state dye-sensitized solar cell with gel electrolyte containing zeolite-X and -A from fly ash. **J. Lim**, G. Choi, S. Lim, J. Moon, U. Baek, J. Park

442. Existence of IO_2H and the role of ice surface in the formation of I_2 . **Y. Baek**, C.H. Choi, K. Kim, W. Choi

SECTION A

San Diego Convention Center
TBD

Green Chemistry & the Environment

Cosponsored by CEI

R. Luque, S. O. Obare, *Organizers*

5:00 - 7:00

443. Characterizing diffusion in cationic hydrogels for bioremediation applications. **J. Counts**, S. Wolfe, K. Hillyer, M.F. Roll, K.V. Waynant, J. Moberly

444. Microbially induced carbonate precipitation assisted by poly-L-lysine: Ecofriendly approach inspired by nature. **T.H. Nawarathna**, K. Nakashima, S. Kawasaki

445. Degradation of tetracycline by ferrate(VI): Reaction kinetics and efficiency evaluation. **K. Park**, D. Kang, Y. So, I. Kim

446. Evaluation of indoor air quality of residential rooms in Beijing. **F. Liu**

447. Water filtration with biomass. **A. Mukhopadhyay**, P. Das, S. Mukhopadhyay

448. Ubiquitous rapid biodegradation of polystyrene by dark (*Tenebrio obscurus*) and yellow (*Tenebrio molitor*) mealworms (Coleoptera: Tenebrionidae). **B. Peng**, Z. Chen, W. Wu, Y. Zhang

449. Electrochemical regeneration of oxidized Fe(II) thiochelatase based nitric oxide absorbent. **S. Cheon**, J. Han, H. Yoon, S. Kim

450. Valorization of food waste and waste activated sludge to high value-added optical pure L-lactic acid stimulated by electron control. **X. Li**

451. Multifunctional odour control gel for H_2S abatement in dewatered sludge. **K. CHENG**, L.T. Luk, M. Arjona Alonso, W. Han, K. Yeung

452. Field study of control-released hydrogel for H_2S suppression in Hong Kong drainage system. **S. Wong**

453. Study on the competitive reactions during SO_3 removal by $\text{NaHSO}_3/\text{Na}_2\text{SO}_3$. **K. He**, Q. Song, Z. Yan, Q. Yao

454. High fluorescence carbon dots from kappa-carrageenan for environmental sensing and bioimaging. **M.A. Sinoy**

455. Investigation on weak magnetic field-enhanced adsorption mechanism of pollutants on magnetic biopolymer/graphene composite gel. **J. Ma**, F. Yu

456. Identifying and overcoming rate-limiting steps of electrochemical stripping for nitrogen recovery from wastewater. **M. Liu**, W. Tarpel

457. Study on the reduction of acidic gases generated from solid refuse fuel (SRF) use plant. **S. Park**, J. Han, W. Eom, Y. Park, **H. Kim**

458. Enantioselective behavior of epoxiconazole fungicide in soil and water mediums and its enantiomeric bioactivity against the targeted pathogens. **A.E. Esmat**

459. Approach of electrochemical synthesis of ammonia from water and nitrogen using iron under ambient conditions. **S. Jeon**, K. Kim, J. Kim, H. Yoon, J. Han

460. Functional group-directed self-installing doors in porous graphene. **Y. Li**, C. Wu

461. $1\text{T}'\text{-MoS}_2$, a promising candidate for sensing NO_x . **Y. Linghu**, C. Wu

462. Design and automatic screening of tetra-branched structures for multiple-site acid gas capture. **C. Li**, D. Lu, C. Wu

463. Determination of heavy metals in the distinct ecological matrix of the biotopes near the "Cavernas del Rio de Camuy" National Park. **J. Torres Ayende**, N.D. Maldonado Pérez, J. Soto Perez

SECTION A

San Diego Convention Center
TBD

Legacy & Emerging Per- & Polyfluoroalkyl Substances: Identification, Fate, Transport, Exposure, & Removal

K. Chu, J. Liu, M. Sun, F. Xiao, *Organizers*

5:00 - 7:00

464. Column studies of PFAS adsorption by a cationic polymer modified organosilica. **C. Hefner**, H.A. Hartmann, E.K. Stebel, P. Edmiston

465. Development and characterization of organosilica adsorbents tailored for removal of perfluoroalkyl substances from water. **M. Klonowski**, E.K. Stebel, H.A. Hartmann, K. Pike, P. Edmiston

466. Evaluation of PFAS-specific organosilica adsorbents using adsorption isotherms and kinetics. **K. Pike**, H.A. Hartmann, M. Klonowski, E.K. Stebel, C. Hefner, P. Edmiston

467. Enhanced reductive defluorination of 6:2 fluorotelomer alcohol using bio-electrochemical systems. **A. Cummings**, R. Tenorio, D. Jiang

468. Influence of multi-process retention on the transport of perfluorooctanesulfonic acid (PFOS) in the presence of non-aqueous phase liquids (NAPLs). **S. Van Glubt**, N. Yan, Y. Wang, M. Brusseau

469. Identification of novel polyfluoroalkyl substances and their byproducts using UPLC–TOF–MS. **F. Xiao**

470. Effect of composting operating parameters on the degradation of PFAS in biodegradable food service products. **F. Hussain**, J. Hazard, J. Velazquez

471. Comprehensive retention model for PFAS transport in subsurface systems. **M.L. Brusseau**

472. Perfluorinated compounds in agricultural soils following years of biosolids applications. **G.R. Johnson**

473. Microbial inhibition of aerobic BTEX biodegradation caused by the influence of fluorinated compounds in aqueous film-forming foams (AFFFs). **K. Tsou**, C.I. Olivares, S. Yi, L. Alvarez-Cohen

474. Extraction of per- and polyfluoroalkyl pollutants from water using paramagnetic ionic liquids. D. Bwambok, **J. Doney**, M. Peralta, J. Woodtelle

475. Delivering an integrated data hub for per- and polyfluoroalkyl (PFAS) chemicals via the US EPA CompTox Chemicals Dashboard. **A.J. Williams**, C. Grulke, K. Mansouri, G. Patlewicz, A. Richard

476. Effects of chloride on electrochemical oxidation of perfluorooctane sulfonate. **L. Wang**, Y. Wang, J. Lu, Q. Huang

477. Key considerations for accurate exposures in toxicological assessments of per- and polyfluoroalkyl substances. **J.N. Rewerts**, T. Anderson, C. McCarthy, C. Salice, J.A. Field

478. Removal and recovery of perfluoroalkyl substances in water by electrocoagulation. **H. Shi**, R.D. Pierce, Q. Huang

479. Novel LC-MS/MS procedure for determination of legacy and emerging polyfluoroalkyl substances in environmental water samples. S.A. Oehrle, K. Organtini, K.J. Rosnack, **M.S. Young**

Nanomaterials & Sustainability

Cosponsored by CEI

S. Ahuja, *Organizer*

5:00 - 7:00

480. Self-polarized ultrathin nylon-11 nanofiber membrane for enhanced capturing of particulate matters. D. Park, P. Park, **J. Nah**

481. Physiological and photochemical effects of TiO₂ nanoparticles on tomato plants under different irradiance. J. Ko, **Y. Hwang**

482. Lead adsorption by electrospun PVA/PAA nanofiber membranes in a fixed-bed column. **S. Zhang**

483. Nanorod zeolitic framework as a luminescent probe for selective detection of carcinogenic hexavalent chromium in aqueous medium. **E. Adotey**, M. Torkmahalleh, M.P. Balanay

484. Fast synthesis of reduced graphene oxide/ carbon nanotubes/iron/silver composites with high catalytic activity for 4-nitrophenol reduction. **X. Tran**, M. Hussain, H. Kim

485. Prussian blue incorporated polyacrylonitrile nanofibers for rapid removal of radioactive ¹³⁷Cs. **S. Kim**, H. Kim, M. Kim

486. Long-term fate of zinc oxide nanoparticles in the presence of nano-iron oxide through the natural sediment under different solution chemistry. **D. Kumari**, A. Kumar, P. Joshi, T. Raychoudhury

487. Time resolved characterization of metal ion-induced nanocellulose gelation by small angle X-ray scattering. **H. He**, T. Rosén, C. Zhan, R. Wang, S. Chodankar, L. Yang, B.S. Hsiao

488. Engineered *Escherichia coli* cell capable of specific binding to metal surface. **K. Nakashima**, Y. Iwata, S. Kawasaki

489. Surface chemistry and phase transformation of nanoscale zero-valent (nZVI) iron in aquatic media. **A. Liu**

490. Characterization and permeation properties of graphene oxide membrane fabricated by various methods for desalination. **S. Lee**, J. Kim, J. Woo, C. Han

491. Photocatalytic core-shell magnetic ZnO nanostructure. **O.D. Máñez-Navarro**, M.A. Mendez-Rojas, J. Sanchez-Salas, D.X. Flores-Cervantes

492. Investigation of the main mineral properties driving MnO_x photoreduction. **S. Benkaddour**, A. Schwartzberg, B. Gilbert, J. Pena

SECTION A
San Diego Convention Center
TBD

Non-targeted Analysis to Understand Fate & Effects of Pharmaceuticals & Emerging Contaminants in Agriculture & Natural Environments

Cosponsored by AGRO
D. S. Aga, J. B. Sallach, *Organizers*

5:00 - 7:00

- 493.** Photochemical dissolution and degradation of industrial crude oil and natural seep oil in seawater. **K. Snyder**, N. Mladenov, E. Hoh
- 494.** Simultaneous separation and determination of the chiral fungicide cyproconazole enantiomers by high-performance liquid chromatography. **H. Zongzhe**
- 495.** Microbial degradation of malachite green in milkfish pond sediments. **B. Chang**, C. Yang, W. Chao, C. Hsieh
- 496.** Occurrence of emerging contaminants in an urban river of Buenos Aires, Argentina. G. Fitó Friedrichs, **E.P. Beiguel**, A. Zalts, J. Montserrat

SECTION A
San Diego Convention Center
TBD

Plastics in Aquatic Environments, Part II: Transport, Fate & Global Impacts

Cosponsored by POLY
J. A. Glaser, K. Ikehata, R. T. Mathers, S. V. Orski, M. A. Pasquinelli, *Organizers*

5:00 - 7:00

- 497.** Heterogeneous oxidative degradation and potential secondary organic aerosol yields of the toxic organic UV filter, octinoxate, by OH, O₃, and UV irradiation. **A.W. Cooper**, A. Kawasaki, S. Kruse, J.H. Slade
- 498.** Degradation of the toxic plastic additive, bisphenol-A, in the aerosol phase through heterogeneous and multiphase OH, O₃, and photosensitized reactions. **S. Kruse**, A. Kawasaki, A.W. Cooper, J.H. Slade
- 499.** Toxicity and pollution generated from decomposed plastic in the ocean. **K. Koizumi**, H. Kimukai, K. Kim, S. Chung, K. Metori, T. Hiaki, M. Nishimura, T. Kusui, **K. Saïdo**
- 500.** Polymers and anthropogenic particles extracted from oceanic water, beach sediments, and fish stomach: Raman microspectroscopy study. **S. Ghosal**

- 501.** Organic leaching from micro plastics, potential effects on microbial growth on the aquifer. **S. Choi**
- 502.** Recycling helps reduce the plastics being dumped in our oceans, plastics in our oceans endanger marine life, environmental engineering is a way to address this problem. **T.V. Clardy**
- 503.** Challenges in electronic plastic waste management practices. **E. Sahle Demessie**, B. Mezgebe, T. Richardson, C. Lee, J.A. Glaser
- 504.** Quantifying and analyzing microfiber pollution in the Lake Michigan watershed. **E. Kostelnik**, J.R. Peller, C.R. Iceman

SECTION A
San Diego Convention Center
TBD

Safeguarding Water Quality in a Climate of Change

Cosponsored by CEI
J. Arrigo, J. W. Moerman, *Organizers*

5:00 - 7:00

- 505.** Integrated water cycle science in the context of global change: Interagency approaches to water quality challenges. **J.W. Moerman**, J. Arrigo, S. Connors, G. Geernaert, W. Higgins
- 506.** Quality data matters: Challenges in effective resource management and solutions through quality assurance. **R. Pisor**, J. Saraceno, T. Treleaven, S. Miller
- 507.** Evolution and mechanisms driving water quality trends across United States watersheds. **M.E. Newcomer**, N. Bouskill, H. Wainwright, B. Arora, T. Maavara, D. Dwivedi, E. Woodburn, K. Williams, R. Carroll, C. Steefel, S. Hubbard
- 508.** Predicting drivers of groundwater Cr(VI) contamination in the Central Valley, CA: Integrated multivariate statistical & geospatial approach. **A.M. Lopez**, J. Caers, S.E. Fendorf
- 509.** Isolation and characterization of microcystin-degrading bacteria from Iowa recreational lakes. **X. Liang**, K. Ikuma
- 510.** Effects of chlorine on hexavalent chromium occurrence in drinking water via oxidation of iron corrosion scales. **C. Tan**, S. Avasarala, H. Liu
- 511.** Toledo Waterways Initiative: Updating infrastructure to improve water quality. **J. Cousino**, E. Kippenhan

SECTION A
San Diego Convention Center
TBD

Sensors & Biosensors for Widespread Environmental Monitoring

Cosponsored by AGRO

T. Li, V. V. Rajasekharan, M. Romero-Gomez, P. L. Schorr, W. Zhang, *Organizers*

5:00 - 7:00

- 512.** Phylogenetic diversity, virulence genes, and antibiotic resistance of *Vibrio parahaemolyticus* in a tropical urban marine estuary in Hawaii. **P. Saingam**, T. Yan
- 513.** Rapid detection of residual antibiotics in wastewater treatment plants by surface enhanced Raman scattering (SERS) analysis. **Y. Huang**, W.J. Thrift, A.S. Cabuslay, R. Ragan, S. Jiang
- 514.** Development of flexible electrochromic oxygen sensor operating at room temperature. **H. Son**, S. Hong, Y. Choi
- 515.** Alpha-(2-hydroxy-5-methylphenylimino)-o-cresol as nano-chemosensor for simultaneous recognition of Al³⁺ and Zn²⁺: Electrochemical and cell-imaging studies. **E. Tecuapa Flores**, C.A. Huerta-Aguilar, T. Pandiyan
- 516.** Detection of *E. coli* 16S ribosomal RNA using duplex specific nuclease-mediated target recycling signal amplification. **H. Gowda**, **A. Shin**, M. Madou, S. Jiang

SECTION A
San Diego Convention Center
TBD

Sensors for Water Quality Assessment in Resource Limited Environments

Cosponsored by AGRO

E. Brack, C. Gomes, E. McLamore, M. S. Wiederoder, *Organizers*

5:00 - 7:00

- 517.** Rapid cell-free protein synthesis based biosensing system for the detection of cadmium. **K. Turner**, S. Walper
- 518.** Smartphone-base paper microfluidic particulometry of norovirus from environmental water samples at single copy level. S. Chung, L.E. Breshears, S. Perea, C.M. Morrison, W.Q. Betancourt, K.A. Reynolds, **J. Yoon**
- 519.** Modification of the SPADNS method to develop a sensor as a dye sensitized strip in assessing fluoride levels in drinking water. **V.S.**

- Samarasiri**, U.R. Kumarasinghe, A. Cooray
- 520.** TLF sensor prototypes: Low-cost sensors for detecting biological contaminants in water. **T. Purvis**, R. Wallace, J. Brown
- 521.** Laser scribed graphene sensors for point of use detection of *Listeria monocytogenes*. **N. Cavallaro**, C.L. Gomes, E.S. McLamore
- 522.** Graphene-anchored cuprous oxide nanoparticles from waste electric cables for electrochemical sensing. **V. Morgan**, D. Vanegas, E.S. McLamore, I. Velez-Torrez

SECTION A
San Diego Convention Center
TBD

Stormwater Treatment & Green Infrastructure: From Research to Practice

R. Ambrose, S. Grant, P. Holden, J. Jay, L. Levin, H. Liu, *Organizers*

5:00 - 7:00

- 523.** Distribution of heavy metals and nutrients in soil, plant, and effluent water in a rain garden. **K. Sung**, C. Kim
- 524.** Reducing storm water pollution with increased green space planning as part of a community driven neighborhood revitalization project. **E. Kippenhan**, B.W. Miringu, A.M. Smith
- 525.** Natural treatment systems for urban stormwater runoff: Relationships between soil microbial communities, environmental conditions, accumulated pollutants, and nitrogen cycling. **M. Feraud**, P. Holden
- 526.** Survey of antibiotic resistant gene and heavy metal coselection in UC campus stormwater biofilters. **M. Rugh**, W. Hung, M. Feraud, S. Avasarala, J. Jay, P. Holden, H. Liu
- 527.** Practice versus promise: An assessment of design and maintenance guidance relative to goals for stormwater natural treatment systems. **P. Holden**, M. Feraud, M. Rippy
- 528.** Perceived services and disservices of natural treatment systems for urban stormwater. M. Rippy, **S. Grant**
- 529.** Classic urban land management hastens decomposition in Southern California. **J. Kurylo**, R. Ambrose

SECTION A
San Diego Convention Center
TBD

**Wastewater-Based Epidemiology:
Opportunities, Challenges & Applications to
Public Health & Safety**

D. A. Burgard, M. Matus, B. Subedi, *Organizers*

5:00 - 7:00

530. Integration of antimicrobial resistant bacterial isolate libraries and metagenomics sequencing for quantitative antimicrobial resistance (amr) risk assessment in cattle manure. **B. Li**

531. Validation and application of a LC-MS/MS method for illicit drug determination in wastewater. **M. Kuloglu**, S. Mercan, T. Tekin, Z. Turkmen, F. Asicioglu

532. Trends in nicotine consumption between 2010 and 2017 in an Australian city using the wastewater-based epidemiology approach. **M. Mackie**, B. Tscharke, J. O'Brien, P. Choi, C. Gartner, K. Thomas, J. Mueller

533. Uncertainties treatment for wastewater-based epidemiological estimation of the consumption of illicit and prescribed neuropsychiatric drugs in two urban communities in Kentucky using ammonium normalized population and monte carlo simulation. T.L. Croft, **R.A. Huffines**, M. Pathak, **B. Subedi**

534. Biobot analytics: Novel sampling and analytical method to quantify opioids and their urinary metabolites in wastewater. **K. Foppe**, N. Endo, M. Matus

SECTION A
San Diego Convention Center
TBD

**Water, Health, & Environmental Justice in
Marginalized Communities**

Cosponsored by CMA and PRES

F. de los Reyes, A. Harris, J. Kearns, *Organizers*

5:00 - 7:00

546. Inner city faith communities as educational hubs via urban water management. M. Berry Du-Four, **E. Kippenhan**, B.W. Miringu

547. Development of a pathogen flow model for risk-based sanitation safety planning and mapping. **M.E. Verbyla**, **I. Musaaazi**, A. Vaidyanathan, L. Mendoza, N. Hofstra, L. Joe, H. Murphy, I. Nansubuga, D. Okaali, J. Ssazi, I. Tumwebaze, J. Rose

548. Novel community engaged system thinking approach to onsite wastewater treatment management for nutrient pollution in the Belizean Cayes. **D.A. Delgado**, C. Prouty, M. Trotz

549. Rapid small-scale column test development for fluoride control using bone-char sorbents. **M. Thompson**, J. Kearns

550. Water, health, and environmental justice in the central valley of California: Geospatial analysis of nitrate contamination and health disparities. **A. Tariqi**, C. Naughton

551. Predicting per/polyfluoroalkyl substance (PFAS) breakthrough in biochar water treatment using fluorescence and UV absorbance as surrogates. **M.T. Aung**, J. Kearns

552. Nanosensors and decision support models paired on a mobile device for establishing a participatory monitoring program on mercury exposure in rural Colombia. **V. Morgan**, **D. Vanegas**, K. McCourt, J. Crews, E. Kuo, L. Casso-Hartmann, I. Velez-Torrez, G. Kiker, E.S. McLamore

553. Using microbial source tracking and antibiotic resistance for environmental justice. **B. Hunter**, L. Rocha Melogno, W. Gerhard, S. Farling, S. Kawadiya, M. Deshusses

SECTION A
San Diego Convention Center
TBD

**Water in the Solid State: Reactions &
Interactions with Impurities**

Cosponsored by PHYS

E. Asenath Smith, W. Choi, K. Kim, *Organizers*

5:00 - 7:00

535. Enhanced dissociation of weak acids in cryogenic ice: Configurational entropy of mobile proton is the driving force. **H. Kang**, Y. Park, S. Shin

536. Sulfuric acid formations by sulfurous acid and hydrogen peroxide in gas phase and on ice surface. **S. Shostak**, Y. Horbatenko, C.H. Choi, K. Kim

537. Redox chemical reaction between chromate and iodide in frozen solution: Mechanism, kinetics, and environmental implications. **H. CHUNG**, J. Kim, K. Kim

538. *In-situ* chemical characterization of impurities in ice using cryo-raman spectroscopy. **B. Kim**, K. Kim

539. Enhanced redox transformation of inorganic iodine species in ice. **K. Kim**

540. Mechanisms of heat transfer in ice containing organic and inorganic matter. **C. Erb**, R. Winter, E. Barnes, R. Lieb-Lappen, E. Asenath Smith

- 541.** Investigating the effects of an insect antifreeze protein on ice nucleation and crystallization. **E. Ambrogi**, E. Asenath Smith, G.R. Hoch, J. Sreter, K. Jovic, K. Varga, P.W. Baures, J. Tsavalas
- 542.** Modification and characterization of polyol based polymers for ice recrystallization inhibition and thermal hysteresis activity. **M. Mousazadeh**, J. Tsavalas, P.W. Baures, K. Varga, E. Asenath Smith
- 543.** Computational study of adhesive properties of bi-material interfaces formed with freshwater ice. **V. Gisladottir**, E. Asenath Smith, G.R. Hoch, M.W. Parker, D.T. O'Connor, R. Haehnel
- 544.** Fe(II) oxidation in aqueous solution under freezing conditions. **S. Choi**, W. Choi, G. Lee
- 545.** Effects of pH and Mn(II) concentration on Mn(II) oxidation under freezing condition. **J. Lee**, Y. Won, W. Choi, G. Lee

Future of Biomacromolecules at a Crossroads of Polymer Science & Biology

Sponsored by POLY, Cosponsored by BIOL, CARB, CELL, COLL, ENVR, MEDI, PHYS and PMSE

WEDNESDAY MORNING – ENVR

SECTION A

San Diego Convention Center
Room 28A

Chemistry & Applications of Free Radical-based Technologies for Water Treatment & Purification

Sulfate Radicals- & Electrochemical Production of Radicals-Based Technologies

Cosponsored by AGRO

Financially supported by Association of Environmental Engineering & Science Professors (AEESP)

D. D. Dionysiou, D. Minakata, K. E. O'Shea, W. Song, *Organizers*

G. Li Puma, *Organizer, Presiding*

K. Doudrick, D. Minakata, *Presiding*

- 8:00** **554.** Comparative evaluation of nitroguanidine removal by UV and oxidants: Hydrogen peroxide, persulfate, and peroxymonosulfate. **A. Terracciano**, C. Christodoulatos, X. Meng, B. Smolinski, P. Arriente
- 8:25** **555.** Comparative study for the degradation of theophylline in a pharmaceutical factory effluent using chemically and thermally persulfate activated systems. **A. Ghauch**, S. Al Hakim, A. Baalbaki, O.N. Tantawi

- 8:50** **556.** Advanced oxidation of trimethoprim in water by iron activated persulfate. **H. Zhang**, K.F. Hayes
- 9:15** **557.** Sulfate radical generation and its application for degradation of acetanilide herbicide as a green technology. **W. Chu**
- 9:40** **558.** Exploring synergisms essential to combined ultrasound-activated persulfate using *in situ* EPR spin trapping. **W.P. Fagan**, F.A. Villamena, L.K. Weavers
- 10:05** Intermission.
- 10:20** **559.** Oxidation of organic compounds by peroxymonosulfate catalyzed by a N,O-doped carbonaceous material. **J. Yang**, J.J. Pignatello, Z. Dang
- 10:45** **560.** Reconciling light delivery with photoelectrocatalytic reactors for water treatment. R. Montenegro, J. Morales-Gomero, P.K. Westerhoff, **S. Segura**
- 11:10** **561.** Withdrawn
- 11:35** **562.** Biofouling control on the chelator modified conductive substrate with applying low potentials. **M. Lin**, S. Mehraeen, G. Cheng, C. Rusinek, B.P. Chaplin

SECTION B

San Diego Convention Center
Room 28B

Legacy & Emerging Per- & Polyfluoroalkyl Substances: Identification, Fate, Transport, Exposure, & Removal

Financially supported by Association of Environmental Engineering & Science Professors (AEESP)

K. Chu, J. Liu, M. Sun, *Organizers*

F. Xiao, *Organizer, Presiding*

- 8:00** Introductory Remarks.
- 8:05** **563.** Enhancing photochemical defluorination of per- and polyfluoroalkyl substances (PFASs). **Z. Liu**, M.J. Bentel, Y. Yu, Y. Men, J. Liu
- 8:30** **564.** Breakdown products from perfluorinated alkyl substances (PFAS) degradation in a plasma-based water treatment process. **R. Singh**, S. Fernando, S. Baygi, N. Multari, S. Thagard, T.M. Holsen
- 8:55** **565.** Hydrothermal treatment: Novel method for destruction and defluorination of per- and polyfluoroalkyl substances (PFAS) in aqueous film-forming foam (AFFF). **S. Hao**, B. Wu, Y. Choi, C.P. Higgins, T.J. Strathmann
- 9:20** **566.** Electrochemical oxidation of perfluorooctanesulfonate (PFOS) on different porous Magnéli phase titanium suboxides anodes. **Y. Wang**, H. Shi, R.D. Pierce, Q. Huang

- 9:45 567.** Chemical degradation of environmentally persistent fluorochemicals in aqueous film-forming foam (AFFF). **M. Harake**, M.J. Bentel, L. Wang, S. Lin, M. Sun, J. Liu
- 10:10** Intermission.
- 10:20 568.** Electrochemical mineralization of perfluorooctanoic acid and perfluorooctane sulfonic acid. **V.F. Pulikkal**, M. Sun
- 10:45 569.** Leaching of poly- and perfluoroalkyl substances from soil subjected to dry-wet and freeze-thaw cycles. **A. Borthakur**, J. Blotvogel, S. Mahendra, S.K. Mohanty
- 11:10 570.** Molecular mechanism of per- and polyfluoroalkyl substances on a modified clay. **B. Yan**, G. Munoz, S. Sauve, J. Liu
- 11:35 571.** Interfacial partition coefficients of PFAS at air-water surface in water-unsaturated porous media. **J. Zhang**, J.N. Rewerts, Z. Yu, C. Schaefer, J.A. Field

SECTION C

San Diego Convention Center
Room 28C

Safeguarding Water Quality in a Climate of Change

Cosponsored by CEI

Financially supported by US Global Change Research Program; Association of Environmental Engineering & Science Professors (AEESP)

J. Arrigo, J. W. Moerman, *Organizers, Presiding*

- 8:00** Introductory Remarks.
- 8:05 572.** Water cycle research and the US global change research program. **J. Kaye**, J. Arrigo, J.W. Moerman, J.K. Entin, C. Avery
- 8:35 573.** NASA water quality monitoring within the current era of the Cyanobacteria Assessment Network (CyAN) and the future era of the Plankton, Aerosol, Clouds, ocean Ecosystem (PACE) mission. **B. Seegers**, J. Werdell
- 8:55 574.** U.S. Geological Survey's next-generation water observing system. **L. Sprague**
- 9:15 575.** Managing agricultural nonpoint sources of contaminants under a changing climate: USDA agricultural research service perspectives. **R.B. Bryant**, A. Buda, J. Baker, D. Bosch, J. Garbrecht, D. Smith, P. Kleinman, T. Tsegaye
- 9:35 576.** WHONDERS: Community resource for studying dynamic river corridors. **J.C. Stegen**, A. Goldman, E. Graham, V. Garayburu-Caruso, K. Wrighton, T. Johnson, H. Ren, X. Chen, T. Scheibe
- 9:55** Intermission.
- 10:15 577.** Influence of redox interfaces on metal(loid) contaminant mobility in shallow alluvial

- groundwater aquifers. **K. Boye**, N. Kumar, V. Noël, J.R. Bargar, S.E. Fendorf
- 10:35 578.** Satellite-based monitoring of water quality in the Chesapeake Bay and its watershed. **N. Pahlevan**, A. Mehrabian, B. Smith, N. Pal, S. Balasubramanian, S.S. Uz
- 10:55 579.** Exploration of climatic impacts on watershed water quality as a control on harmful algal blooms and water sustainability. M.E. Newcomer, **Y. Cheng**
- 11:15 580.** Modeling regional water quality impacts of global climate change and adaptation strategies. **X. Zhang**, J. Li, S. Waldhoff, C. Jefferson
- 11:35 581.** Sensitivity analysis of existing water models to effects of climate change. **J. Thomas**, N. Rao
- 11:55** Closing Remarks.

SECTION D

San Diego Convention Center
Room 28D

Biochar & Hydrochar for Energy, Environmental & Agricultural Applications

Cosponsored by AGRO

Financially supported by Frontiers in Energy Research; Association of Environmental Engineering & Science Professors (AEESP)

N. D. Berge, J. L. Goldfarb, R. Volpe, *Organizers*
A. Shah, *Organizer, Presiding*

- 8:15** Introductory Remarks.
- 8:20 582.** Agro-energy-environmental applications of biochar/hydrochar. **K. Ro**
- 8:45 583.** Environmental assessment of pyrolysis and hydrothermal carbonization of anaerobic digestion effluent. J. Vasco Correa, **A. Shah**
- 9:10 584.** Techno-economic analysis of a combined anaerobic digestion and hydrothermal carbonization system from sewage sludge. L. Huezo, **A. Shah**
- 9:35 585.** Emerging challenges in the application of biochar to agricultural and wastewater treatment. **D.S. Alessi**, K. von Gunten, V. Gondziola, M. Alam, K. Konhauser
- 10:00** Intermission.
- 10:15 586.** Assessing the reversibility of electron storage capacity of biochar by chemical methods. **D. Xin**, M. Xian, P. Chiu
- 10:40 587.** Real-time microbial sensors to characterize saturated and unsaturated environments. **S.R. Burge**, K.D. Hristovski
- 11:05 588.** Compaction affects the performance of biochar-augmented biofilter: Mechanism and implications. **S.K. Mohanty**, H. Le, A. Borthakur, S. Ravi

- 11:30 589.** Environmental oil recovery using engineered douglas fir biochar. **C. Navarathna**, N. Wickramasighe, T. Mlsna
- 11:55** Closing Remarks.

- 11:30 598.** Assessing the effect of oxidation on the photophysical and photochemical properties of dissolved organic matter. **F.L. Rosario**, F. Leresche, K. Couch

SECTION E

San Diego Convention Center
Room 28E

Fundamental Chemical Processes Common to Dissolved Organic Matter & Atmospheric Organic Aerosols

N. Borduas, S. A. Nizkorodov, *Organizers, Presiding*

- 8:00** Introductory Remarks.
- 8:05 590.** Feedbacks between aerosol microphysics and photochemical aging in an iron containing secondary organic aerosol (SOA) proxy. **U.K. Krieger**, J. Dou, B. Luo, T. Peter, P. Corral Arroyo, P.A. Alpert, M. Ammann
- 8:35 591.** Exploring the relationship between the conformation of NOM and fluorescence changes caused by the presence of metals. **L.T. Stirchak**, D.J. Donaldson
- 8:55 592.** Hydroxyl radicals from isoprene hydroxy hydroperoxide (ISOPPOOH) decomposition induced by irons in water. **T. Fang**, P. Lakey, J. Rivera-Rios, F. Keutsch, M. Shiraiwa
- 9:15 593.** Insights onto the complex iron oxide-organic-water interface from *in situ* studies using ATR-FTIR, flow microcalorimetry, and surface complexation modeling. **H.A. Al-Abadleh**
- 9:45** Intermission.
- 10:00 594.** Dust-catalyzed oxidant production and organic transformations in the atmospheric aqueous phase. **S.A. Styler**, M. Abou-Ghanem, A.I. Burnett, C.D. Cote, M. Schmidt, S.R. Schneider, A.L. Aantjes, T.H. Chou, L. Gan, S. Gao, A. Holod, S.M. Jansen van Beek, A.J. Locock, G. Lotfi, M. Lyu, L. Michelat, A.O. Oliyynyk
- 10:30 595.** Challenges with traditional fluorescence quantitation metrics for anthropogenic DOM: Case for re-examining approaches and definitions on unique pools of leachable biosolids organic matter. **S. Fischer**, M. Gonsior, L. Powers, A. Hamilton, J.D. Chorover, M. Ramirez, A. Torrents
- 10:50 596.** Organic aerosol growth via aqueous reactions in the presence of different inorganic aerosols containing ammonium sulfate, sea salt, and airborne mineral dust. **M. Jang**, C. Zhou, S. Han, Z. Yu
- 11:10 597.** Aqueous photochemistry of secondary organic aerosol in the presence of common inorganic salts. **A. Klodt**, D. Romonosky, J. Laskin, A. Laskin, S.A. Nizkorodov

SECTION F

San Diego Convention Center
Room 29A

Artificial Water Channels for Water Purification & Desalination

Financially supported by Association of Environmental Engineering & Science Professors (AEESP)

J. Hou, B. Mi, *Organizers*

M. Barboiu, *Organizer, Presiding*

M. Kumar, *Presiding*

- 8:00 599.** Artificial water channel membranes: Design ideas from biological and biomimetic membrane research. **M. Kumar**, W. Song, C. Lang, R. Hickey
- 8:30 600.** Construction of artificial water channels from organic tubular structures. **J. Hou**
- 9:00 601.** Highly permeable and selective reverse osmosis membranes incorporating artificial water channels. **M. Di Vincenzo**, A. Tiraferri, M. Barboiu
- 9:20 602.** Cluster formation of artificial water channels enable high water/salt permselectivity. **W. Song**, H. Joshi, R. Chowdhury, Y. Shen, J. Hou, A. Aksimentiev, M. Kumar
- 9:40** Intermission.
- 9:50 603.** Water transport through carbon nanotube porins in lipid membranes. **Y. Li**, A. Noy
- 10:10 604.** Probing ion solvation in single-digit nanopores with first-principles simulations. **T. Pham**, C. Zhan, E. Schwegler
- 10:30 605.** Hydroxilic pathways for water permeation: New mechanisms for water purification. **L. Huang**, M. Barboiu
- 10:50 606.** Layer-by-layer assembled graphene oxide membrane with efficient swelling control through water-ethanol mixed system. S. Zheng, **M. Wang**, B. Mi
- 11:10 607.** Removal of neutral pharmaceuticals and PPCPs using graphene oxide membranes: Characterization of diffusion and partitioning coefficient of micropollutant in confined nanochannels. **S. Zheng**, **X. Yang**, **B. Mi**
- 11:30 608.** Membranes with artificial channels based on poly(styrene-*b*- γ -benzyl-L-glutamate). B. Sutisna, P. Bilalis, V. Musteata, **D. Smilgies**, K. Peinemann, N. Hadjichristidis, **S. Nunes**

Novel Polymeric Materials & Polymer-Based Processes for Energy-Efficient Treatment of Water & Resource Recovery

Nanomaterials for Separations

Sponsored by PMSE, Cosponsored by ENVR

From Antibody-Based to Mass Spectrometry-Based Analysis of Emerging Contaminants in Water: Advances & Future Trends

Sponsored by ANYL, Cosponsored by ENVR

Future Insights into Syngas Conversion Catalysis: Symposium in honor of Burtron H. Davis

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

Pollinators in Agroecosystems: Current Science Issues & Risk Assessment Approaches

Sponsored by AGRO, Cosponsored by ENVR

Surfaces & Interfaces in the Environment: Symposium in Honor of Vicki Grassian

Organic-Surface interactions & Organic Aerosols

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Geochemistry of the Urban & Lived Environment

Sponsored by GEOC, Cosponsored by ENVR

Future of Biomacromolecules at a Crossroads of Polymer Science & Biology

Delivery Systems

Sponsored by POLY, Cosponsored by BIOL, CARB, CELL, COLL, ENVR, MEDI, PHYS and PMSE

Advances in Analytical Technologies Supporting Environmental Fate, Metabolism, & Residue Analysis

Sponsored by AGRO, Cosponsored by ENVR

Ecological Considerations of Crop Protection

Sponsored by AGRO, Cosponsored by ENVR

Off-Target Transport of Field Applied Agricultural Chemicals: Study Designs, Monitoring, Modelling, & Risk Assessment

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Pollinators in Agroecosystems: Current Science Issues & Risk Assessment Approaches

Sponsored by AGRO, Cosponsored by ENVR

WEDNESDAY AFTERNOON – ENVR

SECTION A

San Diego Convention Center

Room 28A

Chemistry & Applications of Free Radical-based Technologies for Water Treatment & Purification

Novel Materials Application for Free Radicals-Based Technologies

Cosponsored by AGRO

Financially supported by Association of Environmental Engineering & Science Professors (AEESP)

G. Li Puma, D. Minakata, W. Song, *Organizers*

D. D. Dionysiou, K. E. O'Shea, *Organizers, Presiding*

- 1:30** **609.** Catalytic hydrogel membrane reactor for treating aqueous contaminants. **K. Doudrick**, R. Marks
- 1:55** **610.** Photocatalytic degradation of model organic dyes by strontium barium niobate particles synthesized by solution combustion synthesis. **E. Barnes**, S. Lauren, S. Jones, L. Johnson, J. Flowers, E. Zamora, K. Nash
- 2:20** **611.** Spontaneous oxidative degradation of aromatic compounds on iron oxide nanorods/CNF sheet in dark condition. **Y. Park**, C. Kim, S. Kim, W. Choi
- 2:45** **612.** Laser-induced graphene (LIG) membranes for advanced water and wastewater treatment. **C. Thamaraiselvan**, C. Arnusch
- 3:10** **613.** Highly selective active chlorine generation electrocatalyzed by Co_3O_4 nanoparticles: Mechanistic investigation through *in situ* electrokinetic and spectroscopic analyses. **H. Ha**, K. Jin, S. Park, K. Lee, K. Cho, H. Seo, H. Ahn, Y. Lee, K. Nam
- 3:35** Intermission.
- 3:50** **614.** Unraveling electrochemical chlorination of ammoniacal water. **K. Cho**, S. Hong
- 4:15** **615.** Solar photocatalytic phenol polymerization and hydrogen generation for flocculation of wastewater impurities. **R.E. Patalano**
- 4:40** **616.** Modulations of Bi_2MoO_6 for photocatalytic performance enhancement under visible light illumination. **Q. Li**
- 5:05** **617.** Degradation of 2,4-dichlorophenol by CNT-activated peroxydisulfate: Radical vs. non-radical mechanisms. C. Chen, **Y. Lin**

SECTION B
San Diego Convention Center
Room 28B

Catalysis for Environmental & Energy Applications

Catalysis for Energy Application

Cosponsored by CATL

A. Orlov, A. Savara, Y. Wang, *Organizers, Presiding*

- 1:30** Introductory Remarks.
- 1:35** **618.** Role of H₂S on CO₂ hydrogenation on MoS₂: Kinetic study. **J. Baltrusaitis**, L. Sharma, R. Upadhyay, S. Rangarajan
- 1:55** **619.** Zero valent iron enhances bioelectrochemical biogas upgrading and hydrogen sulfide removal. **C. Dykstra**
- 2:15** **620.** Multipronged approach to enhancing microbial coal-to-methane production from Appalachian Basin coal: Investigating biological amendments and physicochemical coal treatments. **J. Moore**, D. Gulliver
- 2:35** **621.** Efficient head-tail coconversion process for high quality gasoline production via catalytic cracking route. **R. Wang**, Y. Li, G. Jiang, Y. Zhang, A. Duan, Z. Zhao, C. Xu, Y. Wang
- 2:55** **622.** Permeable CNT hollow fiber membrane as a facile strategy for electrocatalytic syngas production from CO₂. **M. Lee**, Y. Kwon, S. Kang
- 3:15** Intermission.
- 3:35** **623.** Development of hydrotalcite-based catalyst for water gas shift reaction and the effect of precursor type on catalytic activity. **S. Kim**, C. Lee, K. Lee
- 3:55** **624.** *In situ* photochemical fabrication of CdS/g-C₃N₄ nanocomposite with high performance for hydrogen evolution under visible light. **L. Chen, B. Chen**
- 4:15** **625.** Photobioelectrochemical systems: Blue ocean approach. **L. Coy Aceves**, B. Corona Vázquez, M.A. Mendez-Rojas, M. Cerro-Lopez, J. Sanchez-Salas
- 4:35** **626.** Quantitative determination of intermolecular attraction between amines and graphene using AFM force spectroscopy. **Y. Zhang, B. Chen**
- 4:55** Concluding Remarks.

SECTION C
San Diego Convention Center
Room 28C

Safeguarding Water Quality in a Climate of Change

Cosponsored by CEI

Financially supported by US Global Change Research Program; Association of Environmental Engineering &

Science Professors (AEESP)

J. Arrigo, J. W. Moerman, *Organizers, Presiding*

- 1:30** **627.** Department of Energy and Water Security grand challenge. **D. Bauer**
- 2:00** **628.** Energy efficient potable reuse: Lowering organic RO membrane fouling and DBP formation when treating anaerobic secondary effluent. **A. Szczuka**, W. Mitch
- 2:20** **629.** Impacts of climate change on drinking water treatment process: Story of unusual high haloacetic acid concentrations in Massachusetts drinking waters. **X. Ma**, P. Wittbold, Y. Sun, G. Moriarty, J.E. Tobiason, D.A. Reckhow
- 2:40** **630.** Effects of changing water chemistry on lead minerals: Implications on lead control in drinking water distribution systems. **J. Orta**, S. Avsarala, H. Liu
- 3:00** **631.** Oil & gas class II wells: Proximities to schools and water contamination. **H. Barravecchia**, J. Buonocore, D. Michanowicz
- 3:20** Intermission.
- 3:40** **632.** Impact of climatic events on water quality and related health outcomes. **J. Jagai**, E. Hilborn, T. Wade
- 4:00** **633.** Protecting groundwater quality from geogenic and emerging contaminants in actively managed aquifers. **S. Fakhreddine**, A. Sherris, A.M. Lopez, A. Wells, R. Holmes, P.S. Nico, C. Babbitt, S.E. Fendorf
- 4:20** **634.** Colloid formation driven by redox processes: Impact on groundwater quality in shallow alluvial aquifers. **V. Noel**, N. Kumar, L. Barragan, K. Boye, J.R. Bargar
- 4:40** **635.** Microbial risk from wildfire residues. **R.L. Valenca**, S.K. Mohanty
- 5:00** **636.** Advanced simulation capabilities to explore pre-and-post fire water quality after the 2017 wine country fires. **M.E. Newcomer**, J. Underwood, R.W. Harvey, T. Schram, M. Smedt, P. Bliznik, C. Ulrich, D. Seymour, M. Trotta, J. Jasperse, S. Hubbard
- 5:20** Discussion.

SECTION D
San Diego Convention Center
Room 28D

Biochar & Hydrochar for Energy, Environmental & Agricultural Applications

Cosponsored by AGRO

Financially supported by Frontiers in Energy Research; Association of Environmental Engineering & Science Professors (AEESP)

N. D. Berge, J. L. Goldfarb, A. Shah, *Organizers*

R. Volpe, *Organizer, Presiding*

- 1:30** Introductory Remarks.
- 1:35** **637.** Adsorption of metals from mining-impacted water onto biochar from different sources. **S.R. Al-Abed**, P. Pinto, M.J. Arambewela, P. Potter, M. Johnson, J. Novak, K. Steve, M. John
- 2:05** **638.** Black carbon-enhanced transformation of chloroacetamide herbicides and safeners by sulfide. **X. Xu**, J. Sivey, W. Xu
- 2:30** **639.** Preparation of novel seaweed biomass-based activated carbon and use for gaseous elemental mercury (Hg⁰) removal. Z. Liu, **Y.G. Adewuyi**, H. Chen, S. Shi, Y. Li, D. Liu, Y. Liu
- 2:55** **640.** Preparation and use of CuO_x- and CeO₂-modified rice straw chars for gaseous elemental mercury (Hg⁰) removal in the presence and absence of ultrasound. W. Xu, **Y.G. Adewuyi**, Y. Liu, Y. Wang
- 3:20** Intermission.
- 3:35** **641.** Ion-selective biochar electrodes for asymmetrical capacitive deionization. **H. Stephanie**, D. Wipf, T. Mlsna
- 4:00** **642.** Biochar combined with polyvalent phage therapy to mitigate antibiotic resistance pathogenic bacteria vertical transfer risk in an undisturbed soil column system. **S. Mingming**, M. Ye, F. Hu
- 4:25** **643.** Assessing flow rate parameters on capacitive deionization of NaCl solution using biomass-derived activated carbon electrodes. M. Maniscalco, **R. Volpe**, A. Messineo
- 4:50** Closing Remarks.

SECTION E

San Diego Convention Center
Room 28E

Fundamental Chemical Processes Common to Dissolved Organic Matter & Atmospheric Organic Aerosols

N. Borduas, S. A. Nizkorodov, *Organizers, Presiding*

- 1:30** Introductory Remarks.
- 1:35** **644.** Photodesulfurization and other photomineralization reactions involving amino acids. **K.P. McNeill**
- 2:05** **645.** Time-resolved singlet oxygen phosphorescence to measure triplet photochemistry in aquatic environments. **K. Moor**, P.R. Erickson, K.P. McNeill
- 2:25** **646.** Photochemical properties of photosensitizers in tropospheric aqueous solution. **T. Felber**, T. Schaefer, H. Herrmann
- 2:45** **647.** Photooxidants in atmospheric drops and particles: Moving beyond solely OH. **C. Anastasio**, R. Kaur
- 3:15** Intermission.

- 3:30** **648.** Development the novel chemical probes for examining the triplet-excited state of organic matters. **W. Song**, H. Zhou, S. Yan
- 4:00** **649.** Photochemical processing of organics at the ocean-atmosphere interface. **S. Blair**, K. Kappes, A. Reed Harris, R. Rapf, E. Pangui, M. Cazaunau, J. Doussin, A. Monod, V. Vaida
- 4:20** **650.** Chemical reactions involving triplet excited states and other reactive species in secondary organic aerosol produced by photooxidation of naphthalene. **V. Baboimian**, R. Gemayel, C. George, D. Fishman, S.A. Nizkorodov
- 4:40** **651.** Photoinduced reactions of anthraquinone-2-sulfonate as model constituents in tropospheric aqueous aerosol. **T. Schaefer**, J.D. Raff, H. Herrmann
- 5:00** **652.** Photochemical production and reactions of halogen oxidants in organic matter-rich saline waters. K. Zhang, **K. Parker**

SECTION F

San Diego Convention Center
Room 29A

Stormwater Treatment & Green Infrastructure: From Research to Practice

R. Ambrose, S. Grant, P. Holden, J. Jay, L. Levin, H. Liu, *Organizers, Presiding*

- 1:30** Introductory Remarks.
- 1:35** **653.** Urban stormwater to enhance water supply. **R.G. Luthy**
- 2:05** **654.** Fighting drought with stormwater: From research to practice. **S. Grant**
- 2:35** **655.** Low-cost polymer-functionalized clay composites for trace organic compound and metal removal during urban stormwater treatment. **J. Ray**, I. Shabtai, M. Teixido, Y. Mishael, D.L. Sedlak
- 2:55** Intermission.
- 3:10** **656.** Waste-derived amendments in stormwater biofilters: Do the benefits outweigh the risks?. **S.K. Mohanty**, M. Ghavanloughajar, M.K. Stenstrom
- 3:30** **657.** Biochar-based bioinfiltration for enhanced and prolonged removal of pesticides from stormwater. **A.C. Portmann**, R. Hankawa, S. Fox, C.P. Higgins
- 3:50** **658.** Efficacy of biochar amended bioretention systems for both urban and agricultural stormwater runoff. **M. Rahman**, N. Truong, S.J. Ergas, M. Nachabe
- 4:10** **659.** Enhanced removal of urban stormwater runoff contaminants using biochar and manganese oxide-coated sand geomedia in a sequential biofiltration system. **M. Teixido**, S. Spahr, R.G. Luthy, D.L. Sedlak
- 4:30** Concluding Remarks.

SECTION G
San Diego Convention Center
Room 31C

Artificial Water Channels for Water Purification & Desalination

Financially supported by Association of Environmental Engineering & Science Professors (AEESP)

M. Barboiu, *Organizer*

J. Hou, B. Mi, *Organizers, Presiding*

- 1:30** **660.** Artificial water channels: Deconvolution of natural aquaporins through synthetic design. **M. Barboiu**
- 2:00** **661.** Biomimetic carbon nanotube water treatment systems utilizing electro-dynamic interfaces. **B. Hinds**
- 2:30** **662.** Functional and scalable carbon nanomembranes (CNMs) are efficient nanoconduits for water purification. **A. Goelzhaeuser**
- 3:00** **663.** Effective removal of emerging cyanotoxins from water using hybrid photocatalytic channels. T. Noeiaghaei, Y. Oh, J. Park, **S. Chae**
- 3:20** **664.** Combining water flux studies with fluorescence techniques to help elucidate the mechanism of membrane biofouling. C. George, **E.M. Stennett**
- 3:40** Intermission.
- 3:50** **665.** Development of hydrophilic nanofiltration membrane for water purification. **W. Sajomsang**, S. Singto, C. Ratanatawanate, S. Thaiboonrod, P. Gonil
- 4:10** **666.** Highly efficient ammonia recovery from wastewater using electrically conducting gas-stripping membranes. **A. Iddya**, D. Hou, Z.J. Ren, J.W. Tester, D. Jassby, A. Gross
- 4:30** **667.** Water vapor permeation of inorganic membranes. **K.J. Lawrence**, P.R. Beaumont, J. Velten
- 4:50** **668.** TiO₂@MoS₂ composite for highly efficient water evaporation and water purification by interfacial solar heating. **R. Chen**, **M. Ye**, **C. Huang**
- 5:10** **669.** Molecular insights into seawater desalination through functionalized nanoporous graphene membranes. **L. Qin**, J.E. Tobiasson, H. Huang

Novel Polymeric Materials & Polymer-Based Processes for Energy-Efficient Treatment of Water & Resource Recovery

Nanomaterials for Separations

Sponsored by PMSE, Cosponsored by ENVR

Sorption & Redox at Mineral-Water Interfaces & the Impact on the Biogeochemical Cycling of Trace & Major Elements

Sponsored by GEOC, Cosponsored by ENVR

Innovative Approaches to Managing the Interface Between Pesticide Use & Non-Target Species Habitat Protection

Sponsored by AGRO, Cosponsored by ENVR

Surfaces & Interfaces in the Environment: Symposium in Honor of Vicki Grassian

Nano in the Environment & Plenary Lecture

Sponsored by COLL, Cosponsored by ENVR and WCC

Future of Biomacromolecules at a Crossroads of Polymer Science & Biology

Biomaterials

Sponsored by POLY, Cosponsored by BIOL, CARB, CELL, COLL, ENVR, MEDI, PHYS and PMSE

THURSDAY MORNING

SECTION C
San Diego Convention Center
Room 28C

Safeguarding Water Quality in a Climate of Change

Cosponsored by CEI

Financially supported by US Global Change Research Program; Association of Environmental Engineering & Science Professors (AEESP)

J. Arrigo, J. W. Moerman, *Organizers, Presiding*

- 8:00** Introductory Remarks.
- 8:05** **670.** Increasing interagency coordination in river monitoring and data access in the United States. **L. Sprague**
- 8:35** **671.** Exploring the effects of streamflow trends and watershed management on changing water quality: National perspective. **J. Murphy**, L. Sprague
- 8:55** **672.** Long-term research assessing water quality and quantity in agricultural landscapes within the Lower Mississippi River Basin. **M.A. Locke**, A. Adviento-Borbe, R. Bingner, R. Lizotte, J. Massey, M. Moore, m. reba, J. Rigby, J. Taylor, P. White, L. Yasarer
- 9:15** **673.** Freshwater salinization syndrome: Causes, consequences, and chemical cocktails. **J.G. Galella**, S.S. Kaushal, K.L. Wood, S. Haq, C. Morel, G.E. Likens, M.L. Pace
- 9:35** **674.** Atmospheric rivers and public health: Observed links between extreme precipitation events and California's coastal water quality. **R. Aguilera**, A. Gershunov, T. Benmarhnia

- 9:55 Intermission.
- 10:10 **675.** Coastal acidification: Moving from a global problem to a coastal water-quality issue. **L. Wickes**
- 10:30 **676.** Cistern health post hurricanes Irma and Maria in the US Virgins Islands. **C. Chanes, D. Morris, S. Latesky**
- 10:50 **677.** Climate variability in relation to floodplain erosion and water quality characteristics of the Ikpa River Basin, Nigeria. **E. Inam, R. Ekpenyong, M. Ekpenyong, A.I. Inyangudoh, N.O. Offiong, U. Udotong, S. Shaibu**
- 11:10 **678.** Quality data matters: Challenges in effective resource management and how DWR is working to address this issue on a statewide scale. **R. Pisor, J. Saraceno**
- 11:30 **679.** Safeguarding water quality through local decision making: Lessons from the Resilience Dialogues. **N. Bennett**
- 11:50 Discussion.

SECTION E

San Diego Convention Center
Room 28E

Fundamental Chemical Processes Common to Dissolved Organic Matter & Atmospheric Organic Aerosols

Financially supported by Association of Environmental Engineering & Science Professors (AEESP)

N. Borduas, S. A. Nizkorodov, *Organizers, Presiding*

- 8:00 Introductory Remarks.
- 8:05 **680.** Ionic strength effects on the reactive uptake of ozone on organic compounds: Implications for air-sea ozone deposition. **S. Gligorovski, M. Mekic, M. Brigante, D. Vione**
- 8:35 **681.** Relationship between the physicochemical properties of an aerosol particle and the exchange of semi-volatile organic molecules. **Y. Qin, J. Wang, Y. Lei, J. Ye, S.T. Martin**
- 8:55 **682.** Characterizing wintertime aerosol composition and sulfate formation, Fairbanks, Alaska. **R. Davey, J. Campbell, R. Weber, J. Mao**
- 9:15 **683.** Exploring surface population of organic molecules of aerosol directly by nonlinear light scattering. **Y. Qian, G. Deng, Y. Rao**
- 9:45 Intermission.
- 10:00 **684.** Cloudy and clear sky particulate matter chemical composition. **A. Carlton, A. Christiansen, B. Henderson**
- 10:30 **685.** Organic solvents facilitate the cloud droplet activation of water-insoluble organic aerosol. **F. Barati, A. Asa-Awuku**
- 10:50 **686.** Organosulfates from dark reactions of isoprene epoxydiols in cloud and fog water. **S.**

Petters, T. Cui, Z. Zhang, A. Gold, V.F. McNeill, J. Surratt, B.J. Turpin

- 11:10 **687.** Measurements of acid and organic partitioning in liquid-liquid phase-separated systems. **B.L. Deming, P.J. Ziemann**
- 11:30 **688.** *In situ* quantification of pH in aerosol droplets. **P.J. Vikesland, L.C. Marr, Q. Huang, H. Wei, H. Guo**

SECTION F

San Diego Convention Center
Room 29A

Stormwater Treatment & Green Infrastructure: From Research to Practice

R. Ambrose, S. Grant, P. Holden, J. Jay, L. Levin, H. Liu, *Organizers, Presiding*

- 8:30 Introductory Remarks.
- 8:35 **689.** Fate of pathogens during managed aquifer recharge. **S. Bradford, S. Sasidharan, j. Simunek, S. Torkzaban**
- 9:05 **690.** Infiltration in roadside drainage ditches. **J. Gulliver, M. Garcia-Serrana, J. Nieber**
- 9:25 **691.** Competing mechanisms affecting transport of copper, zinc, and lead in urban stormwater runoff: Column experiments. **S. Avsarala**
- 9:45 Intermission.
- 10:00 **692.** Enhanced removal of hydrophilic organic contaminants from urban stormwater in biochar-amended biofilters. **S. Spahr, M. Teixido, D.L. Sedlak, R.G. Luthy**
- 10:20 **693.** Molecular characterization of dissolved organic nitrogen removal with biosorption activated media (BAM) based on ultrahigh resolution mass spectrometry. **A.M. McKenna, H. Chen, D. Wen, D. Ordonez, N. Chang**
- 10:40 **694.** Impact of biofouling on the retention of stormwater colloidal contaminants in engineered infiltration system (EIS). **Y. Zhang, S. Wu, S. Preheim**
- 11:00 **695.** Plant uptake and transformation of stormwater emerging organic contaminants. **G.H. LeFevre, C.P. Muerdter, M.M. Powers, H. Zhi**
- 11:20 **696.** Iron enhanced sand filters for removing stormwater phosphate: Results from laboratory, urban, and agricultural studies. **A. Erickson, J.S. Gulliver, P. Weiss**
- 11:40 Concluding Remarks.

Novel Polymeric Materials & Polymer-Based Processes for Energy-Efficient Treatment of Water & Resource Recovery Gas Separation Membranes

Sponsored by PMSE, Cosponsored by ENVR

Advances in Spray Drift Deposition Characterization & Measurement

Sponsored by AGRO, Cosponsored by ENVR

Chemometric Analysis for Aqueous Sample

Sponsored by ANYL, Cosponsored by COMP and ENVR

THURSDAY AFTERNOON – ENVR

SECTION E

San Diego Convention Center
Room 28E

Fundamental Chemical Processes Common to Dissolved Organic Matter & Atmospheric Organic Aerosols

N. Borduas, S. A. Nizkorodov, *Organizers, Presiding*

- 1:00** Introductory Remarks.
- 1:05** **697.** Towards identifying the reactive sites responsible for nitrous acid formation on soil surfaces. R.B. Abney, **J.D. Raff**
- 1:35** **698.** Ozonolysis of various VOCs in the presence of NO and/or OH radicals. **M. Noguchi**, A. Yamasaki
- 1:55** **699.** Incorporation of organic matter into freshwater aerosol: Emissions from harmful algal blooms and impacts on health and climate. **N.E. Olson**, N. May, J. Birbeck, J. Westrick, K.A. Pratt, A.P. Ault
- 2:15** **700.** Salt fat acid bugs: Effects of solutes on reaction rates in atmospheric and environmental condensed phases. **T.F. Kahan**, J.N. Grossman, A. Stathis, K. Blaha
- 2:45** Intermission.
- 3:00** **701.** Modulation of aerosol water content of indoor aerosols and impact on partitioning of water soluble species. **P.F. DeCarlo**, A. Avery, E.F. Katz, L. Ampollini, M.S. Waring
- 3:30** **702.** Withdrawn
- 3:50** **703.** Surface activity and interfacial structure of caryophyllene-derived ozonolysis products. **F. Geiger**, A. Be, A. Bellcross, D. Liu
- 4:10** **704.** Toward a comprehensive picture of heterogeneous chemistry at atmospheric aerosols: Solvation and hydrolysis of glyoxal and methylglyoxal at the liquid water aerosols interface. **I. Gladich**, C. Zhu, J.S. Francisco
- 4:30** **705.** Interconnections of atmospheric aqueous-phase chemistry: Past, present, and future. **H. Herrmann**, T. Schaefer, A. Tilgner

SECTION F

San Diego Convention Center
Room 29A

Stormwater Treatment & Green Infrastructure: From Research to Practice

R. Ambrose, S. Grant, P. Holden, J. Jay, L. Levin, H. Liu,
Organizers, Presiding

- 1:00** Introductory Remarks.
- 1:05** **706.** Biochar-augmented biofilters (BIOCHARGE) to improve pollutant removal from stormwater: Can they improve receiving water quality?. **A. Boehm**, R.G. Luthy, J. Wolfand, C.P. Higgins, T. Hogue, N. Fitzgerald, B. Kranner, W. Eisenstein, B. Ulrich
- 1:35** **707.** IoT enabled data exchange for stormwater systems. P. Venkateswaran, **N. Venkatasubramanian**
- 1:55** **708.** From the laboratory to the field: Study of a modified denitrifying bioretention system. Innovative green stormwater infrastructure for nitrogen removal. **E.V. Lopez-Ponnada**, T.J. Lynn, S.J. Ergas, J.R. Mihelcic
- 2:15** **709.** Carbon uptake and emissions over urban landscapes in San Diego, California: Potential ecosystem service. **J.T. Le**, A. Mehring, L. Levin
- 2:35** Intermission.
- 2:50** **710.** Sediment phosphorus release in stormwater ponds. **V.J. Taguchi**, J.S. Gulliver, J.C. Finlay, B.D. Janke, P. Natarajan, H.G. Stefan
- 3:10** **711.** Enhancing green infrastructure with smart stormwater technology. **E.A. Parker**, S. Grant, A. Sahin, J. Vrugt
- 3:50** **712.** Polychlorinated biphenyls in stormwater sediments: Relationships with land use and particle characteristics. **S. Cao**, S.L. Cappozzi, B.V. Kjellerup, A.P. Davis
- 4:10** Concluding Remarks.

Unmanned Aerial Vehicles (aka Drones): Pesticide Spraying & other Agricultural Applications

Sponsored by AGRO, Cosponsored by ENVR

GEOC

DIVISION OF GEOCHEMISTRY

A. Rouff, *Program Chair*

SUNDAY MORNING – GEOC

SECTION A

San Diego Convention Center
Room 25C

Geogenic & Anthropogenic Sources of Trace Elements within Surface & Groundwater Systems & their Effects on Water Quality

Cosponsored by ENVR

C. Hamilton, *Organizer, Presiding*

- 9:30 Introductory Remarks.
- 9:35 1. Presence of Ca–UO₂–CO₃ ternary complex in brackish groundwater in the Northern Territory, Australia: Transformation and remediation. **J. Ma**, R. Collins, A. Kinsela, A. Jones, D. Waite
- 10:05 2. Biogeochemistry of an alkaline permeable reactive barrier in a boreal fen. **K. von Gunten**, B. Bishop, K. Konhauser, D.S. Alessi
- 10:35 3. Potential chemical impacts of CO₂ intrusion into an unconsolidated aquifer: Column experimental study. **T. Xiao**, W. Jia, R. Esser, B. McPherson
- 11:05 Discussion.
- 11:25 Concluding Remarks.

SUNDAY AFTERNOON – GEOC

SECTION A

San Diego Convention Center
Room 25C

Second Symposium on Applied Geochemical Modeling

E. Chiang, *Organizer*

R. Santos, *Organizer, Presiding*

- 1:00 4. Applications of geochemical modeling: Analytical and critical review of recent scientific literature. **R. Santos**
- 1:30 5. Towards understanding the role of solid interfaces and confinement on fluid organization and transport: Case studies of CO₂ interactions

- with hydrocarbons in confined subsurface porous environments using classical molecular dynamics simulations. **G. Gadikota**, S. Mohammed
- 2:00 6. Geochemical modelling of microbial trace nutrient acquisition by metallophores. **W. Schenkeveld**
- 2:30 Intermission.
- 2:45 7. Modeling EXAFS and XANES spectra of neoformed LDH and metal-enriched phyllosilicate minerals. **M.G. Siebecker**, W. Li, D.L. Sparks, Y. Wang, R. Chaney
- 3:15 8. Critical literature review of geochemical models applied in municipal solid waste management. **F. Araujo**, H.F. Matheus
- 3:35 Concluding Remarks.

MONDAY MORNING – GEOC

SECTION A

San Diego Convention Center
Room 25C

Impacts of Wetland Hydro-Biogeochemistry on Water Quality

T. Flynn, E. J. O'Loughlin, *Organizers, Presiding*

- 8:30 9. Development of a kinetic-thermodynamic model to simulate the mercury cycle in freshwater sediments. **S. Helmrich**, D. Vlassopoulos, C.N. Alpers, P.A. O'Day
- 8:50 10. Competitive dynamics of redox processes in wetland sediments. **A. Moran**, M. Taillefert, E.M. Eitel
- 9:10 11. Seasonality geochemistry cycles in a seasonal sub-arctic wetland underlain by permafrost. **K. Gagne**, J.J. Guerard
- 9:30 12. Integration of omics into a new comprehensive rate law for competitive terminal electron-accepting processes in freshwater sediments. **M. Taillefert**, E.M. Eitel, T.J. Dichristina, H. Shin, F. Stewart, A.D. Bertagnolli, N.V. Patin, K.M. Kemner, S. Brooks, D. Kaplan, C. Pennacchio, S.J. Callister
- 9:50 Intermission.

- 10:05** **13.** Geochemical roles for sediment iron oxides in protecting wetland water quality. **J. Beckler**, A. Stancil, M. Taillefert, J. Hart, D. Hanisak
- 10:25** **14.** Wetland uranium distribution within Tims Branch at the Savannah River site. **C.J. Parker**, D. Kaplan, B.A. Powell
- 10:45** **15.** Iron flocs as biogeochemically dynamic reservoirs of uranium in Tims Branch wetlands, Savannah River Site. **E.J. O’Loughlin**, M. Boyanov, D. Kaplan, P. Weisenhorn, K.M. Kemner
- 11:05** **16.** Redox properties of iron-ligand complexes in dissolved organic matter. **J. Hudson**, **Y. Chin**

MONDAY AFTERNOON – GEOC

SECTION A

San Diego Convention Center
Room 25C

Water, Ice, & Clathrate Hydrate Geochemistry: Molecular Structures, Microscopic Properties, & Energetics

Cosponsored by COLL and PHYS
S. Lee, D. Wu, *Organizers, Presiding*

- 1:35** Introductory Remarks.
- 1:40** **17.** Water and ionic solutions under pressure investigated with first principles simulations. **G.A. Galli**
- 2:10** **18.** Hydration structure at mineral–water interfaces. **S. Lee**, J.N. Bracco, I.C. Bourg, A.G. Stack, P. Fenter
- 2:30** **19.** Coherent X-rays capture water dynamics from glassy to ambient conditions. **F. Perakis**
- 3:00** Intermission.
- 3:20** **20.** Origin of fast dielectric response of water in electrolytes. **P. Zarzycki**, C.A. Colla, M. Prus, K. Kedra-Krolik, B. Gilbert
- 3:40** **21.** Environmental chemical reactions in frozen solutions. **W. Choi**, K. Kim, S. Menacherry, D. Min
- 4:10** **22.** Crystallization of water induced by carbon. **T. Li**, Y. Bi, B. Cao
- 4:40** **23.** Investigation of the influence of ammonia on the stability of cyclopentane and tetrahydrofuran clathrate hydrates using experimental methods. **C. Petuya**, M. Choukroun, T.H. Vu, C. Sotin, A. Davies

TUESDAY MORNING – GEOC

SECTION A

San Diego Convention Center
Room 25C

Water, Ice, & Clathrate Hydrate Geochemistry: Molecular Structures, Microscopic Properties, & Energetics

Cosponsored by COLL and PHYS
S. Lee, D. Wu, *Organizers, Presiding*

- 8:30** **24.** How do surfactants control the nucleation and antiagglomeration of clathrate hydrates?. **V. Molinero**
- 9:00** **25.** Interfacial properties and controls of gas clathrate hydrates. **C.A. Koh**, A. Dapena, J. Delgado-Linares, S. Hu, A. Majid, D. Salmin, J. Wells, D. Wu, L. Zepa
- 9:30** **26.** Visualization of hydrate slurries coupled with slurry viscosity measurements. **A. Abdul Majid**, B. Tanner, D. Wu, C.A. Koh
- 9:50** Intermission.
- 10:05** **27.** Role of surface energy in nucleation of ice and salt hydrates. **A.N. Dhinojwala**
- 10:35** **28.** Homogeneous and heterogeneous nucleation of gas hydrates: Interplay of water structure, dynamics, and guest solubility. **S. Sarupria**
- 11:05** **29.** Ice and hydrate kinetics: From fundamentals to a (bio)geochemical perspective. **M. Ghaani**, M. Lauricella, C. Allen, N. English
- 11:35** **30.** Atomistic-level description of stability and composition of multicomponent clathrate hydrates. **R. Belosludov**, O.S. Subbotin, R.K. Zhdanov, Y.Y. Bozhko, K.V. Gets, Y. Kawazoe, V.R. Belosludov
- 11:55** Concluding Remarks.

TUESDAY AFTERNOON – GEOC

SECTION A

San Diego Convention Center
Room 25C

Advancing the Understanding of Mineral-Water Interfacial Processes through Synergy between Theory & Experiment

K. Yuan, *Organizer*
A. Koishi, *Organizer, Presiding*

- 1:00** **31.** Electrochemical isotope effect – redox driven stable isotope fractionation. **A. Kavner**

- 1:25** 32. Microstructural changes in dissolution/precipitation of CaCO_3 - $\text{CaMg}(\text{CO}_3)_2$ and CaF_2 . **J. Weber**, M.C. Cheshire, V. Distefano, K.C. Littrell, M. Bleuel, I. Ilavsky, A. Ilevlev, A.G. Stack, L. Anovitz
- 1:50** 33. Alkali metal sorption to rutile (110): Experimental and theoretical approach. **I. Johnston**, L.C. Shuller-Nickles, B.A. Powell
- 2:10** 34. Converging on adsorption enthalpies via flow-through microcalorimetry and density functional theory: Adsorption onto rutile (110). **N. Kabengi, J.D. Kubicki**
- 2:35** 35. Cation sorption at barite (001) and (210) water interfaces. **J. Bracco**, S. Lee, J. Weber, M.L. Machesky, A. Kommu, N. Reade, P. Fenter, J.D. Kubicki, A.G. Stack
- 3:00** Intermission.
- 3:10** 36. Molecular insight into the properties of the nanoconfined calcite-solution interface. **Y. Diao**, R.M. Espinosa-Marzal
- 3:30** 37. Anomalous stability of interfacial ice revealed by the freezing of water in confinement. **T. Li**, B. Cao, E. Xu
- 3:55** 38. Atomistic simulations of rotational energetics in turbostratic Wy-montmorillonite clays. **N. Subramanian**, M. Whittaker, L. Lammers, B. Gilbert
- 4:15** 39. Effect of monovalent cations on the adsorption energetics and structure of Sr^{2+} at the muscovite (001)-water interface. **S. Lee**, C. Park, N.C. Sturchio, P. Fenter
- 4:40** 40. X-ray scattering determination of the bastnäs site (001) surface structure. **A.K. Wanhala**, A.G. Stack, J. Stubbs, V.S. Bryantsev, S.G. Srinivasan, S. Roy, P.J. Eng, A.D. Gordon

TUESDAY EVENING – GEOC

SECTION A

San Diego Convention Center

TBD

General Geochemistry

A. Rouff, *Organizer*

6:00 - 8:00

- 41.** Geochemical effects on the adsorption of uranium onto *Shewanella putrefaciens* CN32. **A. Wray**, D.J. Gorman-Lewis
- 42.** Reduction of Sb(V) by a marine bacterium in the presence of sulfite/thiosulfate. **H. Zhang**, Y. Li, X. Hu
- 43.** Characteristics of arsenic oxidation combined with denitrification by anaerobic bacteria. **S. Oh**, H. Moon

- 44.** Impacts of sediment geochemistry on groundwater arsenic in the Hetao basin, Inner Mongolia, China. **W. Feng**
- 45.** Modeling the fate and transport of organic contaminant mixtures in groundwater using stochastic approach. **H. Moon**, J. Joo
- 46.** How natural organic compounds influence zinc retention by iron oxides. **M. Engel**, S.E. Fendorf
- 47.** Association of 16 priority polycyclic aromatic hydrocarbons with humic acid and humin fractions in a peat soil and implications for their long-term retention. **W. Chen**, X. Wang
- 48.** Effects of poultry litter biochar application on the uptakes of phosphorus by rice. **C. Yu**
- 49.** Changing colors of natural bentonite by plant-derived extracts and its potential application in cosmetics materials. **J. Kim**, D. Kim, D. Kim, S. Seo
- 50.** Experimental studies on the formation and substitution kinetics of CH_4 , C_2H_6 , and C_3H_8 clathrates between 1-50 bar and 150-253 K. **T.H. Vu**, M. Choukroun, H.E. Maynard-Casely
- 51.** Comparing scaling formation in different geothermal systems. **J. Lee**, Y. Jang, E. Chung
- 52.** Interfacial premelting of ice in nano composite materials. **M. Mezger**, H. Li, M. Bier

WEDNESDAY MORNING – GEOC

SECTION A

San Diego Convention Center

Room 25C

Advancing the Understanding of Mineral-Water Interfacial Processes through Synergy between Theory & Experiment

A. Koishi, *Organizer*

K. Yuan, *Organizer, Presiding*

- 8:00** 53. Biogeosystem technique new world water paradigm for the water scarcity overcoming. **V.P. Kalinitchenko**, A. Rykhlik
- 8:20** 54. Understanding molecular assembly on mica surfaces: Influence of buried hydroxyls. **A. Tuladhar**, B. Legg, M.D. Baer, Z. Chase, J. Tao, S. Zhang, Z. Wang, C.J. Mundy, H. Wang, J.J. De Yoreo
- 8:45** 55. Surface hydrophobicity and energetics at mica-water interfaces. **A. Koishi**, S. Lee, P. Fenter, A. Fernandez-Martinez, L. Michot, E. Sun, I.C. Bourg
- 9:05** 56. Aluminum hydrolysis at the mica interface and consequences for crystal nucleation and aggregation. **B. Legg**, M.D. Baer, C.J. Mundy, J. Chun, Y. Zhang, S. Huang, Y. Min, J.J. De Yoreo

SECTION A

San Diego Convention Center

Room 25C

Sorption & Redox at Mineral-Water Interfaces & the Impact on the Biogeochemical Cycling of Trace & Major Elements

Cosponsored by ENVR

E. Elzinga, *Organizer, Presiding*

- 1:00 Introductory Remarks.
- 1:05 **69.** Effect of secondary mineralization of ferrihydrite on dark production of ROS via microbially-driven Fenton reaction. **N. Xie**, Y.J. Toporek, T.J. Dichristina, M. Taillefert
- 1:25 **70.** Hydroxamate siderophore interactions with polycrystalline hematite/water interfaces studied using second harmonic and sum frequency generation spectroscopies. **A.L. Mifflin**, J. Brennan, J. Van Ardenne
- 1:45 **71.** Dissolved organic matter affects arsenopyrite dissolution and secondary iron(III) (hydr)oxides formation. **X. Wu**, B. Bowers, D. Kim, B. Lee, Y. Jun
- 2:15 **72.** Redox impacts of humic acids on plutonium interaction with iron oxides. **C. Pan**, M. Zavarin, Y. Jiao, A. Kersting
- 2:35 Intermission.
- 2:50 **73.** Effects of aggregation through freezing, drying, and organic matter on Zn(II) adsorption/retention to iron oxyhydroxide nanoparticles. **C.S. Kim**, S. Hester, T. Le, F. Silva, J. Valenciano
- 3:10 **74.** Sorption of Ni(II) and Zn(II) onto green rust. **E. Elzinga**
- 3:30 **75.** Competitive retention and oxidation of vanadium by iron and manganese oxides. **M.J. Abernathy**, M.V. Schaefer, H. Liu, S. Ying
- 3:50 **76.** Assessing the redox properties of layer-type MnO_x using the probe compound 2,2'-Azino-bis(3-ethylbenzothiazoline-6-sulfonic acid). **S. Benkaddour**, M. Sander, J. Pena
- 4:10 **77.** Determination of stabilization mechanism of heavy metals by basic oxygen furnace slag: Effect of pH, BOF slag content and water content. **S. Kim**, S. Jeong, H. Chung, K. Nam
- 4:30 Concluding Remarks.

- 9:30 **57.** Epitaxial growth of gibbsite sheets on the basal surface of muscovite mica. **J. Stubbs**, B. Legg, S. Lee, P. Dera, J.J. De Yoreo, P. Fenter, P.J. Eng
- 9:55 Intermission.
- 10:05 **58.** Interfacial organization and diffusion of water at surfaces of boehmite (γ-AlO(OH)) and gibbsite (γ-Al(OH)₃) with low miller indices. **W. Smith**, M. Pouvreau, X. Yang, A.E. Clark
- 10:45 **59.** Surface adsorption of aqueous NaOH on mineral surfaces. **X. Yang**, M. Pouvreau, W. Smith, A.E. Clark
- 11:05 **60.** Photochemically-facilitated formation of todorokite with Ca²⁺ incorporation. **Z. Gao**, H. Jung, Y. Jun
- 11:30 **61.** Understanding interfacial structure and nucleation at the quartz/water interface by optical microscopy and DFTB simulations. **K. Yuan**, S. Irle, J.D. Kubicki, A.G. Stack
- 11:50 Concluding Remarks.

SECTION B

San Diego Convention Center

Room 29B

Geochemistry of the Urban & Lived Environment

Cosponsored by ENVR

O. Goswami, A. Rouff, *Organizers, Presiding*

- 9:00 Introductory Remarks.
- 9:05 **62.** Groundwater flooding in coastal urban areas. **V. Prigiobbe**
- 9:35 **63.** Impact of simulated road de-icing salts on release of palladium and platinum from vehicle catalytic converter materials. **D.M. Aruguete**, A.F. Wallace, J. Ferko, G. Gerber, R. Kerr
- 9:55 **64.** Can iron minerals prevent seagrass mortality stemming from urbanization?. **A. Stancil**, J. Hart, D. Hanisak, J. Beckler
- 10:15 **65.** Early career opportunities in sustained climate assessment. **C.W. Avery**
- 10:35 Intermission.
- 10:50 **66.** Withdrawn
- 11:10 **67.** Dynamics of metals in street dust after a mudslide: Case of mining city in Chile. **A.S. Vega**, G. Arce, A. Carkovic, P. Moya, M. Coquery, **P. Pastén**
- 11:30 **68.** Study of urban soil lead in community gardens of Newark, New Jersey. **O. Goswami**, A. Rouff
- 11:50 Concluding Remarks.

SECTION A

San Diego Convention Center
Room 25C

General Geochemistry

A. Rouff, *Organizer, Presiding*

- 8:00** Introductory Remarks.
- 8:05** **78.** Variation of air radiation dose rates from September 2018 to March 2019 inside cabin flights from Singapore to Tokyo. **H. Katsura**
- 8:25** **79.** Iodine diffusive transport through igneous rock. **C.W. Neil**, K. Telfeyan, P. Reimus, H. Boukhalifa, R. Roback, W.P. Brug
- 8:45** **80.** Effect of neutralizing agents on bioaccessibility in the process of *in situ* stabilization for arsenic contaminated soil by co-precipitation with iron oxides. **J. Park**, J. An, K. Nam
- 9:05** **81.** Isolation of microbial cultures from different carbon sources to assess organic matter stability in soil. **J. Thedford**, N. Noor, A. Thompson
- 9:25** **82.** Distribution of biomarker in Enugu Shale, Anambra Basin Nigeria: Implication on hydrocarbon potential. **A.K. Adeyemi**, T.A. Adedosu, G. Ogunbesan, O. Onawunmi
- 9:45** Intermission.
- 10:00** **83.** Influence of alkanes on adsorption characteristics of lithium and adsorbent. **Y. Jang**, J. Lee, E. Chung
- 10:30** **84.** Withdrawn
- 10:50** **85.** Inhibition of microbially induced calcite precipitation by soil solution Cu determined by calcium. **H. Chung**, S. Kim, K. Nam
- 11:10** **86.** Carbonated hydroxyapatite: Effect of crystallization temperature on carbonate content. **Y. Sakhno**, **G. Tosun**, **D. Jaisi**
- 11:30** **87.** Withdrawn
- 11:50** Concluding Remarks.

HIST

DIVISION OF THE HISTORY OF CHEMISTRY

N. Tsarevsky, *Program Chair*

SUNDAY MORNING – HIST

SECTION A

Marriott Marquis San Diego Marina
Coronado Room

Bibliography of Chemistry

Chemical Bibliography

Cosponsored by CINF

G. D. Patterson, *Organizer, Presiding*

R. S. Brashear, *Presiding*

- 8:00 1. Collecting chemical knowledge: History of chemical bibliography and bibliophilism. **R.S. Brashear**
- 8:30 2. Boyle's *Sceptical Chymist*, 1661: Current census. **V.V. Mainz, G.S. Girolami**
- 9:00 3. Byron A Soule's library guide for the chemist: Guide to the use of the chemical literature. **R.A. Egolf**
- 9:30 4. Different editions or different books? The *Regnum minerale* of "Valentin Krautermann". **J.A. Norris**
- 10:00 Intermission.
- 10:15 5. Introduction to the bibliography of chemistry. **G.D. Patterson**
- 10:45 6. When books lie: Unravelling the bibliography of Lemery's *Cours de Chimie*. **J.R. Voelkel**
- 11:15 7. Chemistry books during the sixties: Renaissance-like flowering. **P. Laszlo**
- 11:45 8. Panel discussion: Role of booksellers in the history of chemistry. **G.D. Patterson, J.A. Norris**

SUNDAY AFTERNOON – HIST

SECTION A

Marriott Marquis San Diego Marina
Coronado Room

150 Years of the Periodic Table

Cosponsored by CINF, INOR and PRES

G. Girolami, C. J. Giunta, *Organizers*

V. V. Mainz, *Organizer, Presiding*

- 1:10 Introductory Remarks.
- 1:15 9. Trouble with triads. **W. Jensen**
- 1:45 10. Vis tellurique of Alexandre-Émile Béguyer de Chancourtois. **C.J. Giunta**
- 2:15 11. Periodicity in Britain: Periodic tables of Odling and Newlands. **J. Poole-Sawyer**
- 2:45 Intermission.
- 3:00 12. Gustavus Detlef Hinrichs and his chart of the elements. **G.S. Girolami**
- 3:30 13. Mendeleev in St. Petersburg: Marginality of the periodic system. **M.D. Gordin**
- 4:00 14. Lothar Meyer's path to periodicity. **A.J. Rocke**

Chemical Nomenclature & Representation: Past, Present & Future

Sponsored by CINF, Cosponsored by HIST and NTS

MONDAY MORNING – HIST

SECTION A

Marriott Marquis San Diego Marina
Coronado Room

150 Years of the Periodic Table

Cosponsored by CINF, INOR and PRES

G. Girolami, V. V. Mainz, *Organizers*

C. J. Giunta, *Organizer, Presiding*

- 8:40 Introductory Remarks.
- 8:45 15. Discovery of the elements predicted by Dmitri Mendeleev's table: Scandium, gallium, and germanium. **M. Orna, M. Fontani**
- 9:15 16. Rare earth elements. **A. De Bettencourt Dias**
- 9:45 17. History (and pre-history) of the discovery and chemistry of the noble gases. **J.A. Labinger**
- 10:15 Intermission.
- 10:30 18. Sir John F.W. Herschel and the concept of periodicity. **G.D. Patterson**
- 11:00 19. Hydrogen, helium, and metals: When astronomy met the periodic table. **V.L. Trimble**
- 11:30 20. Hydrogen to oganesson: Philatelic celebration of the periodic table. **D. Rabinovich**

Chemical Nomenclature & Representation: Past, Present & Future

Challenges & Opportunities in Chemical Representation

Sponsored by CINF, Cosponsored by HIST and NTS

MONDAY AFTERNOON – HIST

SECTION A

Marriott Marquis San Diego Marina
Coronado Room

150 Years of the Periodic Table

Cosponsored by CINF, INOR and PRES

C. J. Giunta, V. V. Mainz, *Organizers*

G. Girolami, *Organizer, Presiding*

- 1:40** Introductory Remarks.
- 1:45** **21.** Impact of 20th century physics on the periodic table and questions still outstanding in the 21st century. **E.R. Scerri**
- 2:15** **22.** Uses of the periodic system after radioactivity and the discovery of the neutron: Contrasting views of Lise Meitner and Ida Noddack. **B. Van Tiggelen**
- 2:45** **23.** Mary Elvira Weeks and *The Discovery of the Elements*. **V.V. Mainz**
- 3:15** Intermission.
- 3:30** **24.** From neptunium to mendelevium: Element discovery and the birth of the atomic age. **K. Chapman**
- 4:00** **25.** Transactinide elements: How the 7th row of the periodic table was discovered. **D.A. Shaughnessy**
- 4:30** **26.** Periodic table after period 7. **V.P. Pyykko**

CHAS 40th Anniversary Symposium

Sponsored by CHAS, Cosponsored by HIST

Chemical Nomenclature & Representation: Past, Present & Future

InChI'ng Forward

Sponsored by CINF, Cosponsored by HIST and NTS

MONDAY EVENING – HIST

SECTION A

San Diego Convention Center

TBD

Sci-Mix

N. V. Tsarevsky, *Organizer*

8:00 - 10:00

10, 21. See Previous Listings.

42, 48, 49, 50, 51, 52. See Subsequent Listings.

TUESDAY MORNING – HIST

SECTION A

Marriott Marquis San Diego Marina
Marina Ballroom Salon E

HIST Award

J. Seeman, *Organizer, Presiding*

- 9:00** **27.** Personal reflection on Ted Benfey's early contributions to chemical education. **L.E. Overman**
- 9:30** **28.** Ted Benfey and the Chemical Heritage Foundation. **N.D. Heindel**
- 10:00** **29.** My "TED Talk": Tribute to Ted Benfey and chemistry. **M. Orna**
- 10:30** Intermission.
- 10:40** **30.** Traveling with Ted Benfey: Greensboro, Munich, and Newton. **W. Newman**
- 11:10** **31.** Periodicals, periodical elements, and structures of periodicity: Perspective on the work of Ted Benfey. **A.J. Rocke**
- 11:40** **32.** Ingold, Bartlett, and the status of physical organic chemistry. **S.J. Weininger**

Gerry Meyer: The First 100 Years

Sponsored by SCHB, Cosponsored by BMGT, CHED, ENFL, HIST and SCC

TUESDAY AFTERNOON – HIST

SECTION A

Marriott Marquis San Diego Marina
Marina Ballroom Salon E

HIST Award

J. Seeman, *Organizer, Presiding*

- 1:30 33. German prince and the encouragement of trade, culture, and chemistry in Victorian Britain. **R. Anderson**
- 2:10 34. From Armstrong's reversed electrolysis and heuristic teaching method to O. T. Benfey's solvent salt effects in hydrolysis and the changing American chemistry curriculum. **W. Brock**
- 2:40 35. Recent advances in the history of chemistry. **J. Seeman**
- 3:10 Intermission.
- 3:20 36. Ted Benfey: Friend to colleges, chemistry, and art. **J. Fernandes**
- 3:50 37. Remarks and reminiscences. C. Benfey, **P. Benfey**, S. Benfey
- 4:30 38. My path from organic research chemistry to becoming a science historian. **O.T. Benfey**

Gerry Meyer: The First 100 Years

Sponsored by SCHB, Cosponsored by BMGT, CHED, ENFL, HIST and SCC

WEDNESDAY MORNING – HIST

SECTION A

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 9

150 Years of the Publication of the 1st issue of Zhurnal Russkogo Fiziko-Himicheskogo Obshtestva

Journal of the Russian Chemical Society: First Issues

D. E. Lewis, N. V. Tsarevsky, *Organizers, Presiding*

- 8:45 39. Foundation and early activities of the Russian Chemical Society. **N.V. Tsarevsky**
- 9:15 40. Russia's first professional chemical journal: *Zhurnal Russkogo Khimicheskogo Obshchestva*. **D.E. Lewis**

- 9:45 41. Volkova effect: Women in and behind the pages of the Journal of the Russian Chemical Society. **M.D. Gordin**
- 10:15 Intermission.
- 10:30 42. Salvaging the past: Conversion of low-resolution historical images to line art. **M.J. Adlington**, S.L. Mahoney, M.A. Bergs, S.E. Lomo, D.E. Lewis
- 11:00 43. Borodin's contributions to organic chemistry. **M.C. Stefan**
- 11:30 44. Exploring the reactivity of halogen compounds: Gustavson's contributions to chemistry. **N.V. Tsarevsky**

WEDNESDAY AFTERNOON – HIST

SECTION A

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 9

Tutorial & General Papers

N. V. Tsarevsky, *Organizer, Presiding*

S. C. Rasmussen, *Presiding*

- 1:00 45. Glass in the West: From forest glass to bohemian glass. **S.C. Rasmussen**
- 1:30 46. Lead in the human habitat: Historical perspective. **G.G. Melikyan**, S. Guarina, V. Abed
- 2:00 47. Rachael Bodley: Charter ACS member and medical education pioneer, part 2. **J. Hayes**
- 2:30 48. Withdrawn
- 3:00 Intermission.
- 3:15 49. Withdrawn
- 3:45 50. Withdrawn
- 4:15 51. Clendenin, WV: Birthplace of the Chemical Valley and the efforts to document our history. **M.W. Fultz**, D. Stone
- 4:45 52. Withdrawn

I&EC

DIVISION OF INDUSTRIAL AND ENGINEERING CHEMISTRY

C. Abney and R. Mayes, *Program Chairs*

SUNDAY MORNING – I&EC

SECTION A

Marriott Marquis San Diego Marina
La Costa

I&EC General Papers

Cosponsored by CTA

C. W. Abney, R. T. Mayes, *Organizers*

H. Martin, *Presiding*

- 8:00** Introductory Remarks.
- 8:05** **1.** Leaching of rare earth elements and yttrium from a central Appalachian coal and the ashes obtained at 550–950 °C. **Y. Soong**, R. Lin, B. Howard, M. Keller, E. Roth, P. Wang, E.J. Granite
- 8:25** **2.** Lithium extraction from Alberta oilfield brines. **S. SafariMohsenabad**, A. Seip, D.S. Alessi
- 8:45** **3.** Separation and purification of rare earth elements using diglycolamide based novel extraction chromatographic material. **M. Momen**, **C. Tsouris**, **M.C. Cheshire**, **S. Jansone-Popova**, D.W. DePaoli, B.A. Moyer
- 9:10** **4.** Laboratory investigation of mineral scale deposition kinetics by adopting a plug-flow tube reactor in oilfield chemistry conditions. **P. Zhang**, Y. Liu, A. Kan, M.B. Tomson
- 9:35** **5.** Impact of Ti containing nanoparticles on ocean Fe fertilization: Laboratory investigation of the growth of marine diatom, *Cyclotella meneghiniana*. **E. Hettiarachchi**, S. Ivanov, T. Kieft, G. Rubasinghege
- 9:55** Intermission.
- 10:15** **6.** Effective immobilization of Pb(II) ions onto novel Nigerian moulding clay material supported zerovalent iron nanocomposite (MCM-nZVI): Adsorption and desorption studies. **A.O. Dada**, F.A. Adekola, E.O. Odeunmi, A.S. Ogunlaja
- 10:35** **7.** Withdrawn
- 10:55** **8.** Need for pressure dependent kinetics in steam cracking models. **R. Van de Vijver**, F.H. Vermeire, K. De Ras, S. Ukkandath Aravindakshan, G.B. Marin, K. Van Geem
- 11:15** **9.** Repetitive pool boiling tests: Controlled process to form reduced GO surfaces from GO with tunable surface chemistry and morphology. **A. Gupta**

- 11:35** **10.** New insights into electrochemical ammonia oxidation on Pt(100) from grand-canonical density functional theory. **H. Pillai**, H. Xin

Molten Salt Reactor Chemistry

Radiation Chemistry in Molten Salts

Sponsored by NUCL, Cosponsored by I&EC

Characterization of Plastics in Aquatic Environments

Sponsored by POLY, Cosponsored by ANYL, BIOL, CEI, ENVR, I&EC, PMSE and PRES

SUNDAY AFTERNOON – I&EC

SECTION A

Marriott Marquis San Diego Marina
La Costa

I&EC General Papers

Cosponsored by CTA

C. W. Abney, R. T. Mayes, *Organizers*

H. Martin, *Presiding*

- 1:00** **11.** Phase boundary of gas hydrates: Application in desalination. **R. Zheng**, Z. Fan, X. Li
- 1:20** **12.** Study on the characteristic of reaction between sodium nitrite and ammonium chloride. **C. QIAN**, Y. Wang, Z. Yang, M. Ding
- 1:40** **13.** Evaluating hydrophobin as an antinucleation agent in amorphous drug delivery systems. **Y. Li**, M. Lamm, N. Sallada, B. Berger
- 2:00** **14.** Coating drivers for sealant slide behavior. **L. Steely**, J. Hixenbaugh, F. Maria, R. Rock, C.R. Hickenboth
- 2:20** **15.** Chemical exergy analysis of salinity gradient energy case study: Great Salt Lake. **A. Emdadi**
- 2:40** Intermission.
- 3:00** **16.** Monitoring particle number stability in emulsion polymerizations. **A. Horn**, T.C. Johnston, D. Guironnet

- 3:20** 17. Quantitative XPS examination of UV induced surface modification of TiO₂ sorbents for the increased saturation capacity of sulfur heterocycles. **M. Chi**, B. Tatarchuk
- 3:40** 18. Herbicidal ionic liquids: Synthesis and properties. **M. Niemczak**, J. Pernak
- 4:00** 19. Plasticized melt spinning process for PAN fibers based on task-specific ionic liquids. **H. Martin**, H. Luo, R.T. Mayes, S. Dai
- 4:20** Concluding Remarks.

Molten Salt Reactor Chemistry

Salt Redox Chemistry & Thermodynamics

Sponsored by NUCL, Cosponsored by I&EC

Characterization of Plastics in Aquatic Environments

Sponsored by POLY, Cosponsored by ANYL, BIOL, CEI, ENVR, I&EC, PMSE and PRES

MONDAY MORNING – I&EC

SECTION A

Marriott Marquis San Diego Marina
La Costa

I&EC Graduate Student Award Symposium

Cosponsored by I&EC

P. E. Savage, G. G. Stanley, *Organizers*

M. A. Matthews, *Organizer, Presiding*

M. Abraham, *Presiding*

- 8:00** Introductory Remarks.
- 8:10** 20. Scalable and facile preparation of SSNs for lithium metal stabilization. **D.G. Mackanic**, Z. Yu, Y. Cui, Z. Bao
- 8:30** 21. Interfacial polymerization of a thin lubricious film for improving wettability and lubricity. **Y. Yu**
- 8:50** 22. Dispersion of drug particles and emulsion drops in oleogels for ophthalmic drug delivery. **R. Macoon**, A. Chauhan
- 9:10** 23. Engineering interfacial hydrophobicity by tuning chemical and physical surface properties. **B.C. Dallin**, R. Van Lehn
- 9:30** 24. Ethylene/ethane separation in metal–organic frameworks by computational modeling. **W. You**, D. Sholl, D. Tang, J. Howe
- 9:50** 25. Creation of well-defined “mid-sized” micropores in carbon molecular sieve membranes for organic solvent separations. **Y. Ma**, D. Bhandari, J. Johnson, R.P. Lively

- 10:10** 26. Tetra-*n*-octyl diglycolamide confinement in solid supports for *f*-element separations. **E.R. Bertelsen**, J. Shafer
- 10:30** 27. Phyllosilicate mineral dissolution upon variable alkaline treatment and redox conditions. **S.A. Di Pietro**, H. Emerson, Y. Katsenovich

I&EC Graduate Student Award Symposium

Cosponsored by I&EC

Liquid Assets: The Business of Water

Sponsored by SCHB, Cosponsored by ANYL, BMGT and I&EC

Molten Salt Reactor Chemistry

Industrial Perspectives & Safety Considerations

Sponsored by NUCL, Cosponsored by I&EC

Green & Sustainable Chemistry Theory & Practice: Chemistry & Water

Sponsored by CHED, Cosponsored by CEI and I&EC

MONDAY AFTERNOON – I&EC

SECTION A

Marriott Marquis San Diego Marina
La Costa

I&EC Graduate Student Award Symposium

Cosponsored by I&EC

P. E. Savage, G. G. Stanley, *Organizers*

M. A. Matthews, *Organizer, Presiding*

M. Abraham, *Presiding*

- 1:00** Introductory Remarks.
- 1:05** 28. Process intensification for pharmaceutical manufacturing: How to make drugs cheaper?. **K. Pal**, Z. Nagy
- 1:25** 29. Nanomaterials enable biomolecule delivery in mature plants for high-throughput plant transformation applications. **G.S. Demirer**, H. Zhang, N. Goh, F. Cunningham, Y. Sung, M. Landry
- 1:45** 30. Sustainable chemical production through two-step CO₂ electrolysis. **M. Jouny**, F. Jiao
- 2:05** 31. Demand response operation of electricity-intensive chemical processes for reduced greenhouse gas emissions: Application to an air separation unit. **M. Kelley**, R. Baldick, M. Baldea
- 2:25** 32. Elucidating the role of deep eutectic solvents (reline) towards the synthesis of gold nanoparticles. **S. Datta**, L. Torrente Murciano

- 2:45 33. Modular continuous flow reactor system for large-scale automated synthesis of semiconductor nanomaterials. **A. Vikram**, A. Zahid, A. Khare, T. SinghRachford, D. Shenai, P. Trefonas, M. Shim, P.J. Kenis
- 3:05 Discussion.
- 3:25 Concluding Remarks.

I&EC Graduate Student Award Symposium

Cosponsored by I&EC

Molten Salt Reactor Chemistry

Poster Session

Sponsored by NUCL, Cosponsored by I&EC

MONDAY EVENING – I&EC

SECTION A

San Diego Convention Center
TBD

Sci-Mix

C. W. Abney, R. T. Mayes, *Organizers*

8:00 - 10:00

7, 8, 14, 16, 19, 20, 22, 23, 31. See Previous Listings.
40, 41, 47, 48, 50, 52, 54, 57, 60, 61, 65. See Subsequent Listings.

TUESDAY MORNING – I&EC

SECTION A

Marriott Marquis San Diego Marina
La Costa

Molten Salt Chemistry

Reactivity in Molten Salts

Cosponsored by NUCL

R. Gakhar, J. F. Wishart, *Organizers*

K. Chen-Wiegart, *Organizer, Presiding*

- 8:00 Introductory Remarks.
- 8:05 34. Chemistry of the molten salt reactor fuel. **O. Benes**, P. Soucek, R. Konings
- 8:40 35. Recovery of alkaline-earth fission products from molten salts. **H. Kim**
- 9:10 36. Optical spectroscopic investigation of actinides and fission products in molten salts. **S. Dai**
- 9:40 37. Metal speciation and coordination geometry in molten salts: UV-vis and X-ray absorption studies. **R. Gakhar**, S. Frank, W. Phillips, S. Gill, A. Frenkel, M. Topsakal, V.S. Bryantsev, S.M. Pimblott

- 10:00 Intermission.
- 10:20 38. Impurity analysis in chloride salts using various analytical techniques. **D. Sulejmanovic**, S. Raiman, J.M. Kurley, R.T. Mayes, B. Pint
- 10:40 39. Radiation chemistry and redox reactions in molten salt solutions. **J.F. Wishart**, G.P. Horne, R. Gakhar, J.A. LaVerne, S.M. Pimblott
- 11:00 40. Solid-melt-gas interactions in molten carbonate fuel cell (MCFC). **P. Singh**
- 11:30 41. Computing chemical reaction equilibria in molten salts: Composition of molten carbonate electrolytes in contact with gaseous species. **A. Mondal**, L. Koziol, G. Kiss, T.A. Barckholtz, J.M. Young, A. Panagiotopoulos

TUESDAY AFTERNOON – I&EC

SECTION A

Marriott Marquis San Diego Marina
La Costa

Molten Salt Chemistry

Structure & Properties of Molten Salts

Cosponsored by NUCL

K. Chen-Wiegart, R. Gakhar, *Organizers*

J. F. Wishart, *Organizer, Presiding*

- 1:00 42. *Ab initio* molecular dynamics simulations of molten salt mixtures: Cases of KCl–LiCl and KCl–NaCl systems. **M. Nguyen**, V. Glezakou, R. Rousseau
- 1:20 43. Developing new force fields for molten salts: Toward understanding electrolyte chemistry in the molten carbonate fuel cell. **L. Koziol**, G. Kiss, T.A. Barckholtz, J.M. Young, A. Mondal, A. Panagiotopoulos
- 1:40 44. Bridging the gap between theory and experiments on the structure, dynamics, and thermodynamics of molten salts. **S. Roy**, F. Wu, H. Wang, S. Sharma, Y. Zhang, M.S. Emerson, V.S. Bryantsev, E. Maginn, C.J. Margulis, A.S. Ivanov, S. Gill, S.M. Mahurin
- 2:10 45. Determination of molecular structure and dynamics of molten salts by advanced neutron and X-ray scattering measurements and computer modeling. **B. Khaykovich**, R.T. Mayes, J. Li, G. Zheng
- 2:40 Intermission.
- 3:00 46. Measuring the property of molten salts at operationally relevant temperatures. **W. Chiu**
- 3:30 47. On-line monitoring of molten salts: Process control and fundamental characterization. **S.A. Bryan**, S.D. Branch, H. Felmy, J.M. Wislon, G.J. Lumetta, B.J. Riley, A. Lines

- 4:00 48. Mechanochemical synthesis of high purity anhydrous binary and ternary salt mixtures. **P.W. Halstenberg**, P. Bagri, S.M. Mahurin, R.T. Mayes, S. Dai
- 4:20 49. Utilizing chloroform to purify molten chlorides. **J.M. Kurley**, D. Sulejmanovic, S. Raiman, S. Dai, R.T. Mayes

Chemistry of Disasters

Sponsored by PRES, Cosponsored by CCS, CHAS and I&EC

58. High performance nickel vanadium thin film materials prepared by a cost-effective thermomechanical and chemical process. M. Yuan, **S. Zhao**
59. Sustainability strategies of waste management of petroleum using life cycle analysis. **P. Chongchongprasert**, S. Khaodhiar, A. Charoensaeng
60. Deracemization of sodium chlorate: Effect of enantiomeric excess and crystal size of chiral seeds. **Z. Bowen**, W. Kim, G. Coquerel
61. Molten salt research at ORNL. **R.T. Mayes**

TUESDAY EVENING – I&EC

SECTION A

San Diego Convention Center
TBD

I&EC General Posters

Cosponsored by CTA

C. W. Abney, R. T. Mayes, *Organizers*

6:00 - 8:00

50. Application of spectrophotometric titration for verification of small molecule interaction in relation to amidoximated fibers for uranium extraction from seawater. **K.M. Mote**, P.W. Halstenberg, I. Popovs, S. Dai
51. Structural optimization of thin zeolite films for light gas separations. **P. Lee**, H. Kim
52. Withdrawn
53. Experiments of molybdenum recovery from direct coal liquefaction residue. **C. Wu**, Y. Luo, X. Guo*
54. Orthogonal design and thermal properties of optimum expanded graphite (EG)/calcium chloride hexahydrate composite PCM with good temperature-delay performance. **K. Yuan**, R. Zou
55. Evaluation of non-metallic part in waste printed circuit boards (PCBs) management strategy using combined material flow analysis (MFA) and life cycle assessment (LCA) approach. **W. Rungsitikul**
56. Flue gas analysis by mass spectrometry with carbon monoxide monitoring via an external detector. **I. Beta**, **J. Brenner**, **C. Williams**, **G. Thier**, **J. Wei**, **B. Regel**, L. Kephart
57. Separation of oil-coolant mixture from water using a two-step process of skimming and coagulation. **S. Mortazavian**, h. An, J. Moon

WEDNESDAY MORNING – I&EC

SECTION A

Marriott Marquis San Diego Marina
La Costa

Molten Salt Chemistry

Materials Compatibility & Interfacial Phenomena

Cosponsored by NUCL

K. Chen-Wiegart, J. F. Wishart, *Organizers*

R. Gakhar, *Organizer, Presiding*

- 8:00 62. Characterization of 2LiF-BeF₂ (FLiBe) salt mixture: Methods and error analysis. **R. Scarlet**
- 8:30 63. Basic molten salt research needs to support development of liquid fueled generation-IV nuclear reactors. **M. Simpson**
- 9:00 64. Holistic approach to understanding alloy degradation in molten chloride salts. **S. Raiman**, J.W. McMurray, R.T. Mayes, K.G. Myhre, J.M. Kurley, C.W. Abney, W. Ponder, J. Startt
- 9:30 65. Visualization of molten salt interaction with Ni and Ni-20Cr alloy via multiscale imaging. A. Ronne, L. He, D. Dolzhenkov, M. Ge, X. Xiao, Y. Wang, W. Lee, S.M. Mahurin, **Y. Chen-Wiegart**
- 10:00 Intermission.
- 10:20 66. Molten salt chemistries and their corrosion mitigation for high temperature thermal technologies. **J. Gomez-Vidal**
- 10:50 67. Alloying effects in molten salt corrosion, including porosity formation, and their relation to hot-water corrosion at similar temperature. T. Ghaznavi, **R.C. Newman**
- 11:20 68. Correlating the corrosion behavior to the surface chemistry of Inconel in molten salts. **D. Chidambaram**, W. Phillips
- 11:50 Concluding Remarks.

SECTION A

Marriott Marquis San Diego Marina
La Costa

Keeping Water Safe

Cosponsored by CHAS and PRES

J. M. Pickel, *Organizer, Presiding*

- 1:00 Introductory Remarks.
- 1:10 69. Water purification using the ion-exchange reactivity of nanometric metal oxides. **A.W. Apblett**, C.K. Perkins, H. Albusaidi
- 1:40 70. Innovation transforming lives through the power of clean water. **D.G. Schmidt**
- 2:10 71. Water safety challenges in laboratory. **S. Howell**
- 2:40 Intermission.
- 3:00 72. Flint water crisis now. **M.R. Wilhelm**
- 3:30 73. After flint. **R.M. Izzo**
- 4:00 74. Drinking water quality program at Carnegie Mellon University. **S. Singh**, C. Goyda, R. Cicco

IAC

INTERNATIONAL ACTIVITIES COMMITTEE

SUNDAY AFTERNOON – IAC

Our Element(s): Younger Chemists from Around the World

Sponsored by YCC, Cosponsored by IAC

DIVISION OF INORGANIC CHEMISTRY

N. Radu and S. Koch, *Program Chairs*

SUNDAY MORNING – INOR

SECTION A

Marriott Marquis San Diego Marina
Santa Rosa

Bioinorganic Chemistry: Proteins & Enzymes & Model Systems

S. A. Koch, *Organizer*

M. C. Heffern, S. E. Stieber, *Presiding*

- 8:30** 1. Investigating the dependence of proinsulin C-peptide on metal micronutrients. **M.C. Heffern**
- 8:50** 2. Oxygen uptake in complexes related to [NiFeS] and [NiFeSe] hydrogenase active sites. **X. Yang, T. Le, L.C. Elrod, M.Y. Darensbourg, M. Hall**
- 9:10** 3. Mononuclear Cu-aqua and -hydroxido complexes for multielectron processes. **D.L. Ross, A. Borovik**
- 9:30** 4. Metal-binding pharmacophores utilizing bioisosteres as novel scaffolds for metalloenzyme inhibition. **B. Dick, S. Cohen**
- 9:50** 5. Quantifying nickel nitrosyl coordination modes with X-ray emission spectroscopy and computations. **S.E. Stieber**
- 10:10** Intermission.
- 10:30** 6. Harnessing P450 biocatalysis with Ru(II)-polypyridyl complexes. **L.E. Cheruzel**
- 10:50** 7. Stable end-on (η^1) superoxocopper(II) complexes that display appreciable substrate reactivity. **J. England**
- 11:10** 8. Oxygen intermediates before and after ferryl-oxos in mononuclear nonheme iron enzymes. **S. Iyer, K. Tidemand, S. Goudarzi, H. Christensen, G. Peters, E.I. Solomon**
- 11:30** 9. Dioxygen activation by manganese thiolate complexes with tunable ligands. **C. Poon, M.A. Dedushko, X. Sun, G. Yang, S.A. Toledo, E. Hayes, A. Johansen, J. Rees, S. Stoll, E.V. Rybak-Akimova, J. Kovacs**
- 11:50** 10. Non-heme iron and 2-oxoglutarate-dependent histone demethylases: Understanding reaction mechanisms, ligand binding and dynamics using QM/MM and MD methods. **C. Christov, R. Rajeev, S.S. Chaturvedi, T. Karabencheva-Christova**

- 12:10** 11. Understanding the mechanism of hydrogen peroxide induced carbon monoxide release from a manganese carbonyl. **J. Barrett, P.C. Ford**

SECTION B

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 9

Environmental & Energy-Related Inorganic Chemistry

S. A. Koch, *Organizer*

J. Haber, *Presiding*

- 8:30** 12. Ultrathin MOF nanosheet based composite membranes for carbon capture. **M. Liu, Q. Fu, P. Webley, G. Qiao**
- 8:50** 13. Metal oxide electronic structure determines the direction of electron transfer at dye-sensitized interfaces. **R.E. Bangle, G.J. Meyer**
- 9:10** 14. Coordination environment of a polymer-encapsulated cobalt complex for selective electrochemical CO₂ reduction. **Y. Liu, C.C. McCrory**
- 9:30** 15. 150MPa of high-pressure H₂/CO₂ production by formic acid dehydrogenation and continuous separation. **H. Kawanami, Y. Himeda, M. Iguchi**
- 9:50** 16. Electrocatalytic H₂ evolution in water by co-mimochrome VI*_a, a synthetic mini-protein. **J. Le, V. Firpo, V. Pavone, A. Lombardi, K. Bren**
- 10:10** 17. Functional mapping reveals mechanistic clusters for OER catalysis across (Cu-Mn-Ta-Co-Sn-Fe)O_x composition and pH space. **J. Haber, H.S. Stein, D. Guevarra, A. Shinde, R.J. Jones, J.M. Gregoire**
- 10:30** 18. Open-shell Mo(V) nitrides, phosphides, and carbides: Does radical character dictate coupling chemistry?. **G.A. Bailey, J.A. Buss, T. Agapie**
- 10:50** Intermission.
- 11:00** 19. High performance PDMS pervaporation membranes for recovery of *n*-butanol. **J. Lee, D. Kim, S. Shin, J. Lee**
- 11:20** 20. Electrochemical total oxidation of multi-carbon substrates by an oxidic cobalt catalyst. **T. Keane, C. Brodsky, D.G. Nocera**

- 11:40** **21.** Electrocatalytic water oxidation using (bpy)₂Co-based precursors. **R.L. Holland**, H.M. Tubbs, B.A. McKeown, R.J. Nielsen, W.A. Goddard, T.B. Gunnoe
- 12:00** **22.** Thermodynamic strategies of hydride tuning for CO₂ reduction. **A.L. Ostericher**, C.P. Kubiak
- 12:20** **23.** Determining the site of protonation and the hydricity of active-site model complexes of the tungsten- and molybdenum-containing formate dehydrogenases. **T. Kerr**, J.Y. Yang

SECTION C

Marriott Marquis San Diego Marina
Marina Ballroom Salon F

Chemistry of Materials: Materials for Energy & Catalytic Applications

C. G. Lugmair, *Organizer*
D. Primc, Y. N. Regmi, *Presiding*

- 8:30** **24.** Oxide nanoparticles coated with corrosion resistant metals as anode catalyst layer fillers in proton exchange membrane electrolyzers. **Y.N. Regmi**, E. Tzanetopoulos, N. Danilovic
- 8:50** **25.** Introducing nanocrystalline CeO₂ and Au-CeO₂ in electrocatalytic HER, OER and electro-oxidation of methanol. **K. Deori**
- 9:10** **26.** Improving and understanding the hydrogen evolving activity of a cobalt dithiolene metal-organic framework. **K. Chen**, E. Schneider, C. Downes, J. Goodpaster, S.C. Marinescu
- 9:30** **27.** Synthesis of PtNi tetrahedrons with exceptional activity for hydrogen evolution reaction. **C. Wan**, X. Duan
- 9:50** **28.** Stabilization of reactive Co₄O₄ cubane oxygen-evolution catalysts within porous frameworks. **K.M. Van Allsburg**, A.I. Nguyen, M.W. Terban, M. Bajdich, J. Oktawiec, J. Amtawong, M.S. Ziegler, J.P. Dombrowski, K.V. Lakshmi, W. Drisdell, J. Yano, S.J. Billinge, T. Tilley
- 10:10** Intermission.
- 10:25** **29.** Design of single-site transition metal catalysts for electrochemical oxidation of methane to methanol. **D. Primc**, J. Fornaciari, A.Z. Weber, A.T. Bell
- 10:45** **30.** Electrocatalytic small molecule transformations using multilayer films of discrete molecular catalysts. **J. Kallick**
- 11:05** **31.** Understanding structural features for rapid transport in lithium-ion batteries with niobium oxides. **M. Preefer**, R. Seshadri
- 11:25** **32.** *Operando* X-ray diffraction gives insight into the origin of pseudocapacitance in nano-MoO₂ electrodes. **D. Robertson**, Y. Yao, M. Chin, T.C. Lin, S.H. Tolbert

- 11:45** **33.** Superhydrophilic and superaerophobic metal-organic frameworks for electrocatalytic oxygen evolution. **F. Xie**, J. Ye, M. Eddaoudi, Z. Tang, Y. Han

SECTION E

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 8

Emerging Research in Molecular Synthesis

A. C. Brewer, J. M. Hoover, V. A. Schmidt, J. Y. Yang, *Organizers*
E. B. Hulley, J. Yang, *Presiding*

- 8:30** **34.** Metal carbonyl clusters as catalysts for fast H₂ evolution. **L.A. Berben**
- 9:00** **35.** To tether or not to tether: Frustration of electrophilic transition metal systems. **E.B. Hulley**, W. Christman, L. Pap, T. Morrow, N. Arulsamy
- 9:30** **36.** Developing molecular electrocatalysts and scalable systems for renewable fuels. A. Nichols, S. Hooe, C. Jiang, L. Lieske, **C.W. Machan**
- 10:00** Intermission.
- 10:15** **37.** Storing electrons and protons on redox-active ligands. **A.F. Heyduk**, B.J. Charette
- 10:45** **38.** Chemical and electrochemical studies of half-sandwich rhodium complexes supported by hybrid [P,N] ligands. **J.D. Blakemore**, J. Hopkins, D. Lionetti, V. Day

SECTION F

Marriott Marquis San Diego Marina
Solana

Main Group Chemistry

T. Hudnall, *Organizer*
M. J. Rose, *Presiding*

- 8:30** **39.** Readily available primary aminoboranes as powerful reagents for aldimine synthesis. **G.P. Junor**, E.A. Romero, X. Chen, R. Jazzar, G. Bertrand
- 8:50** **40.** Dispiro-4-bromobenzylaminophosphazenes: Synthesis reactions, spectroscopic and chromatographic properties, crystal structures, biological, and cytotoxic activities. **N. Guven Kuzey**, M. Özgür, N. Asmafiliz, L. Acik, B. Aydin, T. Hokelek, M. Turk, A. Cerci
- 9:10** **41.** New ligand protonation series of aluminum(III) complexes. **N.A. Phan**, L.A. Berben
- 9:30** **42.** Life without solvent: Mechanochemical synthesis of bulky main-group allyl species. **R.F. Koby**, T.P. Hanusa
- 9:50** **43.** Formation of well-defined strong acid sites on oxides. **D. Culver**, W. Huynh, M.P. Conley

- 10:10 Intermission.
- 10:20 **44.** Photocatalytic reactivity of tellurorhodamine chromophore derivatives towards aerobic oxidation of organic substrates. **I. Rettig**, T. McCormick, J. Van, J. Brauer, L. Lutkus, J. Lohman
- 10:40 **45.** Adventures in antimony-3d metal chemistry (Mn to Cu): NIR emission, metal deposition, and spin-orbit coupling. **M.J. Rose**, L. Taylor

SECTION G

Marriott Marquis San Diego Marina
Point Loma

Organometallic Chemistry: Catalysis - Early Transition Metals

N. S. Radu, *Organizer*

A. D. Sadow, *Presiding*

- 8:30 **46.** Zirconium complexes supported by a ferrocene-based ligand as redox switches for hydroamination reactions. **Y. Shen**, P. Diaconescu
- 8:50 **47.** Kinetics And mechanism of catalytic alumination Of 1-alkynes by rare-earth aluminates. **U. Kanbur**, **A.D. Sadow**
- 9:10 **48.** Niobium-catalyzed ether deoxyhalogenation with silicon halides. **B.F. Parker**, H. Tsurugi, J. Arnold, K. Mashima
- 9:30 **49.** Substrate determined mechanism of deoxydehydration of polyols by a Mo(VI) catalyst. **S.M. Kilyanek**, R. Tran, K.A. DeNike
- 9:50 **50.** Synthesis, structure, and reactivity of bulky isocyanides supported unsaturated chromium dianion species. **S. Wang**, J.S. Figueroa
- 10:10 **51.** Synthesis and reactivity of group 4 complexes supported by redox noninnocent anthracene-bisphenoxide ligands. **M. Bruening**, C. Low, T. Agapie
- 10:30 **52.** Homoleptic lanthanide alkyl compounds in homogeneous and interfacial hydroboration catalysis. **A.D. Sadow**
- 10:50 **53.** Ligand substituent effects on the rate of hydrocarbon C-H activation at bent-sandwich tantalum(V) trihydride complexes. **S. Rehbein**

SECTION H

Marriott Marquis San Diego Marina
Cardiff

Organometallic Chemistry: New Ligand Platforms

N. S. Radu, *Organizer*

T. S. Haddad, D. R. Manke, *Presiding*

- 8:30 **54.** Cooperative hydrogenolysis in late transition metal-aluminum heterobimetallic complexes. **R.M. Charles**, T.W. Yokley, N.J. Deyonker, T.P. Brewster
- 8:50 **55.** Synthesizing new “Pacman” ligands for renewable energy applications. **P.E. Sues**, C.A. Ackley, E.M. Archer, N.P. Marshall
- 9:10 **56.** Synthesis and characterization of 1,1'-dicarbodiimidoferocones and their group IV 1,1'-bisguanidinateferrocene complexes. **O. Esarte Palomero**, R.A. Jones
- 9:30 **57.** Electropolymerization of new N-heterocyclic carbene (NHC) complexes of Pd, Pt, Rh and Ir featuring a terthiophene backbone. **W. Wang**, R.A. Jones
- 9:50 **58.** Siloxide podand ligands as a scaffold for molybdenum catalyzed alkyne metathesis: Role of ligand flexibility and Mo-O-Si bond angle on catalyst activity. **R.R. Thompson**, P. Du, R. Kumar, S. Lee
- 10:10 **59.** Synthesis, characterization, and reactivity of iridium-aluminum and rhodium-aluminum heterobimetallic complexes. **T. Brewster**, Z. Li, R.M. Charles, T.W. Yokley, S.L. Tran, N.D. Schley, N.J. Deyonker
- 10:30 **60.** Ligand design for permanent catalytic deactivation. **T.S. Haddad**, A. Romich, J.A. Boatz, R. Blanski, K.B. Ghiassi
- 10:50 **61.** What difference does an extra CH₂ make? Oxidation chemistry of 16- and 18-atom ringed tetra-NHC iron complexes. J. DeJesus, M. Anneser, X. Powers, S.B. Isbill, K. Blatchford, S. Roy, **D.M. Jenkins**
- 11:10 **62.** Diferrocenylmercury-bridged diphosphines: Flexible ambiphilic ligands with a unique stereochemical environment. A. Tagne Kuate, R. Lalancette, **F. Jaekle**
- 11:30 **63.** Design and synthesis of a new hybrid N₂P₂ tetradentate ligand and its metal complexes. **E.E. Marlier**, S.A. Brunclik, M.H. Nevins, A. Reuter, C.M. Seong
- 11:50 **64.** Studies on phosphine ligands containing protic imidazolyl groups for the activation of O-H bonds. **B.E. Silva**, A. Sarbajna, A. Sharma, R.N. Nair, Y. Gong, J. Golen, A.L. Rheingold, D. Grotjahn
- 12:10 **65.** New tren ligands and the reactivity of their metal complexes. **D.R. Manke**
- 12:30 **66.** Sterically hindered β-diketones: Synthesis and applications in catalysis. **A.S. Crossman**, M.P. Marshak

Future Insights into Syngas Conversion Catalysis: Symposium in honor of Burtron H. Davis

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Nanoscale & Molecular Assemblies: Designing Matter to Control Energy Transport

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Advances in Catalysis with Ceria & Other Reducible Oxides

Model Ceria Catalyst

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

SUNDAY AFTERNOON – INOR

SECTION A

Marriott Marquis San Diego Marina
Santa Rosa

Inorganic Young Investigator Awards

A. De Bettencourt Dias, *Organizer, Presiding*

- 1:30** Introductory Remarks.
- 1:35** **67.** Rediscovering the crystal chemistry of higher borides. **G. Akopov**
- 2:00** **68.** Design and synthesis of heterostructured nanoparticle libraries through sequential cation exchange pathways. **J.L. Fenton**, B.C. Steimle, R.E. Schaak
- 2:25** **69.** Fundamental lessons in carbon fixation chemistry: Molybdenum-mediated reduction of C₁ oxygenates. **J.A. Buss**, T. Agapie
- 2:50** **70.** Metal–organic framework functionalization: Toward uniform and tunable heterogeneous catalysts. **P. Ji**, W. Lin
- 3:15** Intermission.
- 3:25** **71.** Comprehensive nanoscale evaluation of layered materials by X-ray microscopy. **L.R. De Jesus**, S. Banerjee, T.E. Mallouk
- 3:50** **72.** Following the catalyst wherever she goes: Forays into the fundamental behavior of active, on-cycle intermediates in Ru-catalyzed olefin metathesis. **G.A. Bailey**, D. Fogg
- 4:15** **73.** Accessing rare metal-ligand multiple bonds of early transition metals: Nucleophilic, electrophilic, and radical reactivity. **L. Grant**, D.J. Mindiola, B. Pinter
- 4:40** **74.** Understanding and redesigning metallic lithium for next-generation batteries. **Y. Liu**, D. Lin, Y. Lin, G. Chen, A. Pei, Y. Li, Y. Cui

SECTION B

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 9

Undergraduate Research at the Frontiers of Inorganic Chemistry

C. Nataro, N. S. Williams, *Organizers, Presiding*

- 1:30** Introductory Remarks.
- 1:35** **75.** Toward the synthesis of unprecedented transition-metal nitride molecules. **K.D. Herring**, G.X. Monasterio, N. Yamamoto, S.C. Addy, A.R. Sumner, A.M. Dew, M.P. Nguyen, R.J. Wilson, **L.G. Beauvais**, M. Bennett
- 1:55** **76.** Cooperative reactivity of a redox-active ditopic diazaborole. **N. Kennedy**, C. Cuthbertson, N. Torquato, D.N. Blauch, M.R. Anstey
- 2:15** **77.** Syntheses, characterization, and reactivity of cobalt(II) SNS pincer complexes. **J.R. Miecznikowski**, M. Lynn, J. Jasinski, E. Reinheimer, B.Q. Mercado
- 2:35** **78.** Evaluation of air-free glassware using the ketyl test. **L. Carlson**, E.D. Douma, P.T. Truong, M.A. Bowring
- 2:55** Intermission.
- 3:10** **79.** Amphiphilic phosphine boronates by C(sp²)–H and C(sp³)–H borylation of a diverse class of tertiary phosphines. **K.C. Morris**, S.E. Wright, H. Eichelberger, S. Richardson-Solorzano, T.B. Clark
- 3:30** **80.** Synthesis of a phenoxazine-based ligand for redox flow battery electrolytes. **C. Hernandez**, D. Thole, D.N. Blauch, M.R. Anstey
- 3:50** **81.** Water and alkyl Grignards mix for an effective cobalt-catalyzed Kumada coupling of N-aryl chlorides. **M.C. Perry**
- 4:10** **82.** Translating lessons learned in the platinum group to base metal complexes featuring sterically-demanding amine bis(phenolate) ligands. **B. Wile**
- 4:30** Concluding Remarks.

SECTION C

Marriott Marquis San Diego Marina
Marina Ballroom Salon F

Organometallics Distinguished Author Symposium

P. J. Chirik, *Organizer, Presiding*

- 1:30** Introductory Remarks.
- 1:35** **83.** Functionalizing strong C–H bonds with nonheme Fe^V=O oxidants, seen and unseen. **L. Que**
- 2:10** **84.** Efficient CO₂ reduction by bioinspired cobalt aminopyridine complexes. **S.C. Marinescu**

- 2:45 Intermission.
 3:00 **85.** Logical ligand design of iron-based complexes used as catalysts for Suzuki-Miyaura cross-coupling reactions. **J.A. Byers**, M.P. Crockett, A.S. Wong
 3:35 **86.** Metal-metal cooperativity in small molecule activations at bimetallic reaction centers. **T. Tilley**

SECTION D

Marriott Marquis San Diego Marina
 Rancho Santa Fe 2

Chemistry of Materials: Nanomaterials

C. G. Lugmair, *Organizer*
 D. Fairen-Jimenez, Z. Lin, *Presiding*

- 1:30 **87.** Design of highly porous metal-organic frameworks for drug and gene delivery. C. Orellana, S. Haddad, M. Teplensky, **D. Fairen-Jimenez**
 1:50 **88.** Syntheses of phase pure ternary layered chalcogenides of Mo and W. **M.M. Li**, S. Ivanov
 2:10 **89.** Solution-processable van der Waals thin film electronics. **Z. Lin**
 2:30 **90.** Graphene oxide aerogels as electrically-heatable, 3D frameworks for inorganic adsorbent nanoparticles. **D. Xia**, R. Menzel
 2:50 **91.** Examining the effect of nanoscale architecture on the thermal conductivity of mesoporous silica thin films. **S. King**, Y. Yan, M. Li, T. Galy, J.S. Kang, M. Marszewski, Y. Li, L. Pilon, Y. Hu, S.H. Tolbert
 3:10 Intermission.
 3:25 **92.** Gold nanobipyramids for noninvasive photothermal killing of bacteria. **C. Yang**, T. Kuo
 3:45 **93.** Fluorescent surfactant for real-time visualization and dynamics studies of boron nitride nanomaterials. **A. Smith McWilliams**, Z. Tang, S. Ergülen, C.A. de los Reyes, M. Pasquali, A.A. Marti
 4:05 **94.** Improving FePt/FePd nanoparticle synthesis for easier processing of magnetic properties. **J.A. Kurish**, S.H. Tolbert
 4:25 **95.** Sharp transition from metallic to non-metallic state in gold nanoclusters with atomically tailored optical properties. **T. Higaki**, M. Zhou, R. Jin

SECTION E

Marriott Marquis San Diego Marina
 Marriott Grand Ballroom Section 8

Emerging Research in Molecular Synthesis

A. C. Brewer, J. M. Hoover, V. A. Schmidt, J. Y. Yang, *Organizers*
 D. C. Lacy, K. J. Stowers, *Presiding*

- 1:30 **96.** Enabling base-metal catalysis through metalloligand design. **C.C. Lu**, M. Vollmer, B. Ramirez
 2:00 **97.** Catalysis at metal-metal bonds. **C. Uyeda**
 2:30 **98.** Copper-carbon interfaces: Highly active catalysts from inorganic-organic hybrid materials. **K.J. Stowers**, C. Nguyen-Sorenson, A.J. Matzger
 3:00 Intermission.
 3:15 **99.** Design principles in synthetic non-heme (di) oxygenases. **D.C. Lacy**
 3:45 **100.** Copper complexes bearing redox active ligands with tunable H-bonding interactions: Synthesis, structure, and reactivity. **I. Garcia-Bosch**

SECTION F

Marriott Marquis San Diego Marina
 Solana

Coordination Chemistry: Characterization & Applications

A. Larsen, *Organizer*
 M. I. Gonzalez, G. Mezei, *Presiding*

- 1:30 **101.** Tertiary phosphines and bisphosphines appended on N-heterocyclic moieties: Transition metal chemistry and catalytic studies. **M.S. Balakrishna**
 1:50 **102.** Nitrogen-rich metal coordination complexes for new applications in explosive initiation. **J.M. Veauthier**
 2:10 **103.** Synthesis, characterization, equilibrium, and antibacterial studies of Co(II) complex with 4-Hydroxy-N'-(3-hydroxy-5-(hydroxy methyl)-2-methylpyridin-4-yl)methylene)benzohydrazide. **V. Chittireddy**
 2:30 **104.** Tuning the anion binding selectivity of nanojars by ligand-shell rigidification and controlled acidification. **G. Mezei**
 2:50 **105.** Co₂(pyrazine-2,3-dicarboxylate)₂(4,4'-bipyridine) 1D porous coordination materials: Enhanced carbon dioxide adsorption at ambient temperature. **S. Urcia-Romero**, R. Arrieta-Perez, A.J. Hernandez
 3:10 Intermission.
 3:15 **106.** Zr/Co early-late heterobimetallic (ELHB) complexes: O₂ activation, CO₂ capture, and beyond. **H. Zhang**, C.M. Thomas
 3:35 **107.** Taming the chlorine radical: Controlling the reactivity of photogenerated chlorine-atom complexes for selective C-H activation. **M.I. Gonzalez**, D. Gygi, Y. Qin, K. Xia, L. Kramer, D.G. Nocera
 3:55 **108.** Modelling surface dinitrogen coordination with a dicobalt macrocycle. **A. Spentzos**, N.C. Tomson

- 4:15 **109.** Study of the catalytic activity of formamidinate bridged Rh₂(II,II) complexes as a function of the trans effect across the Rh–Rh bond in the axial position. **A. Millet**, C. Turro, K.R. Dunbar
- 4:35 **110.** Caught in the act: Capturing C–H bond activation with photocrystallography. **D. Gygi**, M. Gonzalez, K. Xia, S. Hwang, D.G. Nocera

- 5:10 **121.** Copper (II) selective chelators attenuate copper-overload induced oxidative stress *in vivo*. **A. Rakshit**, K. Khatua, V. Shanbhag, P. Comba, A. Datta
- 5:30 **122.** Rhenium isonitrile complexes induce unfolded protein response-mediated apoptosis in cancer cells. **S. Marker**, A.P. King, R. Swanda, J.J. Wilson

SECTION G

Marriott Marquis San Diego Marina
Point Loma

Bioinorganic Chemistry: DNA, RNA & Inorganic Drugs

S. A. Koch, *Organizer*
T. A. Su, *Presiding*

- 1:30 **111.** Photophysical evaluation of biologically active strained ruthenium(II) polypyridyl complexes. **R.S. Khnayzer**
- 1:50 **112.** Versatile roles of extracellular vesicles in cancer biology: New fluorophores as novel selective nucleic base stains for cellular microvesicles. **K. Wardhani**, A. Levina, G.E. Grau, F. Keene, J. Collins, P.A. Lay
- 2:10 **113.** Modular ionophore platform for treating copper deficiency in fatty liver disease. **T.A. Su**, C.J. Chang
- 2:30 **114.** Supramolecular assembly of uridine monophosphate (UMP) and thymidine monophosphate (TMP) with a dinuclear copper(II) receptor. **M. Rhaman**, D.R. Powell, A. Hossain
- 2:50 **115.** Interaction of DNA with reduced graphene oxides: Electrochemical oxidation of guanines. **J. Kim**, M. Choi, S. Lee
- 3:10 Intermission.
- 3:30 **116.** Synthesis and characterization of symmetrical and unsymmetrical copper(II) bis(terpyridine) complexes: Electrochemical and biological studies. **B. Sengottuvelan**, E. Tamilarasu
- 3:50 **117.** Dinuclear-ruthenium(II) complexes as binders of human telomeric dimeric G-quadruplexes. **J. Weynand**, **A. Decottignies**, **J. Dejeu**, **E. Defrancq**, **B. Elias**
- 4:10 **118.** Investigation of rhenium tricarbonyl isonitrile complexes as alternatives to platinum anticancer agents. **A.P. King**, S. Marker, J.J. Wilson
- 4:30 **119.** Oligo tetrapyrrole complexes as efficient photochemotherapeutic agents with remarkably high phototoxicity indices. A. Potocny, R. Riley, E.S. Day, **J. Rosenthal**
- 4:50 **120.** Photocytotoxicity of dirhodium (II,II) complexes featuring formamidinate bridging ligands with halogen substitution. **E. Song**, C. Turro, K.R. Dunbar

SECTION H

Marriott Marquis San Diego Marina
Cardiff

Chemistry of Materials: Metal Organic Frameworks

C. G. Lugmair, *Organizer*
M. L. Aubrey, S. K. Elsaïdi, *Presiding*

- 1:30 **123.** Mixed-metal metal–organic frameworks as multifunctional catalysts. **M. Zaheer**
- 1:50 **124.** Dual-layer MOF@MOF inorganic membranes with tunable gas transport properties for post-combustion CO₂ separation. **S.K. Elsaïdi**, M.H. Mohamed, S. Venna, D. Hopkinson
- 2:10 **125.** Small and smaller: [Pt₁₂]@ZIF-8 releases platinum nanoparticles with exceptional mass activity for oxygen electroreduction. **K. Kratzl**, B. Garlyyev, A. Bandarenka, R. Fischer
- 2:30 **126.** Highly conductive and stable metal–organic frameworks from sulfur chemistry for electrocatalysis applications. **Z. Xu**
- 2:50 **127.** Structural flexibility and tunability in heteronuclear actinide-based metal–organic frameworks (MOFs). **O.A. Ejegbavwo**, M.D. Smith, N.B. Shustova
- 3:10 Intermission.
- 3:25 **128.** Withdrawn
- 3:45 **129.** Sol–gel monolithic metal-organic frameworks with enhanced adsorption properties. T. Tian, B. Connolly, m. Casco, Z. Zeng, J. Tan, J. Silvestre Albero, **D. Fairen-Jimenez**
- 4:05 **130.** Redox doping and electron hopping in conductive metal-organic frameworks. **M.L. Aubrey**, B. Wiers, S. Andrews, T. Sakurai, S. Reyes-Lillo, S. Hamed, C. Yu, L.E. Darago, J.A. Mason, F. Grandjean, G.J. Long, S. Seki, J. Neaton, P. Yang, J.R. Long, M.I. Gonzalez, K. Pedersen, R. Clerac, J. Oktawiec, M. Kapelewski
- 4:25 **131.** MOF/polymer interactions in composite materials visualized *in situ* with solid-state NMR. **J. Moreton**, P. Duan, S. Tavares, R. Semino, G. Maurin, S. Cohen, K. Schmidt-Rohr

150 Years of the Periodic Table

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Nanoscale & Molecular Assemblies: Designing Matter to Control Energy Transport

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Advances in Catalysis with Ceria & Other Reducible Oxides

Theory of Ceria Catalysts

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SUNDAY EVENING – INOR

SECTION A

San Diego Convention Center
TBD

Learning from Nature: Earth-Abundant Metals for Oxidation Catalysis

S. S. David, T. A. Jackson, A. Mukherjee, *Organizers*

5:30 - 7:30

- 132.** Synthetic model for “diamond” core intermediates in nonheme diiron enzymes. **S. Banerjee**, W. Rasheed, L. Que
- 133.** Mechanism of olefin *cis*-dihydroxylation catalyzed by a bio-inspired non-heme iron complex. **J. Chae**, S. Xu, L. Que
- 134.** Stabilizing reactive nonheme oxoiron(IV) complexes supported by a common pentadentate ligand framework. C. Abelson, W. Rasheed, **L. Que**
- 135.** High-valent gold-hydroxo complex capable of O-H and C-H bond oxidation. **M. Lovisari**, A. McDonald
- 136.** X-ray absorption spectroscopy for elucidating the structure of high-valent nonheme iron complexes. **P. Crossland**, S. Banerjee, W. Rasheed, L. Que
- 137.** Characterization of peroxoiron(III)(TMC) complexes. **W. Ching**, L. Que
- 138.** Peeking into how aromatic hydroxylation reactions are performed by synthetic Fe^{IV}(O) complexes. **Y. Sheng**, A. Darksharapu, J. Prakash, L. Que

139. Probing internal motion of Zn(II) bispicen complexes via NMR relaxometry. **T. Jones**, A. Mukherjee

140. To rebound or not in hydrogen atom transfer reactions by synthetic nonheme oxoiron(IV) complexes. **S. Xu**, T. Jo, W. Rasheed, J.E. Klein, L. Que

141. Characterization and reactivity of [Fe^{IV}O(TPA)(L)] and [Fe^{IV}O(TQA)(L)]: Influence of the L ligand. **G.L. Tripodi**, J. Roithová

SECTION B

San Diego Convention Center
TBD

Undergraduate Research at the Frontiers of Inorganic Chemistry

C. Nataro, N. S. Williams, *Organizers*

5:30 - 7:30

- 142.** VIPeR: Community and content for the inorganic classroom. N.S. Williams, **C. Nataro**, A.K. Bentley, H.J. Eppley, E.R. Jamieson, S. Lin, A.R. Johnson, J.M. Pratt, J.R. Raker, B.A. Reisner, S.R. Smith, J.L. Stewart, L.A. Watson
- 143.** Group 13 complexes of 4,6-dihydroxy-10-phenylphenoxazine. **E. Warner**, C. Hernandez, D. Thole, D.N. Blauch, M.R. Anstey
- 144.** Suzuki coupling catalyzed by (8-(dimesitylboryl)quinoline)palladium(0) species: Theoretical analysis. **H.S. Rust**, A.J. Achazi, P. Miro
- 145.** Synthesis of nickel nitrosyl complexes with bidentate N-heterocyclic carbene ligands. **Z. Zhang**, S.E. Stieber
- 146.** Heteroatom pendant bases for ruthenium catalyzed water oxidation. **B.D. Vincenzini**, A.G. Nash, C.J. Breyer, B.E. Silva, D.B. Grotjahn
- 147.** Stability of molecular-electrode conjugates in acids and bases. **S.K. Spence**, L. Hallett, S.M. Kilyanek
- 148.** Synthesis and characterization of metal-organic framework hydrogel composites. **S. Klein**, L. Zarzar, Y. Liu
- 149.** Unique crystalline composites displaying multiple primary zoning events in the solid state and based upon self-assembled coordination polymers: Summary of results. **S.R. Seidel**, A. Zamurd, S. Cornell, K. Godwin, A. Partelow
- 150.** Investigation of strontium doped hydroxyapatite coating methods for iron oxide nanoparticles. **C.E. Chamberlain**, K. Libson, A. Washburn, A.L. Eckermann
- 151.** Tuning magnetic coupling in organic radical-bridged lanthanide single molecule magnets. **E. Mu**, C. Gould, J.R. Long

- 152.** Optimization of light-driven P450 biocatalysts featuring Ru(II)-polypyridine complexes. **B. Foley, M. Nguyen**, M. Kato, L.E. Cheruzel
- 153.** Synthesis of a gallium metallocavitand nanoparticle for bacterial inhibition. **B.M. Forry**, W.D. Shafer

SECTION C

San Diego Convention Center
TBD

Electrochemistry

N. S. Radu, *Organizer*

5:30 - 7:30

- 154.** Electrochemical behaviors of MnBr(CO)₃bpy-COOH in aqueous solution. **D. Zheng**, L. Sepunaru, P.C. Ford
- 155.** Reversible Na-capacity of magnesium-reduced graphitic carbon nitride. B.D. Fahlman, **A.S. Adeyemi**
- 156.** Reversible Li- and Na-capacities of BaTiO₃/p-Si/g-C₃N₄ nanocomposites. B.D. Fahlman, **M.L. Anger**
- 157.** Proton-coupled electrochemistry of catechol-based redox active deep eutectic solvents. **H. Booth**, J.C. Goeltz
- 158.** High concentrations of electroactive TEMPOL in various ionic melts. **J.M. Carter**, J.C. Goeltz

SECTION D

San Diego Convention Center
TBD

Emerging Research in Molecular Synthesis

N. S. Radu, *Organizer*

5:30 - 7:30

- 159.** Synthesis of cyclopropanes using nickel-catalyzed cross-electrophile coupling reactions. **A. Castro**, E. Lucas, K.A. Hewitt, E.R. Jarvo
- 160.** Measuring the influence of metal ion on hydrogen atom reactivity in a series of group 10 complexes with a proton and redox non-innocent ligand. **B. Charette**, A.F. Heyduk
- 161.** Probing promoter effects in E selective alkyne semi-hydrogenation. **S. Desai**, J. Ye, T. Islamoglu, O.K. Farha, D.G. Truhlar, C.C. Lu
- 162.** Development of molecular electrocatalyst for CO₂ reduction based on nitrogen-based macrocyclic ligands. **L. Lieske**, C.W. Machan
- 163.** Electrocatalytic reduction of dioxygen to hydrogen peroxide by a molecular manganese complex with a bipyridine-containing Schiff base ligand. **S.L. Hooe**, A.L. Rheingold, C.W. Machan, D. Dickie

- 164.** Electrocatalytic CO₂ reduction with Fe(III) Schiff base-type complexes containing pendent proton relays. **A. Nichols**, S. Hooe, C.W. Machan

SECTION E

San Diego Convention Center
TBD

Inorganic Catalysts

S. A. Koch, *Organizer*

5:30 - 7:30

- 165.** Homogeneous reduction of atmospheric carbon dioxide by a neutral zinc complex. **S. Cronin**, m. mashuta, M.J. Shaw, R. Buchanan, C.A. Grapperhaus
- 166.** Product and active site studies of biocatalytic copper-based metal-organic frameworks. **R. Tuttle**, H. Rubin, C. Rithner, R.G. Finke, M.M. Reynolds
- 167.** Synthesis of air-stable ruthenium and nickel catalysts. **S. Phuangthong**, J.P. Lanorio
- 168.** Modification of inorganic catalysts' ligand frameworks for connection to polymeric structures. **V.C. Tafuri**, D. Navarro, H. Ordon, M.R. Radlauer
- 169.** Toward (Z)-alkene isomerization. **E. Delgado**, E.R. Paulson, A.L. Rheingold, D.B. Grotjahn
- 170.** Computational study of the pKa of transition metal-methyl C-H bonds. **W.M. Grumbles**, T.R. Cundari
- 171.** Niobium-doped TiO₂: Effect of an interstitial oxygen atom on charge state of niobium. **X. Liu**
- 172.** Withdrawn
- 173.** Seed-induced synthesis of functional MFI zeolite materials: Method, mechanism, and catalytic property. **H. Zhang**, Z. Ye, Y. Tang
- 174.** Alkali metal-doped series of Linde-Type L zeolites via hydrothermal processes. **Y. Koh**, W.D. Shafer
- 175.** Transition metal dichalcogenides as heterogeneous catalysts for the hydrogenation of nitroarenes. **A. Darling**, Y. Sun, R.E. Schaak
- 176.** Exploring salen ligand type inspired from purple-acid phosphatase towards catalyzing pesticides hydrolysis with zinc complexes. **M.M. Allard**, N.T. Le
- 177.** Zr- and Hf-based polyhedral oligomeric silsesquioxanes (POSS) as thermally robust catalysts in the Meerwein-Ponndorf-Verley reduction. **S. Garg**, C. Krempner
- 178.** Molecular catalysts for CO₂ reduction to CO. **A. Zhanaidarova**, C.P. Kubiak
- 179.** Ferrocene-chelating heteroscorpionate complexes in catalysis. **N. Adhami**

180. Photophysical properties of rhenium(i) diimine dicarbonyl complexes containing phenanthroline and bipyridine ligands. **H. Atallah**, F.N. Castellano, C.M. Taliaferro

181. Solid-state NMR and density functional theory approaches for the elucidation of structure for inorganic complexes. **W. Huynh**, D. Culver, M.P. Conley

SECTION F

San Diego Convention Center

TBD

Chemistry of Materials

C. G. Lugmair, *Organizer*

5:30 - 7:30

182. Hydrothermal crystal growth and characterization of rare earth rhenium and tungsten oxides.

M.T. Kolambage, C.D. McMillen, J.W. Kolis

183. Generalizable top-down nanostructuring method of bulk oxides: Sequential oxygen-nitrogen exchange reaction. **H. Kim**, J. Bang

184. Incorporating excess lithium into LiMn_2O_4 via thermally induced grain fining: Promoted lithium-ion diffusion in Li-excess LiMn_2O_4 . **G. Lee**, J. Bang

185. Highly conductive and stretchable nanocomposite using Ag-Au core-shell nanowires: Applications in wearable and implantable devices.

S. Han, T. Hyeon

186. Two polymorphs of 4,4',5,5'-tetraamino-3,3'-bi-1,2,4-triazolium dinitroformate and their energetic properties. **Y. Xu**, M. Lu

187. Solid-phase detoxification of chemical warfare agents using zirconium-based metal organic frameworks and the moisture effects—analyze via digestion. **H. Wang**, J.J. Mahle, T.M. Tovar, G.W. Peterson, M.G. Hall, J.B. DeCoste, J. Buchanan, C.J. Karwacki

188. Synthesis and electrochromic properties of morphology-controlled vanadium dioxide nanoparticles. **D. Roh**

189. Single-component frameworks for heterogeneous catalytic hydrolysis of organophosphates in pure water. **S. Garibay**, O.K. Farha, J.B. DeCoste

190. Defect-free MOF-based mixed matrix membranes obtained by corona crosslinking. **Y. Katayama**, K.C. Bentz, S. Cohen

191. Heterometallic multinuclear metal-organic frameworks. **O.A. Ejegbavwo**, N.B. Shustova

192. Sierpinski molecules, carbon schwarzites and porous materials for catalytic and electronic applications. **Z. Xu**

193. Hybrid polymer/inorganic nanoparticle composite nanofibers through cooperative non-covalent interactions. **L. Meng**, Y. Qin

194. Charge-separated metal-organic frameworks: Design and application. **S. Thapa**, Y. Qin

195. Exploring O_2 adsorption in cobalt triazolate frameworks. **J. Oktawiec**, H.Z. Jiang, J. Vitillo, D. Reed, L.E. Darago, B.A. Trump, V. Bernales, H. Li, K. Colwell, H. Furukawa, C.M. Brown, L. Gagliardi, J.R. Long

196. Chemical vapour deposition of zinc oxysulfide for photovoltaics. **M.A. Bhide**, C.J. Carmalt, C.E. Knapp

197. Montmorillonite synthesized from natural bentonite. **S. Seo**, J. Kim

198. Effect of heavy atom on the photophysics of porphyrin coordination complexes. **A. Aggarwal**, C. Farley, C.M. Drain

199. Improving PbS QD SWIR photodetectors using thermal annealing. J. Jin, **G. Hwang**

200. Development of the facile ITO coating method on flexible substrates using PDMS (polydimethylsiloxane) nanostructures and the spin-coating approaches. **H. Seo**, S. Sul, S. Lee, S. Chae, J. Jung

201. Seeded growth of metal nitrides on noble metal nanoparticles to form complex nanoscale heterostructures. **R.W. Lord**, C.F. Holder, J.L. Fenton, R.E. Schaak

202. Selective post-synthetic modification of copper sulfide regions in heterostructured nanoparticles. **A.G. Butterfield**, B.C. Steimle, R.E. Schaak

203. Synthesis, structures and properties of some recently characterized borates. **D. Neiner**, Y. Sevryugina, D.M. Schubert

204. Engineering metastable precursors of two-dimensional MBenes. **L. Alameda**, R.E. Schaak

205. Novel electrospun $\text{Ti}_3\text{C}_2\text{Tx}$ MXene titania nanocomposites. **S. Debow**, **B.G. DeLacy**, W.R. Creasy, Y. Gogotsi, K. Maleski, D. Kuhn, Z. Zachary

206. Nanoballs featuring Lewis acidic and basic sites as efficient bifunctional catalysts for tandem deacetalization-Knoevenagel reaction. **G. Verma**, S. Kumar, Z. Niu, W. Gao, L. Wojtas, S. Ma

207. New crystalline porous materials and their gas sorption properties. **X. Bu**, H. Yang, P. Feng

Organometallic Chemistry: Catalysis

N. S. Radu, *Organizer*

5:30 - 7:30

- 208.** DFT study of double bond cleavage induced by silyl migration in Fe complex. **N. Koga**, A.A. Dahy
- 209.** Computational study of methane C-H activation by main group and mixed main group-transition metal complexes. C. Carter, **T.R. Cundari**
- 210.** Colloidal DMF-protected metal nanoparticles for their use as catalyst in organic transformations. **Y. Obora**
- 211.** Indium and yttrium alkoxide catalysts for redox switchable ring opening polymerization. **S. Deng**, P. Diaconescu
- 212.** Phosphines on sulfated zirconia: Probes for Brønsted acidity and precursors to catalytically active olefin polymerization sites. **J.E. Rodriguez**, M.P. Conley
- 213.** Manganese-catalyzed transfer hydrogenation of nitriles with secondary alcohols as the hydrogen source. **J.A. Garduno**, J.J. Garcia
- 214.** Incorporating iridium pincer complexes in polymeric scaffolds for site-isolated catalytic alkane dehydrogenation. **J. Hickey**, T.Z. Myint, M.R. Radlauer
- 215.** High efficient pincer oxo-rhenium catalyst for hydrosilylation. **M. Xiong**, M. Abu-Omar
- 216.** Bioinspired trimetallic cobalt triphenylhexathiol complex for CO₂ reduction reaction. **J. Intrator**, N.M. Orchanian, A.J. Clough, S.C. Marinescu

Organometallic Chemistry: Applications to Materials & Polymer Science

N. S. Radu, *Organizer*

5:30 - 7:30

- 217.** Incorporation of functionalized rhenium(I) bipyridine catalysts into polycarbonates via chain transfer chemistry. **G. Bhat**, T.M. Folsom, A.Z. Rashad, D.J. Darensbourg
- 218.** Synthesis and chemical vapour deposition of precursors to zinc oxysulfide. **M.A. Bhide**, C.J. Carmalt, C.E. Knapp

Bioinorganic Chemistry

S. A. Koch, *Organizer*

5:30 - 7:30

- 219.** Better resolution of hyperfine lines for high-spin cobalt at low frequency, L-band: [Co(D4)(dca)]. S. Hernández-Anzaldo, A.K. Girón Moreno, Y. Reyes-Ortega, **W.E. Antholine**
- 220.** Interplay of folding, reduction potential, and tryptophan fluorescence in azurin variants. **N.J. McCormick**, A. Cembran, S.M. Berry
- 221.** Oxidation of phenols by redox-active copper complexes with tunable hydrogen bonding donor groups. **K. Rajabimoghadam**, I. Garcia-Bosch
- 222.** Metal oximate and amidoximate complexes for the catalytic cleavage of carboxylic and phosphate esters. E. Alpízar-Juárez, **P. Gomez-Tagle**
- 223.** Diastereomeric suite of triscatecholate siderophores: Origin and physiological relevance of Fe(III)-complex chirality. **P. Stow**, Z. Reitz, E. Thomsen, A. Butler
- 224.** Reactive intermediates in multicopper oxidase catalysis. **J. Shin**, J.R. Winkler, H.B. Gray
- 225.** Combined molecular dynamics and quantum mechanical/molecular mechanical studies on histone demethylation by KDM4A enzymes. **R. Ramanan**, S.S. Chaturvedi, T. Karabencheva-Christova, C. Christov
- 226.** Influence of ligand structure and stereochemistry on the photoreactivity of Fe(III)-siderophore complexes containing β-hydroxyaspartic acid. **C.D. Hardy**, J. Suk, A. Butler
- 227.** Computational insights into catalytic mechanism of Nε-methyl lysine demethylation by PHF8. **S.S. Chaturvedi**, R. Ramanan, T. Karabencheva-Christova, C. Christov
- 228.** Exploring the mechanism of DNA repair by ALKBH2 enzyme: Multilevel modeling study. **S.O. Waheed**, R. Ramanan, C. Christov, T. Karabencheva-Christova
- 229.** Long wavelength light induced CO-release from binuclear rhenium–manganese carbonyl complex. **X. Jiang**, **J. Barrett**, **P.C. Ford**
- 230.** Application of graphene quantum dots for NIR light triggered intracellular release of nitric oxide. **C. Guzman**, P. Huang

SECTION A

Marriott Marquis San Diego Marina
Marina Ballroom Salon F

ACS Award in Pure Chemistry: Symposium in Honor of Danna Freedman

H. Karunadasa, J. Zadrozny, *Organizers, Presiding*

- 8:30 Introductory Remarks.
- 8:35 **231.** Platform-based surface ligands for inorganic nanocrystals. **J.A. Mason**, G. Stec, S. Thapa, J. Lee
- 9:00 **232.** Organic mixed-valency across a five charge states of group 13 complexes. A. Arnold, R. Saylor, D. Britt, T. Bass, **L.A. Berben**
- 9:25 **233.** Chalcogenide based coordination polymers. **J.S. Anderson**, J. Xie, N. Horwitz
- 9:50 Intermission.
- 10:05 **234.** Stibonium cations as Z-type ligands for late transition metals: Impact on catalytic properties. **F.P. Gabbai**
- 10:30 **235.** Efficient single molecule dirhodium photocatalyst for H₂ generation using low energy visible to near-IR light. T.J. Whitemore, C. Xue, **C. Turro**
- 10:55 **236.** Metal semiquinoid magnets: From molecules to materials. L. Liu, J. DeGayner, B. Coleman, Y. Wang, A.E. Thorarinsdottir, I. Jeon, **D. Harris**
- 11:20 **237.** Nickel-catalyzed coupling promoted by substrate photoexcitation. **J.A. Kalow**
- 11:45 Concluding Remarks.

SECTION B

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 9

Learning from Nature: Earth-Abundant Metals for Oxidation Catalysis

Financially supported by INOR
S. S. David, A. Mukherjee, *Organizers*
T. A. Jackson, *Organizer, Presiding*

- 8:30 **238.** Molecular catalysts for water oxidation using first-row transition metals. **G.W. Brudvig**, K.J. Fisher, H.M. Lant, T. Michaelos, L.S. Sharninghausen, R.H. Crabtree
- 9:00 **239.** *Operando* X-ray spectroscopic studies of heterogeneous water oxidation catalysts. **S. DeBeer**
- 9:30 **240.** Molecular complexity in inorganic chemistry: Utilizing non-covalent interactions into the molecular designs of metal complexes. **A. Borovik**
- 10:00 Intermission.

- 10:10 **241.** Mechanistic and structural analysis of how nonheme-iron enzymes direct different oxidation reactions. **J.M. Bollinger**, A. Boal, C. Krebs, A. Silakov
- 10:40 **242.** Oxygen intermediates in Cu and Fe zeolites: Correlations to metalloenzymes. **E.I. Solomon**, B.E. Snyder, H.M. Rhoda
- 11:10 **243.** MUTYH & its metal cofactors: Mitigating menacing mutations and mediating DNA damage responses. **S.S. David**

SECTION C

Marriott Marquis San Diego Marina
Solana

Inorganic Chemistry Lectureship

W. B. Tolman, *Organizer, Presiding*

- 8:30 Introductory Remarks.
- 8:35 **244.** Gold (I) anticancer agents: Building blocks for the synthesis of bimetallic compounds, bioconjugates and nanocarrier payloads. Preclinical studies. **M. Contel**
- 9:05 **245.** Nanoparticles and polymer-based nanozymes: Harnessing the power of transition metal catalysis for bioorthogonal chemistry. **V.M. Rotello**
- 9:35 **246.** Iridium luminescent gold nanoparticles in bioimaging and detection. S. King, S. Claire, I. Theofilou, T. Chauhan, R. Bicknell, S. Botchway, P. Murray, **Z. Pikramenou**
- 10:05 Intermission.
- 10:20 **247.** Radiometal-based radiopharmaceuticals for cancer imaging. **J. Lewis**
- 10:50 **248.** Metallo-supramolecular DNA and RNA recognition combined with nanoscience to achieve bioactivity. **M.J. Hannon**
- 11:20 **249.** Unveiling the beauty of gold for biomedical applications: From molecular to supramolecular inorganic chemistry. **A. Casini**
- 11:50 Concluding Remarks.

SECTION D

Marriott Marquis San Diego Marina
Rancho Santa Fe 2

Inorganic Chemistry for Sustainable Energy & Environment

L. A. Berben, *Organizer*
C. P. Kubiak, *Presiding*

- 8:30 **250.** Fractionation of biomass and upgrading of lignin and cellulose streams. **M.M. Abu-Omar**, J. Truong, R. Nishide, B. Liu, S. Zhao

- 9:00** 251. Approaches to the synthesis of weak chemical bonds and application to the synthesis and oxidation of ammonia. **P.J. Chirik**
- 9:30** 252. Molecular control of interfacial energy catalysis. M. Jackson, C.J. Kaminsky, S. Oh, M. Pegis, J. Rosenberg, P. Smith, **Y. Surendranath**
- 10:00** Intermission.
- 10:20** 253. Nitrate-mediated photooxidation of alcohols on CdS nanowires. **B.M. Bartlett**
- 10:50** 254. Managing reactivity of hydrides in CO₂ reduction to formate. **L.A. Berben**
- 11:20** 255. Carbon dioxide mineralization: Strategy for the provision of building materials, and for carbon management globally. **G.N. Sant**, E. Callagon La Plante, D. Jassby, M. Bauchy, D. Simonetti

SECTION E

Marriott Marquis San Diego Marina
Santa Rosa

Emerging Research in Molecular Synthesis

A. C. Brewer, J. M. Hoover, V. A. Schmidt, J. Y. Yang,
Organizers
M. Dai, C. Roberts, *Presiding*

- 8:30** 256. Nickel-catalyzed stereospecific cross-coupling and cross-electrophile coupling reactions. **E.R. Jarvo**
- 9:00** 257. Understanding the mechanism of nickel catalyzed cross-coupling and cross-electrophile coupling reactions. **N. Hazari**
- 9:30** 258. Using first row transition metals for challenging bond breaking and forming reactions. **C. Roberts**, M.S. Sanford
- 10:00** Intermission.
- 10:15** 259. Building structural complexity via novel palladium-catalyzed carbonylative reactions. **M. Dai**
- 10:45** 260. Novel pyridine-modified 12-membered pyridinophane ligands control iron catalyzed C-C coupling reactivity. **K.N. Green**, M. Mekhail, A. Yepremyan

SECTION F

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 8

Electrochemistry

N. S. Radu, *Organizer*
J. C. Goeltz, J. A. Maurer, *Presiding*

- 8:30** 261. Unique interfacial thermodynamics of few-layer 2D MoS₂ for (photo)electrochemical catalysis. **M. Carroll**

- 8:50** 262. Mechanism of copper dissolution by nitric acid: Unraveling a century of hypotheses. **R. Carlson**, P. Yang, S.M. Clegg, E.R. Batista
- 9:10** 263. Core-shell structured zero-valent manganese (ZVM)-sulfur nanohybrid materials for superior performance supercapacitor. K. Jena, **S. Al Hassan**
- 9:30** 264. Immobilization of a molecular proton reduction catalyst onto high-surface area silicon photoelectrodes. **C. Hanna**, N.R. Neale, J.Y. Yang
- 9:50** 265. Proton-coupled and proton-independent redox active deep eutectic solvents. **J.C. Goeltz**
- 10:10** 266. High voltage redox flow batteries: Shattering the kinetic stability window of aqueous electrolyte. **M.P. Marshak**, B.H. Robb, J.M. Farrell
- 10:30** 267. *In situ* nanostructuring and stabilization of polycrystalline copper electrodes with organic salt additives promotes CO₂ reduction to ethylene. **A. Thevenon**, A. Rosas-Hernández, J. Peters, T. Agapie
- 10:50** 268. Effects of solution pH and film thickness on electrocatalytic CO₂ reduction activity by polymer encapsulated cobalt phthalocyanine. **T. Soucy**, C.C. McCrory
- 11:10** 269. Electrodeposition of refractory metals from deep eutectic solvents. **J.A. Maurer**
- 11:30** 270. Fine tuning HER and CO₂RR reaction dynamics via co-substrate addition to Fe tetraphenyl porphyrin. **C.G. Margarit**, C. Costentin, D.G. Nocera
- 11:50** 271. Electrochemical and electrocatalytic analysis of Ru(II) complexes with redox-active S₂N₂ ligands: Applications towards CO₂ reduction. **J.A. Luna**, K.D. Spielvogel, S.M. Loria, F.B. Evans, L.P. Weisburn, G. Durgaprasad, J.M. Keith, M.R. Ringenberg, S.K. Shaw, S.R. Daly

SECTION G

Marriott Marquis San Diego Marina
Point Loma

Organometallic Chemistry: Catalysis - Late Transition Metals

N. S. Radu, *Organizer*

- 8:30** 272. Proton coupled electron transfer by a gold(III)-hydroxide complex. **M. Lovisari**, A. McDonald
- 8:50** 273. Nickel-mediated activation of N-H and O-H bonds. **P. Zhao**, S. Acharya, R.S. Manan
- 9:10** 274. Nickel-catalyzed cross-electrophile coupling reaction of mesylates for cyclopropane synthesis. **T.A. Thane**, A. Sanford, T. McGinnis, E.R. Jarvo
- 9:30** 275. Robust and efficient iridium catalysts having pyridylpyrazole ligands for dehydrogenation of formic acid. **Y. Himeda**, N. Onishi, R. Kanega, E. Fujita

- 9:50 276.** New catalytic route to dehydrogenate alkanes by PCP-pincer iridium complexes using proton and electron acceptors. **A. Shada**, A.S. Goldman
- 10:10 277.** Alkyne hydroarylations catalyzed by low-valent, co complexes: Mechanism and catalysis. **B.A. Suslick**, T. Tilley
- 10:30 278.** Olefin hydroarylation catalyzed by palladium(II) catalysts: Investigation of the reaction selectivity and comparison with Rh catalysts. **X. Jia**, A. Foley, W. Zhu, B.A. Vaughan, B.A. McKeown, T.B. Gunnoe
- 10:50 279.** Chemical innovation at heraeus precious metals: Case studies of process and performance improvements from product development. **P.B. Kettler**, R. Walter, P. Walter, M. Gock
- 11:10 280.** Observation of a photogenerated nitrenoid intermediates in C–H amination. **D.C. Powers**
- 11:30 281.** Environmentally friendly rhodium(I) model catalysts. Z.G. Morerwa, A. Roodt, **G.J. Venter**

SECTION H

Marriott Marquis San Diego Marina
Cardiff

Coordination Chemistry: Synthesis & Characterization

A. Larsen, *Organizer*
J. England, K. V. Waynant, *Presiding*

- 8:30 282.** Bio-inspired approach to ligand design: Folding single-chain peptoids to chelate a multimetallic cluster. **A.I. Nguyen**, R.K. Spencer, R.N. Zuckermann
- 8:50 283.** Structure study of uranyl bisphosphonate-based ligands as potential uranium decorporation agents. **G. Ye**
- 9:10 284.** Electron transfer studies of tris(*N*-arylacetamide) metal complexes. **A.F. Cannella**, D.C. Lacy
- 9:30 285.** Building a better understanding of binding in redox-active arylazothioformamide ligand systems. **K.V. Waynant**, J. Moberly, M.F. Roll, K.L. Gutman, V. Groner
- 9:50 286.** Tetranuclear transition metal clusters with direct metal-metal interactions: Synthesis, electronic structure, and magnetism. **K. Chakarawet**, J. Marbey, S. Hill, J.R. Long
- 10:10** Intermission.
- 10:15 287.** Carbodicarbene ligand redox noninnocence in highly oxidized first-row transition metal complexes. **J. England**
- 10:35 288.** Synthesis and characterization of homobimetallic redox-active macrocycle transition metal complexes with increasing pocket size. **L.M. Thierer**, P. Cui, S. Brooks, Q. Wang, S. Zhang, M. Gau, B. Manor, P. Carroll, N.C. Tomson

- 10:55 289.** Tuning properties of coordination cages via ligand functionalization. **G.A. Taggart**
- 11:15 290.** Linear cobalt(II) dialkyl complex with a non-Aufbau ground state and very large magnetic anisotropy. **P. Bunting**, M. Atanasov, E. Damgaard-Møller, M. Perfetti, I. Crassee, M. Orlita, J. Overgaard, J. van Slageren, F. Neese, J.R. Long
- 11:35 291.** Spectroscopic and photochemical investigations of a thiolate-bridged dinuclear Rh(II,II) complex featuring reversible redox events. **R.P. Coll**, B.S. Dolinar, K.R. Dunbar

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MONDAY AFTERNOON – INOR

SECTION A

Marriott Marquis San Diego Marina
Marina Ballroom Salon F

ACS Award in Pure Chemistry: Symposium in Honor of Danna Freedman

H. Karunadasa, J. Zadrozny, *Organizers, Presiding*

- 1:30** Introductory Remarks.
- 1:35 292.** Lanthanide-based single-molecule magnets with high blocking temperatures. C. Gould, P. Bunting, A. Vincent, S. Demir, K.R. McClain, L. Darago, K. Chakarawet, M. Gonzalez, K.R. Meihaus, J. Zadrozny, M. Nippe, J.D. Rinehart, S. Teat, B.G. Harvey, W.J. Evans, **J.R. Long**
- 2:00 293.** Control of magnetic relaxation via spin bath design. **J. Zadrozny**
- 2:25 294.** Halide perovskites under pressure. A. Jaffe, Y. Lin, W. Mao, **H. Karunadasa**
- 2:50 295.** Developing a mild and modular route to chemically modified electrodes for photoelectrochemical cells. C. Hanna, **J.Y. Yang**
- 3:15** Intermission.
- 3:30 296.** Tunable metal oxide materials via assembly of $[\text{NaP}_5\text{W}_{30}\text{O}_{110}]^{14-}$. **A.M. Schimpf**

- 3:55 297. Making flexible, transparent electronic devices a reality: Organic polymers, heterojunctions, oxides and beyond. **T.J. Marks**
- 4:20 298. On the selectivity of the reduction of CO₂ on gold electrodes. **D.G. Nocera**
- 4:45 Concluding Remarks.

SECTION B

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 9

Learning from Nature: Earth-Abundant Metals for Oxidation Catalysis

S. S. David, T. A. Jackson, *Organizers*
A. Mukherjee, *Organizer, Presiding*

- 1:30 299. New insights into oxidation catalysis with copper. **M.T. Kieber-Emmons**, D. Ramirez, P. VanNatta, G. Ali, A. Velarde
- 1:55 300. Geometric and electronic structure contributions to reactivity of Mn–oxygen intermediates. **T.A. Jackson**, J. Parham, M. Denler
- 2:20 301. Copper(I)-dioxygen adduct stabilization and substrate oxidative reactivity. **K.D. Karlin**
- 2:50 302. Reactivity of an alkyl thiolate-ligated Fe^{III}-superoxo intermediate derived from dioxygen. **J. Kovacs**, M.N. Blakely, M.A. Dedushko, P. Poon, A. Downing, D. Rogers, P. Gannon
- 3:20 Intermission.
- 3:30 303. Going a step beyond nature: Catalyzing aldehyde deformylation with a non-enzymatic metal. **C.R. Goldsmith**, A.C. Saunders
- 3:55 304. Intermediates in aromatic hydroxylation catalyzed by a Rieske monooxygenase. M.S. Rogers, **J.D. Lipscomb**
- 4:25 305. Differentiating between radical rebound hydroxylation versus H-atom transfer with non-heme iron(III)-hydroxo complexes. **A.R. Fout**, M.J. Drummond
- 4:50 306. Site and enantioselective C-H oxidations inspired in nature. M. Milan, M. Scianfanelli, A. Palone, G. Olivo, X. Ribas, M. Bietti, **M. Costas**
- 5:20 307. Cu-promoted hydroxylation of sp² and sp³ C–H bonds: From enzyme modeling to synthetic applications. **I. Garcia-Bosch**

SECTION C

Marriott Marquis San Diego Marina
Solana

Inorganic Nanoscience Award Symposium

J. Millstone, *Organizer, Presiding*

- 1:30 308. Plasmonic metal oxide nanocrystals. **D.J. Milliron**
- 2:15 309. Details of ligands on nanocrystal surfaces. **C.J. Murphy**
- 2:45 310. Inverse design of interactions for assembly. **T. Truskett**
- 3:15 311. Exploiting interfacial assemblies of nanoparticle surfactants to design reconfigurable materials and devices. **B. Helms**, W. Feng, J. Forth, T.P. Russell
- 3:45 Intermission.
- 4:00 312. Prospects and challenges for unity quantum yield nanocrystal lumophores. **P. Alivisatos**
- 4:30 313. Synthesis of multi-component nanocrystals and their application as catalysts to store energy in chemicals. **R. Buonsanti**
- 5:00 314. Dopants and defects in colloidal semiconductor nanocrystals. **D.R. Gamelin**

SECTION D

Marriott Marquis San Diego Marina
Rancho Santa Fe 2

Inorganic Chemistry for Sustainable Energy & Environment

L. A. Berben, *Organizer, Presiding*

- 1:30 315. Selective reduction of CO₂ to water by molecular catalysts attached to carbon surfaces. **C.P. Kubiak**, A. Zhanaidarova
- 2:00 316. Sustainable and renewable carbon and nitrogen cycles for fuel and crop production. **D.G. Nocera**
- 2:30 317. Advances and research challenges in chemical and materials research for renewable energy conversion, storage, and utilization. **W. Tumas**
- 3:00 Intermission.
- 3:20 318. Mechanisms for the activation of supported oxometal complexes for olefin metathesis. **S.L. Scott**, F. Zhang, L. Li, C. Vandervelden, B. Peters
- 3:50 319. Conductive metal-organic frameworks for electrocatalytic H₂ evolution. **S.C. Marinescu**
- 4:20 320. Mechanistic studies of technologically-relevant dye-sensitized and cocatalyst-containing photocatalytic materials. J.M. Cardon, W. Gaieck, K. Tkaczibson, N. Farhang, S. Keene, S. Luo, H. Chen, **S. Ardo**

4:50 321. Controlling the electrocatalytic reduction of O_2 to H_2O/H_2O_2 using nontraditional porphyrinoid scaffolds. Q. Cai, J. Eddy, T. Qiu, **J. Rosenthal**

4:15 Intermission.

4:25 332. Coherent electronic dynamics in atomically precise nanoclusters. **K.L. Knappenberger**

SECTION E

Marriott Marquis San Diego Marina
Santa Rosa

Emerging Research in Molecular Synthesis

A. C. Brewer, V. A. Schmidt, J. Y. Yang, *Organizers*

J. M. Hoover, *Organizer, Presiding*

I. Tonks, *Presiding*

- 1:30 322.** Cross-electrophile coupling to form Csp^3 - Csp^2 bonds. **D.J. Weix**
- 2:00 323.** Cross-coupling with three components and in three dimensions. **K.M. Engle**
- 2:30 324.** Unraveling the mechanism of catalytic decarboxylative coupling reactions. **J.M. Hoover**
- 3:00** Intermission.
- 3:15 325.** Complex molecule synthesis via the enantioselective hydroformylation/hydroacylation/aldol sequence. **C.R. Landis**
- 3:45 326.** Incorporating aryne chemistry into Ti redox catalytic reactions: Ti-catalyzed synthesis of substituted naphthalenes via *in situ* generated arynes. **I. Tonks**, B. Reiner
- 4:15 327.** Identifying catalysts and reactor conditions for tailored polymer rheology. **S.E. Smith**, A. Mohan, G. Kiss, J.M. Soulages

SECTION F

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 8

Surface Chemistry & Structure in Ligand Protected Nanoparticles

C. J. Johnson, *Organizer*

B. Lear, *Organizer, Presiding*

- 1:30** Introductory Remarks.
- 1:35 328.** Atomically precise gold nanoclusters: Surface structure and implications. **R. Jin**
- 2:20 329.** Atomically-precise nanocluster electronic structure and reactivity from atomically-impure syntheses. **C.J. Johnson**, A. Cirri, H. Morales, C. Kmiotek
- 2:50** Intermission.
- 3:00 330.** Effects of surface structure on the chirality and luminescence of thiolate- and phosphine-stabilized gold nanoclusters. **C.M. Aikens**
- 3:45 331.** Chemical control over the electronic structure of discrete gold nanoclusters: Effects of composition, ligand, and solvent environment. **A. Cirri**, H. Morales, C. Kmiotek, C.J. Johnson

SECTION G

Marriott Marquis San Diego Marina
Point Loma

Charge & Substrate Transport in 3D Electrocatalytic Materials

Cosponsored by CATL and ENFL

A. Hall, C. C. McCrory, *Organizers*

V. Thoi, *Organizer, Presiding*

- 1:30** Introductory Remarks.
- 1:35 333.** Designing catalysts for water splitting based on electronic structure considerations. **S. Banerjee**
- 2:00 334.** How do interactions between protic cations and polarized bismuth cathodes control the pathway of CO_2 reduction?. **J. Rosenthal**
- 2:25 335.** Accessing 3-D in transition-metal phosphide catalysts for water splitting: Challenges and opportunities. C. Acquah, S. Mutinda, R. Liyanage, D. Li, **S.L. Brock**
- 2:50 336.** Modulating electrode-electrolyte interfaces for energy conversion reactions. **V. Thoi**
- 3:15** Intermission.
- 3:30 337.** Water electrolysis on metal oxides for energy conversion: Materials and mechanisms. **P. Strasser**
- 3:55 338.** Interfacing metals and compounds for enhancing hydrogen electrochemistry. **Y. Sun**
- 4:20 339.** Tailoring the surface of metal nanoparticles for selective electrocatalysis. **C.W. Li**

SECTION H

Marriott Marquis San Diego Marina
Cardiff

Lanthanide & Actinide Chemistry

A. De Bettencourt Dias, *Organizer*

K. Carter, D. Mills, *Presiding*

- 1:30 340.** Electronic structures of bent, formally two-coordinate lanthanide(III) cations. H. Nicholas, M. Vonci, C. Goodwin, S. Loo, S. Murphy, D. Cassim, R.E. Winpenny, E. McInnes, N. Chilton, **D. Mills**
- 1:50 341.** New insights into solid-phase transformations in the uranyl peroxide system. **T.L. Spano**, A. Miskowicz, J.L. Niedziela, M.W. Ambrogio, B.B. Anderson
- 2:10 342.** Uncovering unprecedented uranium species: From water-stable uranyl(V) to U(IV) POM clusters. **R. Faizova**, L. Chatelain, R. Scopelliti, M. Mazzanti

- 2:30 343.** Guest-dependent single-crystal-to-single-crystal phase transitions in a two-dimensional uranyl-based metal–organic framework. **S. Hanna**, X. Zhang, K. Otake, R.J. Drout, P. Li, T. Islamoglu, O.K. Farha
- 2:50 344.** Synthesis of an unusual square planar Th(III) complex. **D.N. Huh**, J.W. Ziller, W.J. Evans
- 3:10** Intermission.
- 3:20 345.** Interactions of unsaturated hydrocarbon ligands with low valent uranium centers. **J.M. Boncella**, A.M. Tondreau, B.S. Billow
- 3:40 346.** Tuning reactivity of nitride bridged uranium complexes with amide and siloxide ligands. **C.T. Palumbo**, L. Barluzzi, R. Scopelliti, M. Mazzanti
- 4:00 347.** Reactivity of uranyl triperoxide monomers. **A. Arteaga**, N. Martin, L.N. Zakharov, M.D. Nyman
- 4:20 348.** Structural chemistry of uranium(IV)-furoate complexes. **N.A. Vanagas**, K.E. Knope
- 4:40 349.** Organometallic chemistry of lanthanides: Oxidation states in trompe l'oeil and magnetic sandwiches. **G. Nocton**
- 5:00 350.** Condensed and gas phase coordination chemistry of bioinspired chelators with early actinides. **K. Carter**, J. Jian, M. Pynch, T. Forbes, W. Dejong, J.K. Gibson, R.J. Abergel

150 Years of the Periodic Table

Sponsored by HIST, Cosponsored by CINF, INOR and PRES

Nanoscale & Molecular Assemblies: Designing Matter to Control Energy Transport

Sponsored by PHYS, Cosponsored by INOR

Advances in Catalysis with Ceria & Other Reducible Oxides

Reactions and Other Metal Oxides

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

MONDAY EVENING – INOR

SECTION A

San Diego Convention Center

TBD

Sci-Mix

S. A. Koch, N. S. Radu, *Organizers*

8:00 - 10:00

134, 138, 139, 141, 143, 145, 146, 147, 150, 152, 154, 155, 157, 158, 159, 162, 163, 164, 165, 169, 170, 183, 184, 187, 190, 191, 193, 199, 201, 204, 206, 212, 213, 214, 220, 222, 223, 224, 225, 227,

228, 229. See Previous Listings.

476, 477, 478, 480, 484, 486, 487, 490, 492, 494, 500, 501, 503, 504, 506, 507, 509, 510, 514, 515, 517, 523, 524, 534, 539, 540, 541. See Subsequent Listings.

TUESDAY MORNING – INOR

SECTION A

Marriott Marquis San Diego Marina
Marina Ballroom Salon F

ACS Award in Pure Chemistry: Symposium in Honor of Danna Freedman

Cosponsored by PHYS

H. Karunadasa, J. Zdrozny, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 351. Applications of coordination chemistry principles to molecular magnetism. **K.R. Dunbar**

9:00 352. Giant spins as magnetic nodes and building blocks. **T. Betley**

9:25 353. Rationalizing the magnetism of multinuclear single-molecule magnets containing strong single-ion sources of anisotropy through the use of the anisotropic building unit [ErCOT]⁺ (COT²⁻ = 1,3,5,7-cyclooctatetraenide dianion). **J.D. Rinehart**, J. Hilgar, M.G. Bernbeck, A.K. Butts

9:50 354. Quantum magnetism enabled by chemistry: From quantum spin liquids to topological spin waves. **Y. Lee**

10:15 Intermission.

10:30 355. Let's get together! Making bonds between small molecules at multimetallic centers. **L.J. Murray**

10:55 356. Quantum sensing using diamond color centers. **H. Park**

11:20 357. Award Address (ACS Award in Pure Chemistry sponsored by the Alpha Chi Sigma Fraternity and the Alpha Chi Sigma Educational Foundation): Approaching challenges in physics with inorganic chemistry. **D.E. Freedman**, M.J. Amdur, K. Collins, S. Coste, M. Fataftah, R.A. Klein, D. Laorenza, T. Pearson, S. Petry, A. Tamerius, C. Yu, A. Altman, L. Sun, J.P. Walsh, J. Zdrozny, M. Graham, S. Clarke

SECTION B

Marriott Marquis San Diego Marina
Solana

Chemistry of Materials: Nanomaterials

C. G. Lugmair, *Organizer*

E. A. Hernandez-Pagan, M. A. Mahmoud, *Presiding*

- 8:30 358.** Single-component quasicrystalline nanocrystal superlattices by the flexible polygon tiling rule. **Y. Nagaoka**, O. Chen, H. Zhu
- 8:50 359.** Synthesis of ZnS quantum dots: Towards shelling and heterostructures. **E. Bennett**, J.S. Owen
- 9:10 360.** Correlated series of Au/Ag nanoclusters revealing the evolutionary patterns of asymmetric Ag doping. **Y. Li**
- 9:30 361.** Size-controllable and uniform gold bumpy nanocubes for single-particle-level surface enhanced Raman scattering sensitivity. **Y. Lee**, K. Nam
- 9:50 362.** Modulation of tungsten precursor reactivity for control over size and phase of WSe₂ nanocrystals. **J.Q. Geisenhoff**, A.M. Schimpf
- 10:10** Intermission.
- 10:25 363.** Expanding colloidal hybrid nanoparticles to metal phosphide systems. **E.A. Hernandez-Pagan**, R.E. Schaak
- 10:45 364.** Photoreduction of iron oxide nanocrystals. **H. Jung**, B. Zhou, A.M. Schimpf
- 11:05 365.** Asymmetric deposition of platinum atoms on gold nanorods induced by a substrate for synthesis of anisotropic bimetallic nanostructures. **M.A. Mahmoud**
- 11:25 366.** Triplet exciton transfer in PbS/CdS core-shell quantum dots with surface-appended chromophores. **C.M. Papa**, S. Garakyaraghi, F.N. Castellano

SECTION C

Marriott Marquis San Diego Marina
Marina Ballroom Salon D

Chemistry of Material Lectureship & Best Paper Award

J. M. Buriak, A. De Bettencourt Dias, C. Toro, *Organizers*,
Presiding

- 8:30** Introductory Remarks.
- 8:35 367.** Functional properties from molecular dynamics in hybrid perovskite halides. E. Mozur, I.W. Oswald, A. Koegel, A. Maughan, **J.R. Neilson**
- 9:10 368.** Competing interactions: Octahedral tilting, organic-inorganic coupling, and charge transport in vacancy-ordered double perovskites. **A. Maughan**, A. Ganose, A.M. Candia, J. Granger, D.O. Scanlon, J.R. Neilson
- 9:45 369.** Atomic pair distribution function (PDF) analysis of nanostructured and disordered materials. **S. Billinge**
- 10:10** Intermission.
- 10:20 370.** Tuning the bandgaps of halide double perovskites. A. Slavney, B. Connor, L. Leppert, J. Neaton, **H. Karunadasa**

- 10:45 371.** Defect and carrier transport properties of emerging bismuth based photovoltaics. **A. Ganose**
- 11:10 372.** Structural complexities in solids: Understanding functionality through local distortions in perovskite and pyrochlore materials. **G. Laurita**
- 11:35 373.** Key structural and chemical features of defect-tolerant semiconductors. **P. Gorai**

SECTION D

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 9

Inorganic Chemistry for Sustainable Energy & Environment

L. A. Berben, *Organizer*
S. C. Marinescu, *Presiding*

- 8:30 374.** Strategies to enhance electrochemical ammonia production on the surfaces of non-noble metal electrocatalysts. Y. Jang, **K. Choi**
- 9:00 375.** CO₂ as a trigger for controlling the properties of surfaces and coatings. **P.G. Jessop**, M.F. Cunningham
- 9:30 376.** Developing alternatives to oil as feedstocks for our chemicals and liquid fuels. **K.I. Goldberg**
- 10:00** Intermission.
- 10:20 377.** Metal-organic frameworks in light harvesting and energy transfer. **A.J. Morris**, P. Usov, S. Shaikh
- 10:50 378.** Renewable methane from green energy and CO₂: Commercial-scale solution to decarbonize our planet with biological methanation. **M.B. Hein**

SECTION E

Marriott Marquis San Diego Marina
Santa Rosa

Emerging Research in Molecular Synthesis

A. C. Brewer, J. M. Hoover, J. Y. Yang, *Organizers*
V. A. Schmidt, *Organizer*, *Presiding*
M. Emmert, *Presiding*

- 8:30 379.** Beyond static DFT calculations for organometallic reactions in catalysis. **D.H. Ess**
- 9:00 380.** Cu-catalyzed MLCT enabled photocycloadditions of non-conjugated pi-systems. **V.A. Schmidt**
- 9:30 381.** Development of the copper-catalyzed carboamination reaction. **K.L. Hull**
- 10:00** Intermission.
- 10:15 382.** Developing data-driven reaction analysis tools for reaction optimization and interrogation. **M.S. Sigman**

- 10:45 383.** Mechanistic insights into Fe catalyzed late-stage functionalization of amine C-H bonds. **M. Emmert**, C.J. Legacy, M. Frenette, F. Greenaway
- 11:15 384.** Catalyst development for the decarboxylative functionalization of (hetero)arenes. **J.J. Topczewski**, R. Daley, E. Liu

SECTION F

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 8

Surface Chemistry & Structure in Ligand Protected Nanoparticles

C. J. Johnson, B. Lear, *Organizers*
A. Cirri, *Presiding*

- 8:30 385.** How many organic molecules are there on gold nanocrystals? Results from both imaging and NMR. **C.J. Murphy**
- 9:15 386.** Visualizing dynamic reorganization of surface-bound ligands on gold nanorods. **K.A. Willets**
- 10:00** Intermission.
- 10:10 387.** Ligand control of the electronic structure near the Fermi energy in metallic nanoparticles. **B.J. Lear**
- 10:40 388.** Elucidating the role of ligand functionality in phosphine-protected gold clusters using mass spectrometry. **G.E. Johnson**, J. Laskin, H. Hernandez
- 11:10** Intermission.
- 11:20 389.** Dimensionality in surface functionalization. D.P. Goronzy, T. Base, K.N. Houk, **P.S. Weiss**

SECTION G

Marriott Marquis San Diego Marina
Marina Ballroom Salon G

Charge & Substrate Transport in 3D Electrocatalytic Materials

Cosponsored by CATL and ENFL
A. Hall, V. Thoi, *Organizers*
C. C. McCrory, *Organizer, Presiding*

- 8:30 390.** Using polymer encapsulation to influence the mechanism, activity, and selectivity of electrocatalytic CO₂ reduction by molecular catalysts. **C.C. McCrory**
- 8:55 391.** Developing materials to promote substrate channeling of intermediates in electrocatalytic cascades. **S.D. Minteer**
- 9:20 392.** Ultrathin oxide overlayers for tunable electrocatalysis. **D. Esposito**
- 9:45 393.** Exploiting transport limitations to enhance CO₂-to-fuels selectivity. A. Wuttig, Y. Yoon, M. Schreier, S. Hall, **Y. Surendranath**

- 10:10** Intermission.
- 10:25 394.** Making porous MOFs electrically conductive. **J.T. Hupp**, S. Goswami
- 10:50 395.** Bridging homogeneous and heterogeneous catalysis with pincerMOFs. **C.R. Wade**, A. Kassie, B. Reiner
- 11:15 396.** Redox hopping electron and ion transport in metal-organic framework materials. **A.J. Morris**, P. Celis Salazar, M. Cai

SECTION H

Marriott Marquis San Diego Marina
Cardiff

Inorganic Catalysts

S. A. Koch, *Organizer*

- 8:30 397.** Development of molecular electrocatalyst for CO₂ reduction based on polypyridyl and nitrogen-based macrocyclic ligands. **L. Lieske**, A.L. Rheingold, C.W. Machan
- 8:50 398.** Electrocatalytic reduction of dioxygen to hydrogen peroxide by a molecular manganese complex with a bipyridine-containing Schiff base ligand. **S.L. Hooe**, A.L. Rheingold, C.W. Machan, D. Dickie
- 9:10 399.** Effect of s-block metal ion on redox properties of Mn(V) salen-crown ether complexes: Methane activation. **A. Najafian**, T. Cundari
- 9:30 400.** Synthetic [2Fe2S] biomimetics in metallopolymers as hydrogen evolution electrocatalysts. **K. Clary**, M. Karayilan, R.S. Glass, J. Pyun, D.L. Lichtenberger
- 9:50 401.** Systematic study of proton-coupled electron transfer in tris(triazolyl)borate mid-late 3d, 4d-transition metals complexes: Computational study. **A. Nazemi**, T.R. Cundari
- 10:10 402.** Turning off hydrogen evolution: Effects of secondary sphere electrostatic interactions on catalyst product selectivity. **J. Barlow**, J.Y. Yang
- 10:30** Intermission.
- 10:40 403.** Ionic strength of large polyions. **D.L. Collins-Wildman**, Y.V. Geletii, C.L. Hill
- 11:00 404.** Pincer supported iron complexes for dinitrogen activation. **A.M. Lugosan**, D. Dickie, M. Zeller, W. Lee
- 11:20 405.** Mechanism of photoreduction of CO₂ to CH₄ with iron-porphyrin catalyst. **L. Dang**, Z. Lu
- 11:40 406.** Pd Single atom catalyst for small molecule transformations under practical conditions. G. Ding, **Q. Zhang**
- 12:00 407.** Weaker interaction between second sphere and proton donor leads to increased selectivity and activity in Fe(III) Schiff base complexes for

CO₂ reduction to formate. **A. Nichols**, S. Hooe, C.W. Machan

- 12:20 408.** Electrocatalysis with Ni(P₂N₂)₂ complexes attached to the electrode through the phosphine moiety. **F.M. Brunner**, C.P. Kubiak

Future Insights into Syngas Conversion Catalysis: Symposium in honor of Burtron H. Davis

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

Nanoscale & Molecular Assemblies: Designing Matter to Control Energy Transport

Sponsored by PHYS, Cosponsored by INOR

Advances in Catalysis with Ceria & Other Reducible Oxides

Reactions and Other Metal Oxides

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

TUESDAY AFTERNOON – INOR

SECTION A

Marriott Marquis San Diego Marina
Marina Ballroom Salon F

Chemistry of Materials: Synthesis & Properties

C. G. Lugmair, *Organizer*

K. R. Kittilstved, C. E. Knapp, *Presiding*

- 1:30 409.** Phenylalanine-based metallo-hydrogels with photo-switchable arylazopyrazole ligands. **K.Y. Ghebreyessus**, A. Sallee
- 1:50 410.** Synthesis and optoelectronic properties of complex metal oxide A₂M₂O₇ nanoparticles. **Y. Mao**
- 2:10 411.** Trigonal bisdithiazolyl radicals as building blocks towards three-dimensional magnetic exchange networks. **N.J. Yutronkie**, D. Bates, P. Dube, S. Winter, C.M. Robertson, R.T. Oakley, J. Brusso
- 2:30 412.** Revealing the speciation of dopant ions in metal thiophenolate clusters. F. Kato, **K.R. Kittilstved**
- 2:50 413.** From molecules to materials: Effect of precursor design on functional device synthesis. **C.E. Knapp**, H.R. Tinker, Y. Zhou, M.A. Bhide, S.P. Douglas, K.L. Mears
- 3:10** Intermission.
- 3:25 414.** Tunable cyclic Si-N hybrid materials. **C.P. Folster**, P.N. Nguyen, M.A. Siegler, R.S. Klausen

- 3:45 415.** Tunable optical and magnetic properties in redox-switchable all-inorganic polyoxometalate frameworks. **C. Lemmon**, A.M. Schimpf
- 4:05 416.** Tunable polyoxometalate-based frameworks: Synthesis, structural characterization, and modulation of optical and electronic properties. **L. Chen**, **M. Turo**, K. San, J. Wang, M. Gembicky, A.M. Schimpf
- 4:25 417.** Synthesis of high-quality, single-crystalline polyoxovanadate-based frameworks. **K.A. San**, A.M. Schimpf
- 4:45 418.** Sustainable synthesis of high purity silicon carbide with carbon fiber production residual and a sandstone. **K. Sun**, X. He, T. Wang, W. Lu, M. Fan
- 5:05 419.** Withdrawn

SECTION B

Marriott Marquis San Diego Marina
Solana

Learning from Nature: Earth-Abundant Metals for Oxidation Catalysis

T. A. Jackson, A. Mukherjee, *Organizers*

S. S. David, *Organizer, Presiding*

- 1:30 420.** Gas phase tackling of the oxo-wall. **J. Roithova**
- 2:00 421.** Oxidation of hydrocarbons by high-valent metal-halide complexes. **A.R. McDonald**
- 2:25 422.** Small molecule activation at transition metal centers: Structure-function correlations. **K. Ray**
- 2:50** Intermission.
- 3:00 423.** Scope and mechanism of C-H bond activation by bio-inspired copper complexes and peroxides. **A. Mukherjee**, N. Singh, N. Botcha
- 3:25 424.** Spectroscopic investigations of metal binding and oxygen activation in the heterobimetallic Mn/Fe R2lox proteins. **H.S. Shafaat**, E. Miller, C. Ghosh, J.M. Hazel, Z.R. Smith, N. Trivelas
- 3:50 425.** Proton-coupled electron transfer mechanisms in copper-oxygen chemistry. **W.B. Tolman**
- 4:20 426.** Adventures in exploring the high-valent nonheme iron-oxo landscape. **L. Que**

SECTION C

Marriott Marquis San Diego Marina
Marina Ballroom Salon D

Chemistry of Materials: Metal Organic Frameworks

C. G. Lugmair, *Organizer*

B. R. Barnett, D. C. Powers, *Presiding*

- 1:30 427.** Withdrawn

- 1:50 428.** Structural control of metal-organic framework bearing *N*-heterocyclic carbene precursor and immobilization of NHC-metal complexes. **H. Kim**, E. Lee
- 2:10 429.** De novo synthesis of homo and heterometallic titanium organic frameworks with high-throughput methodologies. J. Castells-Gil, N. Padial, N. Almora-Barrios, **C. Marti-Gastaldo**
- 2:30 430.** Particle size and defect control in nanoparticulate UiO-66 via modulator-free synthetic conditions. **G.E. Decker**, Z. Stillman, C.A. Fromen, E.D. Bloch
- 2:50 431.** Responsive metal-organic frameworks incorporating redox-active Mo₂(INA)₄ molecular building units. **F.J. Claire**, M.A. Solomos, T. Kempa Intermission.
- 3:10 432.** Ultrathin films of layered coordination polymers: Charge transport and spin crossover at the nanoscale. V. Rubio-Giménez, G. Escorcia-Ariza, N. Almora-Barrios, M. Galbiati, C. Bartual-Murgui, **S. Tatay**, C. Marti-Gastaldo
- 3:45 433.** Probing substrate diffusion in interstitial MOF chemistry with kinetic isotope effects. **D.C. Powers**
- 4:05 434.** Leveraging π -basicity in metal-organic frameworks for ambient temperature hydrogen storage: Structural, thermodynamic and kinetic insights. **B.R. Barnett**, J.R. Long
- 4:25 435.** Fabrication and characterization of a defect-free mixed matrix membrane by facile mixing PPSU with ZIF-8 core-shell microspheres for solvent-resistant nanofiltration. **J. Dai**, S. Li, L. Wang, J. Lei
- 4:45 436.** Harnessing metal-metal interactions in metal organic framework based catalysts. **S. Desai**, J. Ye, T. Webber, T. Islamoglu, O.K. Farha, D.G. Truhlar, R. Penn, C.C. Lu

SECTION D

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 9

Emerging Research in Molecular Synthesis

A. C. Brewer, J. M. Hoover, J. Y. Yang, *Organizers*
V. A. Schmidt, *Organizer, Presiding*

- 1:30 437.** Carbenes as powerful transition metal surrogates. **G. Bertrand**
- 2:00 438.** Accessing ambiphilic phosphine boronates by phosphine-directed C–H borylation. **T.B. Clark**, S.E. Wright, S. Richardson-Solorzano, K.C. Morris, W. Schumacher, T.N. Stewart
- 2:30 439.** Manipulation of main group element fragments with transition metal isocyanides. **J.S. Figueroa**
- 3:00** Intermission.

- 3:15 440.** Playing with charges: Electrostatically tethered reactive ion pairs. **V. Lavallo**
- 3:45 441.** Main group-mediated olefin functionalization reactions. **A.E. Wendlandt**

SECTION E

Marriott Marquis San Diego Marina
Santa Rosa

Surface Chemistry & Structure in Ligand Protected Nanoparticles

B. Lear, *Organizer*
C. J. Johnson, *Organizer, Presiding*

- 1:30 442.** Synthetic and postsynthetic chemistry of silver monolayer-protected clusters. **T.P. Bigioni**
- 2:00 443.** Switchable surfactants for the preparation of monodisperse nanoparticles. **S.R. Saunders**, K. Bryant
- 2:30 444.** Laser synthesis and spectroscopy of ligand-coated nanoclusters and nanomaterials. **M.A. Duncan**
- 3:00** Intermission.
- 3:10 445.** Precise synthesis of platinum and alloy clusters and elucidation of their structures. **Y. Negishi**
- 3:55 446.** Monitoring nanoparticle-driven chemistry with ultrafast surface-enhanced Raman spectroscopy. **R.R. Frontiera**
- 4:40** Intermission.
- 4:50 447.** Surface chemistry and image dipoles in PbS quantum dots during resonant relaxation of excited intraband states. **J.B. Asbury**
- 5:20** Concluding Remarks.

SECTION F

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 8

Charge & Substrate Transport in 3D Electrocatalytic Materials

Cosponsored by CATL and ENFL
C. C. McCrory, V. Thoi, *Organizers*
A. Hall, *Organizer, Presiding*

- 1:30 448.** Enhancing the real-time detection of phase changes in lithium-graphite intercalated compounds through derivative *operando* (dOp) NMR cyclic voltammetry. **A. Co**, J. Lorie Lopez, P. Grandinetti
- 1:55 449.** Accessing catalytically active ordered intermetallics electrochemically driven non-equilibrium phase transformations. **A. Hall**

- 2:20 450.** Bicarbonate electroreduction in a flow cell. **C.P. Berlinguette**
- 2:45 451.** Control over H⁺/OH⁻ recombination in bipolar ion-exchange membranes enables extremely low overpotential reactivity for water dissociation or efficient light-driven ion pumping. W. White, R. Kautz, L. Schulte, S. Luo, R. Bhide, J. Glancy, L. Renna, **S. Ardo**
- 3:10** Intermission.
- 3:25 452.** 3D design in electrocatalysis. N. Becknell, P. Papa Lopes, D. Jung, D. Strmcnik, N. Markovic, **V. Stamenkovic**
- 3:50 453.** Understanding lithium-mediated ammonia synthesis. **K. Manthiram**, N. Lazouski, Z. Schiffer, K. Williams
- 4:15 454.** Assembly of Au nanoparticles on Cu nanowires to tune CO₂ reduction product from CO, C₂H₄ to CH₃CHO. **S. Sun**

SECTION G

Marriott Marquis San Diego Marina
Marina Ballroom Salon G

Coordination Chemistry: Characterization & Applications

A. Larsen, *Organizer*

F. N. Castellano, C. J. Stein, *Presiding*

- 1:30 455.** Photochemical upconversion with metal-to-ligand charge transfer sensitizers. **F.N. Castellano**
- 1:50 456.** Water-soluble lanthanide (Eu, Tb, Sm) bioprobes combining a pyclen or TACN framework and conjugated antennas for two-photon imaging. **J. Shaya**, N. Hamon, R. Tripier, O. Maury
- 2:10 457.** Investigation of AlCl₃-XCl (X = Cu, Ag) solutions in aromatics by ²⁷Al NMR spectroscopy. **W. Luo**, Z. Liu, X. Meng, R. Zhang, H. Liu, C. Xu
- 2:30 458.** Mimicking thiol gold nanoparticles with atomically-precise tunable organometallic equivalents. **J. Stauber**, E.A. Qian, J. Logan, D. Fujita, Y. Han, P. Kral, A.M. Spokoyny
- 2:50 459.** Indium(III) complex of N, N'-bis(salicylidene) ethylenediamine as chemo-sensor for selective recognition of HSO₄⁻ and hemolytic toxicity (red blood cells) studies. **T. Pandiyan**, C.A. Huerta-Aguilar, S. Huerta-Jose
- 3:10** Intermission.
- 3:30 460.** Copper-benzoquinoid coordination polymer as electrode material for lithium-ion batteries. **C. CHANG**, T. Chen
- 3:50 461.** Synthesis and reactivity of cobalt N-heterocyclic phosphonium/phosphido complexes. **A. Poitras**, C.M. Thomas

- 4:10 462.** Orbital entanglement analysis of exchange-coupled transition-metal complexes. **C.J. Stein**, V. Krewald, D.A. Pantazis

SECTION H

Marriott Marquis San Diego Marina
Cardiff

Organometallic Chemistry: Synthesis & Characterization: Late Transition Metals

N. S. Radu, *Organizer*

- 1:30 463.** Introducing the +1 oxidation state for derivatized 3d metallocene monoanions. C. Goodwin, M. Vonci, H. Nicholas, S. Greer, N. Chilton, **D. Mills**
- 1:50 464.** Extrusion of dicobalt silicide cores via activation of all bonds at RSiH₃ (R = H, Ph) by [(tris-Phosphinoborate)Co]⁻. **R.C. Handford**, P. Smith, T. Tilley
- 2:10 465.** Synthesis and reactivity of a rare Ni(I) methyl complex. **R. Witzke**, T. Tilley
- 2:30 466.** Synthesis and characterization and reactivity of nickel(II)-calix[n]arene (n=4-6) complexes. **J.A. Carter**, B.A. Martinez Ortega
- 2:50 467.** Formation of a Ni-C four-membered metallacycle and its reactivity toward X-Y bond activation. **X. Xing**, N.C. Tomson
- 3:10 468.** Synthesis of cyclic (amino)(aryl)carbene copper(I) complexes. **J. Lorkowski**, U. Radius, C. Pietraszuk
- 3:30 469.** Designing N-heterocycle functionalized phosphinoferrrocene ligands. **A. Sarbajna**, B.E. Silva, A.L. Rheingold, D. Grotjahn
- 3:50 470.** Coordination of diatomic boron monofluoride to iron. **M.J. Drance**, J.S. Figueroa
- 4:10 471.** Structure and Reactivity of Group IX Three-Coordinate Monoanions. **M.L. Neville**, C. Chan, J.S. Figueroa
- 4:30 472.** Low valent cobalt isocyanides: Exploration of cobalt phosphide cluster building blocks. **C. Chan**, J.S. Figueroa
- 4:50 473.** Withdrawn
- 5:10 474.** Synthesis and reactivity of a well-defined mixed-valent copper (0)/(I) nanocluster. **J.L. Peltier**, R.F. Jazzar, G. Bertrand

Future Insights into Syngas Conversion Catalysis: Symposium in honor of Burtron H. Davis

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

SECTION A

San Diego Convention Center

TBD

Coordination Chemistry: Characterization & Applications

A. Larsen, *Organizer*

5:30 - 7:30

- 475.** Synthesis, characterization, and antibacterial studies of Fe(III) complex of 3-nitro-N'-((3-hydroxy-5-(hydroxymethyl)-2-methylpyridin-4-yl) methylene)benzohydrazide. **V. Chittireddy**
- 476.** Rhenium(I) supramolecular rectangles for ion-sensing applications. **S.A. Dhanpat**, A. Kumar
- 477.** Ligand-assisted dissolution of gold in organic solvents. **E. Heliövaara**, M. Räisänen, T. Repo
- 478.** Polypyridine bridged ruthenium dimers as inner-sphere ketone transfer hydrogenation catalysts. **C.H. Weeks**, E.P. Kelson
- 479.** Electrochemical and spectroelectrochemical studies of electrodes modified with ruthenium nitrosyl complexes. **S.B. Ritter**, M.J. Shaw

SECTION B

San Diego Convention Center

TBD

Coordination Chemistry: Synthesis & Characterization

A. Larsen, *Organizer*

5:30 - 7:30

- 480.** Some MOFs with substituted biphenyldicarboxylic acid to show novel topologies. X. He, S. Zhang, **D. Zhu**
- 481.** Preparation of mixed-metal thiocyanate of SnCu(SCN) for opto/electronic applications. **C. Wechwithayakhlung**, S. Horike, P. Pattanasattayavong
- 482.** Synthesis and characterization of palladium mononuclear complexes with electron donor (N,O) species. **C. Jimenez**, J. Aviña, R. Guzmán-Mejía, R. Herrera, J. González-campos
- 483.** Perfect C_3 symmetric sulfate complex with a urea-based hexafunctional synthetic receptor. **A. Hossain**, B. Portis, C.R. Johnson, M. Emami Khansari, A. Jahan, D.R. Powell
- 484.** Effect of a coordinating pyridine moiety on the SAP and TSAP isomer proportions of bimodal Ln(III) complexes. **M. Poveda**, Z. Steinberg, O. Evbuomwan

485. Supramolecular architectures and coordination polymers based on metallacrown complexes: Magnetic and sorption properties. A.V. Pavlishchuk, M. Zeller, L. Carella, E. Rentschler, L.K. Thompson, **A.W. Addison**

486. Synthesis of fluorinated cobalt oxo cubanes: Catalysts for water oxidation. **A. Rahman**, T. Tilley

487. Synthesis of substituted bipyridylphosphine oxides via palladium(II) cross-coupling: Method development and application to coordination chemistry. **T. Grutza**, M. Bezpalko, W.S. Kassel

488. Synthesis of lanthanide molybdates via reaction of molybdenum(VI) oxide with aqueous acetate salts. **K. Alrashidi**

489. Synthesis, characterization, and electrochemistry of a ruthenium saloph nitrosyl complex. **K. Shrestha**, M.J. Shaw

490. Synthesis and characterization of a series of 5-methoxypyridyl-substituted phosphines and associated metal complexes. **L. Warring**, W.S. Kassel, M. Bezpalko

491. Synthesis and characterization of tris(2-pyridyl)phosphine oxide (OPPy₃) complexes of select lanthanide(III) nitrates with potential application in molecular sensing. **C. Cox**, M. Bezpalko, W.S. Kassel

492. Anilino-pyridine ligand framework: Steric and electronic effects on the coordination chemistry to late transition metals. **M. Bezpalko**, W.S. Kassel

493. Systematic study of steric and electronic effects in substituted trispyridylphosphine ligands using molybdenum carbonyl complexes. **J. Leonard**, M. Bezpalko, W.S. Kassel

SECTION C

San Diego Convention Center

TBD

Environmental & Energy-Related Inorganic Chemistry

S. A. Koch, *Organizer*

5:30 - 7:30

494. Tetraphenylphosphonium metal halide perovskites synthesis and crystal structures. **S.A. Althobaiti**

495. Electrocatalytic reduction of carbon dioxide at a 2D rhenium covalent organic framework. **M. Rahman**

496. Electrocatalytic alcohol oxidation by Co_(3-x)M_xO₄ catalysts. **M. Riehs**, S.E. Michaud, C.C. McCrory

- 497.** Time dependence of iron-binding compound production in marine microorganisms under competitive growth conditions. **J.D. Martin**, S. Littlejohn, K. Brown
- 498.** Tin polyesters: Polyimide blends as a dielectric material for energy storage application. **A.A. Deshmukh**, S. Nasreen, M. Baczkowski, G.M. Treich, M. Tefferi, C. Anastasia, Y. Cao, G. Sotzing

SECTION D

San Diego Convention Center
TBD

Main Group Chemistry

T. Hudnall, *Organizer*

5:30 - 7:30

- 499.** Synthesis and their characteristics of 1,1-disubstituted-2,5-bis(trimethylsilyl)ethynyl-3,4-diphenyl-siloles. J.W. Lim, **Y.T. Park**
- 500.** Binary zinc borates and their industrial use. **D.M. Schubert**, M.B. Jacobs
- 501.** Full-color luminescent dimethylamino-substituted difluoroboron β -diketonate complexes as environment-sensitive probes. **F. Wang**, S. Chung, C.A. DeRosa, D. Song, C.L. Fraser
- 502.** Antibacterial performance and mechanism of inorganic salt cations. Z. Ding, **X. Zhao**, **Y. Zhang**
- 503.** 1,8-Naphthalenediol derived boronic esters and inclusion properties of the 4,4'-bipyridine based Lewis acid-base complexes with different aromatic guest molecules. **C. Manankandayalage**, C. Krempner

SECTION E

San Diego Convention Center
TBD

Lanthanide & Actinide Chemistry

A. De Bettencourt Dias, *Organizer*

5:30 - 7:30

- 504.** Synchrotron and electron microscopy microstructural characterization of PuO_2 . **M.A. DeVore**, J.L. Venzie, B.A. Powell, L.C. Shuller-Nickles, J. Fortner, M. Newville
- 505.** Understanding the effect of ligand environment on the tunability europium(II)-containing visible-light photocatalysts. **R. Barraza**, M.J. Allen
- 506.** Lanthanide extraction from fly ash using coordination chemistry. **J. Hovey**, M. Dardona, T.M. Dittrich, M.J. Allen
- 507.** Slow magnetic relaxation in mono- and multinuclear uranium metallocene complexes. **D.**

- Lussier**, M. Boreen, K. Chakarawet, J. Arnold, D.K. Shuh, J.R. Long
- 508.** Lanthanide- and Ln doped bismuth-organic complexes: Structural motifs, visible excitation, and luminescence color tuning via dual emission pathways. **R.L. Ayscue**, C. Verwiel, K.E. Knope
- 509.** F-element Fagan-Nugent coupling chemistry. **J.K. Pagano**, K.A. Erickson, J.L. Kiplinger
- 510.** Organoactinide complexes of uranium and neptunium. **A. Myers**, J.R. Walensky
- 511.** Comparative insertion reactivity of small molecules into thorium-nitrogen and thorium-phosphorus bonds. **M. Tarlton**, J.R. Walensky
- 512.** Functionalization of cyclooctatetraene aimed to improve erbium single molecule magnet behavior. **A. Butts**

SECTION F

San Diego Convention Center
TBD

Nanoscience

B. G. Trewyn, *Organizer*

5:30 - 7:30

- 513.** Garlic based two photon nanoprobe for targeted triple-negative breast cancer imaging. **S. Begum**, A. Pramanik, K. Gates, Y. Gao, P.C. Ray
- 514.** Continuous growth of iron-oxo clusters to iron oxide nanoparticles: Insights on iron oxide nanoparticle formation at the early stage. **H. Chang**, T. Hyeon
- 515.** Holey graphene noble metal nanoparticle composites via crystalline polymer templated etching. **D. White**, S. Burkert, S. Hwang, A. Star
- 516.** Microwave-assisted synthesis of Mn- and rare earth ion-doped CsPbX_3 ($X = \text{Br}, \text{Cl}$) perovskite nanocrystals. **K.Y. Ghebreyessus**, L. Flagg, U. Hommerich
- 517.** Controlling nanocomposite magnetism through magnetic orientation within a polymeric matrix. **T. Zand**
- 518.** Magnetic characterization of iron-doped polydopamine nanoparticles. **K.S. Cay**, J.D. Rinehart, P.C. Bunting, Y. Xie
- 519.** High-performance superparamagnetic Co-Mn-Zn ferrite nanoparticles for magnetic hyperthermia therapy of cancer. **J. Pan**, P. Hu, J. Shi, Q. Wu
- 520.** Fe- and Sn-doped titania nanoparticles for metal-ion battery applications. B.D. Fahlman, **M.K. Islam**
- 521.** Microwave-assisted flow synthesis of titania nanotubes. **Y. Luo**, **M. Calzado Delgado**, K. Yeung

522. Investigation of the influence of sonochemical parameters and initial temperature study on (ZnxAgyInz)₂ synthesis mechanism. **H. JUNG**, S. Sul, J. Jung, J. Park

523. Engineering pseudo spin valve magnetoresistance in colloidal prepared nanoparticle films. **B. Zhou**, J.D. Rinehart

524. Synthesis of barium ferrite nanoparticles for new magnetic materials. **K.M. Kirkpatrick**, P.C. Bunting, J.D. Rinehart

SECTION G

San Diego Convention Center
TBD

Organometallic Chemistry: New Ligand Platforms

N. S. Radu, *Organizer*

5:30 - 7:30

525. Dipyritylmethane derivatives as ligands for highly efficient iridium catalyzed sp³ C–H borylation. **M.R. Jones**, N.D. Schley

526. Synthesis and characterization of terpyridine intermediate and derivatives for metal coordination. **M. Moghadasnia**

527. Strong magnetic exchange in dinuclear transition metal-Me₆tren single-molecule magnets facilitated by a radical bridging ligand. **K. Chakarawet**, J.R. Long

SECTION H

San Diego Convention Center
TBD

Organometallic Chemistry: Synthesis & Characterization: Late Transition Metals

N. S. Radu, *Organizer*

5:30 - 7:30

528. Ferrocene-based heteroscorpionate nickel complexes for atom transfer radical polymerization. **S. Li**, P. Diaconescu

529. Evidence of carbon dioxide insertion into palladium-phenyl complex. **K. Zhang**, **W. Williams**, **D. Dickie**, **D.H. Ess**, **T.B. Gunnoe**

530. Use of silyl-calixarene derivative compound as precursor for the synthesis of transition metal-calixarene complexes. **B.M. Olivo**, B.A. Martinez Ortega

531. Synthesis, reactivity, and magnetism of carbene-cobalt complexes. **A. Mantanona**, K.S. Cay, J.D. Rinehart

532. Synthesis, characterization, and photophysical properties of platinum(II) complexes with thiophene and halide ligands. **C. Mastrocinque**, M. Greenberg, **C.M. Anderson**, J. Tanski

SECTION I

San Diego Convention Center
TBD

Organometallic Chemistry: Synthesis & Characterization: Early Transition Metals

N. S. Radu, *Organizer*

5:30 - 7:30

533. Aromatic substituent effects modulate catalytic activity of synthetic [NiFe]-Hydrogenase mimics. **C.R. Forbes**, L. Gan, N.S. Herringer, T.L. Groy, P. Tarakeshwar, A.K. Jones

534. Tantalafuran supported by a linked cyclopentadienyl-carboranyl ligand: Synthesis and structure. **J. Yang**, Z. Xie

535. Synthesis and characterization of precursors for the electrochemical deposition of refractory metals out of ionic liquids. **C. Egger**, R. Reich, O. Schneider, F.E. Kuehn

536. Synthesis and structures of thermolabile organotitanium monoalkyl phosphates: Solvent effect on nuclearity, utility as epoxidation catalysts and single-source molecular precursors for TiP₂O₇. **S. Verma**, G. Bhat, R. Murugavel

537. Experimental and computational mechanistic and structural studies on substituted bis(cyclopentadienyl)tantalum(v) trihydrides for hydrocarbon activation. **S. Rehbein**

SECTION J

San Diego Convention Center
TBD

Solid-State Inorganic Chemistry

C. G. Lugmair, V. Poltavets, *Organizers*

5:30 - 7:30

538. Establishing the complex crystal chemistry of the coinage metals through synthesis, computation, and data-driven analysis. **S. Lotfi**, A. Mansouri Tehrani, J. Brgoch

539. Synthesis of ternary metal tetrel-pnictides using arc-melted precursors. **G. Akopov**, J. Mark, B. McBride, K. Kovnir

540. Tuning the thermoelectric properties of 2D layered GeAs. **S. Lee**, B. Owens-Baird, K. Kovnir

- 541.** New ternary transition metal selenide Na_2MoSe_4 : Computational and experimental study. **E.I. Palos**, R.I. Hernández Lima, J. Guerrero Sánchez, G. Alonso Nuñez, A. Reyes Serrato
- 542.** Flexible and hierarchical structured MnO_2 @ ZrO_2 nanofibrous membranes with high catalytic performance. **X. Zhang**, X. Wang, J. Yu, B. Ding

WEDNESDAY MORNING – INOR

SECTION A

Marriott Marquis San Diego Marina
Marina Ballroom Salon F

Environmental & Energy-Related Inorganic Chemistry

S. A. Koch, *Organizer*
A. J. Morris, *Presiding*

- 8:30** **543.** Electrocatalytic water oxidation by a trinuclear copper complex. **A. Geer**, X. Jia, B.A. McKeown, R.J. Nielsen, W.A. Goddard, T.B. Gunnoe
- 8:50** **544.** Electrocatalytic CO_2 reduction by cobalt bis(pyridylmonoimine) complexes: Effects of ligand structure on catalytic activity. **W. Nie**, C.C. McCrory
- 9:10** **545.** Effects of surface modification of p-type silicon on the photoelectrochemical reduction of CO_2 with group VII catalysts. **C. Miller**, S. Okuno, P. Cheung, C.P. Kubiak
- 9:30** **546.** Molecular control over excited-state supramolecular assembly. **M. Turlington**, L. Troian-Gautier, R. Sampaio, E.E. Beauvilliers, G.J. Meyer
- 9:50** **547.** Sustainable simplified process for production of vanadium oxides (V_2O_5 , VO_2 , and V_2O_3). **H.S. Devi**, A. Mishra, M.S. Reza, M. Singh
- 10:10** Intermission.
- 10:15** **548.** Mixed-valency across supramolecular systems: Stabilizing soft interactions with electron delocalization. **J.M. Palasz**, F.M. Brunner, C.P. Kubiak
- 10:35** **549.** Enhancing Si(111) photocathode performance with surface dipoles and surface density of states. **M.J. Rose**, D. Boucher
- 10:55** **550.** Copper-dioxygen chemistry using novel tren-based, tris(phosphinimine) ligands. **A. Weberg**, N.C. Tomson, S. McCollom
- 11:15** **551.** Design and studies of novel iron-based complexes for hydrogen photo-evolution. **A. Aydogan**, O. Schott, G. Hanan, M. Singleton, B. Elias
- 11:35** **552.** Taming a high valent tetra-nickel cluster for PCET of small molecules. **S. Jacob**, G. Menard
- 11:55** **553.** High nuclearity Co/Mn oxo clusters: Potential water oxidation catalysts. **P. Mahalay**, G. Maayan, K.A. Abboud, G. Christou

SECTION B

Marriott Marquis San Diego Marina
Solana

Bioinorganic Chemistry: Proteins & Enzymes & Model Systems

S. A. Koch, *Organizer*
T. Karabencheva-Christova, *Presiding*

- 8:30** **554.** Structural and spectroscopic insights into the reaction mechanism of carotenoid cleaving oxygenases. P. Kiser, **E.R. Farquhar**
- 8:50** **555.** Spectroscopic insights into the unusually high reactivity of the $S = 1$ $[\text{Fe}^{\text{IV}}(\text{O})(\text{Me}_3\text{NTB})]^{2+}$ complex that shed light on the oxidation mechanism of ferryl complexes. **S. Banerjee**, W. Rasheed, L. Que
- 9:10** **556.** Cu-dependent hydroxylation combined with 6-membered intramolecular cyclization under benign reaction conditions. **R. Trammell**, I. Garcia-Bosch, A. Cordova, P. Polunin, B. Blackmore
- 9:30** **557.** Genomic analysis of siderophore Fe(II)/ α -ketoglutarate-dependent Aminoacyl β -Hydroxylases reveals functional subtypes. **Z.L. Reitz**, A. Butler
- 9:50** **558.** Mechanistic investigation of stereoselective olefin cyclopropanation catalyzed by an engineered carbene transferase. **A. Tinoco**, R. Fasan
- 10:10** Intermission.
- 10:30** **559.** Modeling copper active sites in biology: Synthesis and reactivity of bioinspired mononuclear copper(II) complexes. **T. Jones**, A. Mukherjee
- 10:50** **560.** Withdrawn
- 11:10** **561.** Insights into the linkage between the catalytic reaction cycle and proton pumping in ba_3 cytochrome c oxidase: combining DFT, electrostatics, molecular dynamics, and new X-ray structures. **L. Noodleman**, W. Han Du, Y. Chen, D. McRee, K. Hartfield, A.W. Goetz, T. Goh, T. Doukov, A. Cohen, V. Cherezov, M. Soltis, P. Padayatti
- 11:30** **562.** Selective removal of endogenous CO *in vitro* and *in vivo* by aqueous hemoprotein model complexes. **H. Kitagishi**
- 11:50** **563.** Synthesis and characterization of heterobimetallic Fe–O–Mn complexes: Modeling RNR 1c and R2lox. **P. Crossland**, A. Zhou, L. Que
- 12:10** **564.** Withdrawn

SECTION C

Marriott Marquis San Diego Marina
Marina Ballroom Salon D

Organometallic Chemistry: Synthesis & Characterization: Early Transition Metals

N. S. Radu, *Organizer*

- 8:30** **565.** Stable ethylene-carbon dioxide group 6 metal complexes. **P.J. Perez**, M. Alvarez
- 8:50** **566.** Tungsten-ligand bond strengths for 2p elements, a DFT and *ab initio* study. **C. Moulder**, K. Kafle, T. Cundari
- 9:10** **567.** Organomanganese phosphine-phenol(ate) complexes: Coordination chemistry, and catalysis. **K. Kadassery**, S.N. MacMillan, D.C. Lacy
- 9:30** **568.** Synthesis and characterization of mono(oxazoline)-substituted cyclopentadienyl zirconium complexes. **Y. Chu**, N. Eedugurala, A.D. Sadow
- 9:50** **569.** Organometallic complexes of early transition metals supported by bulky acetylacetonate ligands. **S.M. Krajewski**, M.P. Marshak

SECTION D

Marriott Marquis San Diego Marina
San Diego Ballroom Salon C

Chemistry of Materials: Metal Organic Frameworks

C. G. Lugmair, *Organizer*
E. D. Bloch, J. Rimsza, *Presiding*

- 8:30** **570.** Theoretical study of porphyrin-based MOF structure for storage, separation, and drug delivery applications. **R. Belosludov**
- 9:10** **571.** Gold nanoparticles in the NU-1000 metal organic framework: Structures and O₂ activation. **R.D. Senanayake**, R. Snurr, C.J. Cramer
- 9:30** **572.** Hierarchical self-assembly of supramolecular coordination polymers using giant metal-organic nanocapsules as building blocks. **C. Zhang**, F. Wang, R. Patil, C.L. Barnes, T. Li, J.L. Atwood
- 9:50** **573.** Liquid-phase separations of fluoroarenes in metal-organic frameworks. **P.J. Milner**, M. Gonzalez, J.R. Long
- 10:10** Intermission.
- 10:25** **574.** Gas storage in porous coordination cages. **E.D. Bloch**
- 10:45** **575.** Low-valent coordination networks with *m*-terphenyl isocyanides based linkers. **A. Arroyave**
- 11:05** **576.** Probing metal-organic framework growth process with competitive nucleation. **M.C. Wasson**, J. Lyu, T. Islamoglu, O.K. Farha
- 11:25** **577.** Acid gas adsorption and structural characterization of RE-DOBDC MOFs via density functional theory. D.J. Vogel, T.M. Nenoff, **J. Rimsza**

SECTION E

Marriott Marquis San Diego Marina
Santa Rosa

Chemistry of Materials: Nanomaterials

C. G. Lugmair, *Organizer*
S. Chen, Y. Mao, *Presiding*

- 8:30** **578.** Kinetically controlled sequential seeded growth as a route toward metal dendrimers. **J.D. Smith**, M.M. Scanlan, S.E. Skrabalak
- 8:50** **579.** Tunable library of aminophosphines provides mechanistic insights on InP nanocrystal nucleation and growth. **B. McMurtry**, J. De Roo, J.K. Teglas, K. Qian, A. Swarnakar, J.S. Owen
- 9:10** **580.** Scalable solid-state synthesis of SnS₂/graphene nanostructured hybrids for high performance supercapacitor applications. **S. Al Hassan**, S. Lonkar, V. Pillai
- 9:30** **581.** Synthesis and characterization of nanoscale europium barium titanate (Eu_{0.5}Ba_{0.5}TiO₃). **N. Farahmand**, S. O'Brien, J. Lombardi, F.A. Pearsall, L. Yang, S.J. Billinge, Z. Gai
- 9:50** **582.** Crystallinity and size control of colloidal germanium nanoparticles from organogermanium halide reagents. **B. Pescara**, K. Mazzio, K. Lips, S. Raoux
- 10:10** **583.** Transformation of cuprous oxide microcrystals into hollow copper nanoshells by facet-selective extraction of photoexcited charges. **C. Qin**, B. Campbell, M. Shen, T. Zhao, B. Sadtler
- 10:30** Intermission.
- 10:35** **584.** Mesoporous silica coated CuFe₂O₄ nanoparticles: Synthesis, characterization and application in gas phase H₂S removal. **G. Basina**, D. Abdullah Ali Gaber, S. Abdullah Ali Gaber, V. Tzitzios, C. Gioti, A. Mourkas, I. Ismail, I. Panagiotopoulos, M.A. Karakassides, **Y. Fowad AlWahedi**
- 10:55** **585.** Enzyme immobilization with reduced confinement in metal-organic frameworks. **S. Chen**, W. Lo, L. Chou, F. Shieh, C. Tsung
- 11:15** **586.** Molten-salt synthesis of pyrochlore RE₂Hf₂O₇ nanoparticles. **Y. Mao**, M. Pokhrel, K. Wahid, S. Gupta

SECTION F

Marriott Marquis San Diego Marina
Marina Ballroom Salon E

Coordination Chemistry: Synthesis & Characterization

A. Larsen, *Organizer*
T. Betley, M. Stollenz, *Presiding*

- 8:30 587.** Correlation of formal oxidation state with the N-N bond distance of chromium dinitrogen complexes. **F. Ahmadi Darani**, K.H. Theopold
- 8:50 588.** Aromaticity in bis(imino)pyridine complexes. **T. Bass**, T.J. Sherbow, C.R. Carr, L.A. Berben
- 9:10 589.** Interaction between bimetallic sites in bimetallic composite ionic liquids. **Y. Zhang**, X. Meng, R. Zhang, H. Liu, C. Xu, Z. Liu
- 9:30 590.** Heteroleptic calladium(II) complexes of the redox-active propentdyopent scaffold supported by intramolecular hydrogen bonding. **C. Curtis**, E. Tomat
- 10:10** Intermission.
- 10:15 591.** To multiply bond or not. **T. Betley**
- 10:35 592.** Investigation on the stability of a series of BODIPYs in acidic conditions: Experimental and computational study into the role of the substituents at boron. **M. Wang**, D.R. Mason, P.N. Bobadova-Parvanova, M. Vicente
- 10:55 593.** Synthetic investigation of competing magnetic interactions in 2D metal-organic frameworks. **K. Collins**, M. Fataftah, D.E. Freedman
- 11:15 594.** Lewis-acid-catalyzed BODIPY boron functionalization utilizing trimethylsilyl nucleophiles. **G. Zhang**, M. Wang, F.R. Fronczek, K.M. Smith, M. Vicente

SECTION G

Marriott Marquis San Diego Marina
Marina Ballroom Salon G

Inorganic Catalysts

S. A. Koch, *Organizer*

- 8:30 595.** New classes of homo- and heteroleptic Cu(I) metal-to-ligand charge transfer photosensitizers. **F.N. Castellano**
- 8:50 596.** Real-time detection of large Abeta oligomers using photoluminescence anisotropy. **B. Jiang**, A. Aliyan, A. Smith, A. Marti, I. Gonzalez-Moreno
- 9:10 597.** Delayed photoluminescence in metal-conjugated fluorophores. **M. Yang**, M. Zamkov, H.M. Mattoussi
- 9:30 598.** Methane C–H activation via cyclic (alkyl) (amino)carbenes (CAACs) and CAAC- supported transition metal complexes: Computational study. **Z. Sun**, T.R. Cundari
- 9:50 599.** Photoinitiated oxidation of halides to halogen using ruthenium trisbipyridyl complexes as catalysts. C. Chen, **I. Chang**
- 10:10 600.** New approaches to hydrocarbon feedstock conversion: Bifunctional Pd complexes for tunable heterolytic C-H activation. **R. Tenney**, W. Christman, N. Arulsamy, E.B. Hulley

- 10:30 601.** High-throughput screening of MOF catalysts. **J. Palomba**, S. Cohen, M. Kalaj
- 10:50** Intermission.
- 11:00 602.** Molecular cobalt complexes with pentadentate ligands for electro- and photocatalytic hydrogen generation in aqueous solution. **P. Wang**, G. Liang, E. Towles, D. Li, C. Boyd, K. Hill, B. Shaver, W. Grubbs, C.E. Webster, X. Zhao
- 11:20 603.** Electrochemical and computational investigation of aromatically bridged [2Fe-2S] clusters for electrocatalytic hydrogen production. **M.O. Hamilton**, J.M. Kiselka, M. Karayilan, R.S. Glass, J. Pyun, D.L. Lichtenberger
- 11:40 604.** Effect of hydrogen bonds on photocatalysis of CO₂ reduction. **P. Cheung**, T. Zeng, C.P. Kubiak
- 12:00 605.** Chemically driven water oxidation by mononuclear Ru(II) complexes and deactivation pathway. **A. KUNDU**, S. Mandal
- 12:20 606.** Synthesis and reactivity studies of molybdenum(VI) and rhenium(V) oxo complexes as bioinspired oxo transfer catalysts. **M. Hossain**, J. Schachner, M.O. Haukka, A. Lehtonen, N. Mösch-Zanetti, E. Nordlander

SECTION H

Marriott Marquis San Diego Marina
Cardiff

Nanoscience

B. G. Trewyn, *Organizer*

- 8:30 607.** Revealing the peculiar solubility of some atomically-precise gold nanoclusters. **M.J. Cowan**, T. Higaki, R. Jin, G. Mpourmpakis
- 8:50 608.** Nonthermal plasma-synthesized PB co-doped Si NCs: New approach to non-toxic NIR-emitters. **G. Pach**, R. Limpens, N.R. Neale
- 9:10 609.** Structural identification and quality assessment of graphene derivatives by X-Ray diffraction. **I. Sengupta**, S. S S Sharat Kumar, S. Pal, S. Chakraborty
- 9:30 610.** Capitalization on self-assembly for the preparation of rhenium carbonyl-based nanoparticles for theranostic applications. **K. Chan**
- 9:50 611.** Probing the interior nanoscale heating mechanism of a magnetic core in mesoporous silica drug-delivery nanoparticles using fluorescence depolarization. **F. Lin**, J.I. Zink
- 10:10 612.** Mosquito bite prevention through graphene barrier layers. **C. Castilho**, D. Li, M. Liu, Y. Liu, H. Gao, R. Hurt

Future Insights into Syngas Conversion Catalysis: Symposium in honor of Burtron H. Davis

Sponsored by CATL, Cosponsored by ENFL, ENVR, INOR and
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Nanoscale & Molecular Assemblies: Designing Matter to Control Energy Transport

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Understanding the Role of Water in Solid Acid- Base Catalysis

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WEDNESDAY AFTERNOON – INOR

SECTION A

Marriott Marquis San Diego Marina
Marina Ballroom Salon F

Bioinorganic Chemistry: Proteins & Enzymes & Model Systems

S. A. Koch, *Organizer*

M. J. Rose, *Presiding*

- 1:30** **613.** Acid pK_a -dependence O–O bond lysis of a nonheme Fe^{III}–OOH species: Analogy to the formation of heme compound I. **S. Xu**, A. Darksharapu, W. Rasheed, L. Que
- 1:50** **614.** Investigating the mechanism of formation of a rare thiolate-ligated Fe(III)-sulfenate. **A. Downing**, M.N. Blakely, J. Kovacs
- 2:10** **615.** Functional hydride transfer in anthracene scaffold-based synthetic models of [Fe]-hydrogenase. **M.J. Rose**, S. Kerns, J. Seo
- 2:30** **616.** Investigation of the binding of nitrogen-based exogenous ligands in iron complexes within a C_3 -symmetrical phosphinic amide tripodal ligand. **C. Sun**, A. Borovik
- 2:50** **617.** From organometallic carbides to nitrogenase-inspired clusters: Sulfurization of Fe₆ and Fe₅Mo carbides. **M.J. Rose**, C. Joseph
- 3:10** Intermission.
- 3:30** **618.** Artificial iron proteins using biotin–streptavidin technology. **K. Miller**, A. Borovik
- 3:50** **619.** Tetranuclear Mn₄O₄ complexes as models of the oxygen evolving complex of photosystem II. **A. Shiau**, H. Lee, P. Oyala, T. Agapie
- 4:10** **620.** Spectroscopic characterization of thiolate ligated iron-dioxygen and oxo-atom donor intermediates. **M. Dedushko**
- 4:30** **621.** Fluorescent probes for New Delhi metallo-β-lactamases to explore bacterial zinc homeostasis. **R. Mehta**, P. Thomas, W. Fast, E.L. Que

- 4:50** **622.** High valent non-heme iron-oxido and -hydroxido complexes. **J. Lee**, V. Oswald, S. Biswas, M.P. Hendrich, A. Borovik
- 5:10** **623.** Principles of metal selectivity bias and cluster assembly in metallothionein metal thiolate clusters. J.S. Calvo, N. York, B.S. Pierce, **G. Meloni**

SECTION B

Marriott Marquis San Diego Marina
Solana

Chemistry of Materials: Materials for Energy & Catalytic Applications

C. G. Lugmair, *Organizer*

A. J. Karkamkar, R. M. Kennedy, *Presiding*

- 1:30** **624.** Facile solvent free synthesis of iron porphyrin COFs for CO₂ reduction. **P. Cheung**, S. Lee, C.P. Kubiak
- 1:50** **625.** Covalent organic frameworks composed of rhenium bipyridine and metal porphyrins: Designing heterobimetallic frameworks with two distinct metal sites. **E. Johnson**, R.M. Haiges, S.C. Marinescu
- 2:10** **626.** Surface-immobilized conjugated polymers incorporating rhenium bipyridine motifs for electrocatalytic and photocatalytic CO₂ reduction. **N.M. Orchanian**, L.E. Hong, J. Skrainka, J. Esterhuizen, D. Popov, S.C. Marinescu
- 2:30** **627.** Electrocatalytic CO₂ reduction in water using Re complex catalyst with polymer ion gels electrode. **S. Sato**, B.J. McNicholas, R.H. Grubbs
- 2:50** Intermission.
- 3:05** **628.** Catalytic hydrogenation of CO₂ to methanol using tandem catalysis involving encapsulated ruthenium complexes in the metal-organic framework UiO-66. **T. Rayder**, E.H. Adillon, C. Tsung, J.A. Byers
- 3:25** **629.** Catalytic upcycling of waste polymers by supported metal catalysts. **R.M. Kennedy**, G. Celik, R. Hackler, S.C. Ammal, M. Ferrandon, A.M. LaPointe, A.D. Sadow, A. Heyden, K.R. Poepfelmeier, M. Delferro
- 3:45** **630.** CO₂ reduction to CO by rhenium catalyst and various attachment strategies to carbon electrode surfaces. **A. Zhanidarova**, C.P. Kubiak
- 4:05** **631.** Alternative ammonia storage materials for SCR of NO_x. **A.J. Karkamkar**
- 4:25** **632.** Exploration of p-type delafossite CuMO₂ oxides as photocatalysts. **Y. Mao**
- 4:45** **633.** Electron localization and transport through ruthenium polypyridyl dye-sensitized core/shell SnO₂/TiO₂ mesoporous thin films. **E. James**, M. Bennett, G.J. Meyer

SECTION C

Marriott Marquis San Diego Marina
Marina Ballroom Salon D

Chemistry of Materials: Metal Organic Frameworks

C. G. Lugmair, *Organizer*

M. I. Gonzalez, M. Wriedt, *Presiding*

- 1:30** 634. Metal-organic frameworks as templates for the controlled growth of catalytically active copper nanoparticles. **L. Redfern**, O.K. Farha
- 1:50** 635. Controlled encapsulation of biomolecules into nanoporous materials. **C. Tsung**
- 2:10** 636. Confinement of atomically-defined metal halide sheets in a metal-organic framework. **M.I. Gonzalez**, A. Turkiewicz, L.E. Darago, J. Oktawiec, K. Bustillo, F. Grandjean, G.J. Long, J.R. Long
- 2:30** 637. Framework structure defines the excitonic properties of MOFs. **P. Deria**, J. Yu
- 2:50** 638. Synthesis and enhanced performance of metal-organic framework hybrid materials. **Y. Liu**, S. Klein, K. Nelms, J. Sosa
- 3:10** Intermission.
- 3:25** 639. Old linkers new tricks: Evolution of 14-Connect Zr₆ secondary building units. M.J. Hurlock, **Q. Zhang**
- 3:45** 640. Photodoping as a route to storing electrons in metal-organic frameworks. **C.H. Hendon**
- 4:05** 641. Energy and charge transfer dynamics in porphyrin: MOF composite. **X. Li**, J. Yu, P. Deria

SECTION D

Marriott Marquis San Diego Marina
San Diego Ballroom Salon C

Organometallic Chemistry: Catalysis - Late Transition Metals

N. S. Radu, *Organizer*

- 1:30** 642. Rhenium bipyridine catalysts with hydrogen bonding pendant amines for CO₂ reduction. **A. Hellman**, S.C. Marinescu, R.M. Haiges
- 1:50** 643. Generation of active palladium(0) catalyst species from air-stable palladium(II) precatalysts and their application in cross-coupling reactions. **K.H. Shaughnessy**
- 2:10** 644. Novel metal-catalyzed nitrene transfer reactions: Increasing molecular complexity. **P.J. Perez**, M. Diaz-Requejo, M.R. Rodríguez, A. Moreno
- 2:30** 645. Optimizing ene-yne metathesis reactions: Understanding how optimal conditions shift with substrate. **K. Basemann**, B. Schmidt, T.L. Windus, A.D. Sadow

- 2:50** 646. Chasing copper hydrides. J.L. Peltier, E.A. Romero, d. munz, **R.F. Jazzar**, G. Bertrand
- 3:10** 647. Co-catalytic effects in iron-mediated hydrogenation of electron-rich carbonyl compounds. U. Jayarathne, N. Hazari, **W.H. Bernskoetter**
- 3:30** 648. Development of molecular electrocatalysts for energy-related transformations. **K.M. Waldie**, S. Katipamula, M. Zou, S. Warriar
- 3:50** 649. Comparison of reactivity of iron alkoxide complexes towards azoarene synthesis. **D. Wannipurage**, S. Kurup, M. Yousif, S. Groysman, R.L. Lord
- 4:10** 650. Development of group 9 transition metal based catalysts for the oxidative alkenylation of arenes. **W. Zhu**, J. Chen, X. Jia, D. Dickie, T.B. Gunnoe

SECTION E

Marriott Marquis San Diego Marina
Santa Rosa

Chemistry of Materials: Nanomaterials

C. G. Lugmair, *Organizer*

M. Friedfeld, *Presiding*

- 1:30** 651. Systematic tailoring of CdSe quantum dot-molecule composites for triplet energy transfer reactions. **D.T. Yonemoto**, F.N. Castellano
- 1:50** 652. Conversion of InP clusters to nanomaterials and its role in the design of alloyed III-V nanomaterials for emissive applications. **M. Friedfeld**, J. Stein, D. Johnson, B. Cossairt
- 2:10** 653. Nucleation kinetics and molecular mechanism in transition-metal nanoparticle formation: Intriguing, informative case of a bimetallic precursor, $\{[(1,5\text{-COD})\text{Ir}(\text{HPO}_4)]_2\}^{2-}$. **C. Whitehead**, R.G. Finke
- 2:30** 654. Attaining tunability of colloidal copper phosphide nanocrystals through synthetic design and post-synthetic redox modulation. **A. Rachkov**, A.M. Schimpf
- 2:50** 655. Functionalization of boron-nitride nanomaterials using reductive conditions. C.A. de los Reyes, K. Hernandez, C. Martinez, A. Smith McWilliams, M. Pasquali, **A.A. Marti**
- 3:10** Intermission.
- 3:25** 656. Stitching quantum dots in formamide as an alternative route to make heterostructures. **P. Moroz**, M. Zamkov, J. Cassidy, D. Porotnikov
- 3:45** 657. Withdrawn
- 4:05** 658. Applications of the nanoconfinement effect in explosive stabilization, chemical dosimeters, and water treatment. **A.W. Apblett**, N.F. Materer, E. Kadossov, R. Butt

- 4:25 **659.** Colloidal CuFeS₂ nanocrystals: Synthesis and insights into the intermediate Fe d-band that influences its optical properties. **S. Ghosh**, D.J. Milliron

SECTION F

Marriott Marquis San Diego Marina
Marina Ballroom Salon E

Coordination Chemistry: Synthesis & Characterization

A. Larsen, *Organizer*

R. Hernandez Sanchez, *Presiding*

- 1:30 **660.** Some novel bioactive carboxylate metal complexes: Synthesis, structural elucidation and antimicrobial properties. **J.A. Obaleye**
- 1:50 **661.** Ruthenium–cobalt oxo cubane bearing a terminal Ru^V–oxo. **J. Amtawong**, D. Balcells, J. Wilcoxon, N. Biggins, R. Britt, T. Tilley
- 2:10 **662.** Thermochemical properties of mixed anion crystals of bis(cyclohexyl isocyanide) gold(I) complexes. **P.M. Luong**, V. Moshayedi, M.M. Olmstead, A.L. Balch
- 2:30 **663.** Reaction of iron ions with 2-oximinocarboxylates: Kinetics of complex formation and the thermal conversion of the products to metal oxides. **W. Alamier**, A.W. Apblett
- 2:50 **664.** Atomically-defined nanoscale materials. **R. Hernandez Sanchez**
- 3:10 Intermission.
- 3:30 **665.** Questions of noninnocence and ease of azo reduction in diruthenium frameworks. **F.F. Fatima Khan**, G.K. Lahiri
- 3:50 **666.** Accessing a new molecular scaffold for Fe(II) spin-state switching through post-synthetic modification. **B. Livesay**, M.P. Shores
- 4:10 **667.** Fe^{II} spin-crossover complexes as temperature- and pH-responsive ¹⁹F chemical shift magnetic resonance probes. **A.E. Thorarinsdottir**, A.I. Gaudette, D. Harris
- 4:30 **668.** NHC–, CAAC–, and CDC–alkaline earth metal complexes as reagents for bond activation. L.A. Freeman, J. Walley, G. Wang, G. Breiner, D. Dickie, **R.J. Gilliard**

SECTION G

Marriott Marquis San Diego Marina
Marina Ballroom Salon G

Lanthanide & Actinide Chemistry

A. De Bettencourt Dias, *Organizer*

D. A. Penchoff, D. Stamberga, *Presiding*

- 1:30 **669.** Predicting stability constants for terbium(III) complexes with 4-substituted dipicolinic acid analogues using density functional theory. **H. Chen**, R. Shi, H. Ow
- 1:50 **670.** High-throughput screening to achieve benchtop separations for selected rare earth elements. **J. Nelson**, T. Cheisson, H. Rugh, M. Gau, P. Carroll, E.J. Schelter
- 2:10 **671.** Ion coupled plasma mass spectrometry detection of the isotachophoretic separation of nonradioactive lanthanides in a capillary and a microfluidic device. **H.E. Lackey**, D. Bottenus, S.D. Branch, M. Liezers, S.D. Shen, A. Lines
- 2:30 **672.** Complexation of lanthanides and actinides: Theoretical perspective on predicting binding selectivity. **D.A. Penchoff**, C. Peterson, G.K. Schweitzer, D.M. Jenkins, R. Harrison, H.L. Hall
- 2:50 **673.** Tetravalent cerium complexes and clusters. **J.N. Wacker**, A.S. Ditter, S.A. Kozimor, K.E. Knope
- 3:10 **674.** Crucial impact of cerium reduction on photoluminescence properties. **R. Gãnois**, R. Gautier, F. Massuyeau, S. Jobic
- 3:30 **675.** Isolation and assessment of the cytotoxicity of oligothieryl-based luminescent lanthanide complexes. **K. Johnson**, C.V. Rodrigues, M.O. Rodrigues, V.C. Lombardi, A. De Bettencourt Dias
- 3:50 **676.** Separation of rare earth elements using novel diglycolamide ligands. **D. Stamberga**, C. Albisser, M.R. Healy, K.L. Lyon, I. Popovs, S. Jansone-Popova
- 4:10 **677.** Highly functional rare Earth starting materials. **R. Beattie**, J.K. Pagano, K.A. Erickson, S.K. Cope, B. Scott, D.E. Morris, J.L. Kiplinger
- 4:30 **678.** Peroxide-selective O₂ reduction via metal-coupled electron transfer with rare earth triflates. **M.J. Lueckheide**, M.Z. Ertem, J.R. Robinson
- 4:50 **679.** ErCOT: An anisotropic metal-ligand pair for targeted molecular magnet design. **M.G. Bernbeck**, J. Hilgar, J.D. Rinehart

SECTION H

Marriott Marquis San Diego Marina
Cardiff

Main Group Chemistry

T. Hudnall, *Organizer*

R. J. Gilliard, C. E. Knapp, *Presiding*

- 1:30 **680.** Eclipsed digermynes as building blocks to construct catenated multinuclear germanium chains and rings. Y. Wey, G. Huang, J. Yu, **Y. Tsai**
- 1:50 **681.** Cyclodiphosphazanes in metal–organic frameworks. **M.S. Balakrishna**
- 2:10 **682.** Inorganic rings of group 13 and 14 elements as a platform for molecular hybrid materials. W. Yang, K.E. Krantz, D. Dickie, **R.J. Gilliard**

- 2:30 683.** Iron, cobalt, and nickel complexes with silylene ligands. **C. Cui**, Y. Bai
- 2:50** Intermission.
- 3:00 684.** Investigations into the synthesis, reactivity, and thermolysis of heterobimetallic precursors. **K.L. Mears**, C.E. Knapp, C.J. Carmalt
- 3:20 685.** Designer aluminium compounds for use as precursors in low temperature metal coatings. **S.P. Douglas**, C.E. Knapp
- 3:40 686.** Synthesis and characterization of selenium and tellurium containing organic materials toward sensors and emitters. **G. Hoover**, B. Drummond, S. Jones, D. Credgington, D.S. Seferos
- 4:00 687.** Precursor design, synthesis, and reactivity: Tuning molecules for low temperature conversion to functional materials. **C.E. Knapp**, H.R. Tinker, Y. Zhou, M.A. Bhide, S.P. Douglas, K.L. Mears

Understanding the Role of Water in Solid Acid-Base Catalysis

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Nanoscale & Molecular Assemblies: Designing Matter to Control Energy Transport

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THURSDAY MORNING – INOR

SECTION A

Marriott Marquis San Diego Marina
Marina Ballroom Salon F

Chemistry of Materials: Synthesis & Properties

C. G. Lugmair, *Organizer*
A. Hendrickson, *Presiding*

- 8:30 688.** Withdrawn
- 8:50 689.** Lead-free all-inorganic Ag doped cesium bismuth iodide perovskite for resistive switching with ultra-low operating voltage and high on/off ratio by preconditioned metal conducting filament. **J. Han**
- 9:10 690.** Designer gallium precursors towards functional materials. **K.L. Mears**, C.E. Knapp, C.J. Carmalt
- 9:30 691.** Synthesis and structural characterization of nano coordinated Cd(II) complexes. **M. Raja**
- 9:50** Intermission.
- 10:05 692.** Ultrathin PdAg single-crystalline nanowires enhance ethanol oxidation electrocatalysis. **H. Lv**, Y. Wang, D. Xu, B. Liu

- 10:25 693.** Accelerating the discovery of type II porous liquids using high-throughput automation. **R. Kearsley**, B.M. Alston, M.E. Briggs, R.L. Greenaway, A.I. Cooper
- 10:45 694.** Synthesis and design of semiconductor-core crystalline Bragg fibers. **A. Hendrickson**, M. Coco, J. Krug, C. Mathewson, S.C. Aro, S. McDaniel, J. Mauro, P. Sazio, G. Cook, V. Gopalan, J.V. Badding
- 11:05 695.** *In silico* design of new functional materials. V. Korolev, **A. Mitrofanov**, A. Eliseev, B. Sattarov, V. Tkachenko
- 11:25 696.** Experimental screening for discovery of low dimensional metal halides with intense white-light emission. **R. Gautier**

SECTION B

Marriott Marquis San Diego Marina
Solana

Organometallic Chemistry: Applications to Materials & Polymer Science

- N. S. Radu, *Organizer*
- 8:30 697.** ‘Super-bulky’ ligands: Coordination chemistry and application in ring-opening polymerization reactions. **C. Bakewell**
- 8:50 698.** Mechanistic and kinetic studies of ring-opening metathesis polymerization with third-generation Grubbs catalysts. D. Walsh, M. Hyatt, **D. Guironnet**
- 9:10 699.** Chemical mapping and optimization of redox switchable metal complexes for ring-opening polymerization. **A. Lai**, N. Fey, P. Diaconescu
- 9:30 700.** Electrochemically controlled redox-switchable ring-opening polymerization. **Z. Hern**, C. Liu, P. Diaconescu
- 9:50 701.** Increasing stereocontrol in lactide polymerization with flexible catalysts. P. Daneshmand, **F. Schaper**
- 10:10 702.** Redox switchable (co)polymerization reactions with a zirconium compound. **R. Dai**, P. Diaconescu
- 10:30 703.** CVD functionalization of graphene using transition metal carbonyls: Facile route to generate bandgaps. **K. Vinodgopal**, K. Robinson, X. You, J. Atkin, M. Terrones, D. Grasseschi, S.C. Sendlinger
- 10:50 704.** Nickel-based bimetallic catalysts for Olefin polymerization. **S. Xiong**, T. Agapie
- 11:10 705.** Introducing complexity to polysilanes using fused ring building blocks: Poly(siladecalin). **E. Marro**, R.S. Klausen

SECTION C
Marriott Marquis San Diego Marina
Marina Ballroom Salon D

Chemistry of Materials: Materials for Energy & Catalytic Applications

C. G. Lugmair, *Organizer*

V. Doan-Nguyen, R. Mishra, *Presiding*

- 8:30** **706.** Oxide ion conductors in the hexagonal perovskite family. **A. McLaughlin**, E. Wildman, S. Fop
- 8:50** **707.** MOF crystal branching: Novel solution to counteracting plasticization in MOF-polymer mixed-matrix membranes. **K. Zhang**, B.J. Sundell, D. Harrigan, S.C. Hayden, W. Chi, Z. Smith
- 9:10** **708.** Dual functions of water in stabilizing the metal-pentazolate hydrates $[M(N_5)_2(H_2O)_4]4H_2O$ (M = Mn, Fe, Co, and Zn) high-energy density materials. **M. Cheng**
- 9:30** **709.** Quinone-based metal-organic materials for energy storage and gas separation. **T. Chen**
- 9:50** **710.** Nanoporous ceramic membranes for redox flow batteries. **S. Candelaria**, K.L. Corp, A. Salunkhe, G.M. Newbloom
- 10:10** Intermission.
- 10:25** **711.** Generation of well-defined electrophilic surface sites on sulfated zirconium oxide. **M.P. Conley**
- 10:45** **712.** Structural evolution of transition metal trisulfide electrode materials. **V. Doan-Nguyen**
- 11:05** **713.** New look at an old compound: X-ray photocrystallography studies of potassium ferrioxalate upon photolysis in the solid state. **M. Nava**, M. Gonzalez, E.J. Johnson, D.G. Nocera
- 11:25** **714.** Storing solar energy: Photochemical oxygen capture and thermal release. **T. McCormick**, L. Lutkus
- 11:45** **715.** $KBaTeBiO_6$: Lead-free, inorganic double-perovskite semiconductor for photovoltaic applications. A.S. Thind, S. Kavadiya, M. Kouhnavard, R. Wheelus, S.B. Cho, L. Lin, A.Y. Borisevich, G. Pilania, P. Biswas, **R. Mishra**

SECTION D
Marriott Marquis San Diego Marina
San Diego Ballroom Salon C

Nanoscience

B. G. Trewyn, *Organizer*

- 8:30** **716.** Prussian blue analogues for templated nanoparticle growth. **E.T. Nguyen**, D.A. Hardy, G.F. Strouse
- 8:50** **717.** Probing the electronic states of small metallic nanoparticles using conduction electron spin resonance. **S.S. Cruz**, B. Lear

- 9:10** **718.** Electrolyte-induced conformational change of alkanethiolate ligands on gold nanoparticles in organic solutions. **V. Tanygin**, B. Lear
- 9:30** **719.** Bottom-up design of metal oxide and peroxide nanoclusters using neural networks. **P. Miro**
- 9:50** **720.** Carbon capture with MgO(111). **R.M. Richards**
- 10:10** **721.** STEM-in-SEM methods for 2D material defect and reliability studies. **E. Mansfield**, J.D. Holm
- 10:30** **722.** Active plasmonics based devices using metal oxide nanocrystals: Fundamentals and applications. **A. Agrawal**, D.J. Milliron

SECTION E
Marriott Marquis San Diego Marina
Santa Rosa

Solid-State Inorganic Chemistry

C. G. Lugmair, V. Poltavets, *Organizers*

R. Compton, T. Ortner, *Presiding*

- 8:30** **723.** Vacuum transport of transition metal-doped ZnSe fiber lasers. **A. Hendrickson**, J. Krug, C.J. Mathewson, M. Coco, S.C. Aro, S. McDaniel, P. Sazio, J. Mauro, G. Cook, V. Gopalan, J.V. Badding
- 8:50** **724.** New methods for measuring absolute optical constants using loose powders: Implementation, validation, and renewable energy applications. **P. Khalifah**, T. Glotch
- 9:10** **725.** Tuning the photoluminescence by controlling the oxidation states of dopants. **R. Gautier**
- 9:30** **726.** Withdrawn
- 9:50** **727.** Dimensional reduction of halide double perovskites. **B. Connor**, L. Leppert, M.D. Smith, J. Neaton, H. Karunadasa
- 10:10** **728.** Redox properties of dysprosium 3+/4+ in barium zirconate. **J.R. O'Brien**, S. Ricote, L. Krishna
- 10:30** Intermission.
- 10:45** **729.** Structural and physical properties of $CaLaMReO_6$. F. Yuan, **C.M. Thompson**
- 11:05** **730.** Geometrically frustrated magnetism in transition metal borides. **A. Iyer**, Y. Zhang, B. Fokwa
- 11:25** **731.** Varying the fermi level in gadolinium transition-metal aluminides. **G. Agbaworvi**, C. Thompson
- 11:45** **732.** Topotactic transformations of heterolayered borides. **L. Alameda**, R.E. Schaak
- 12:00** **733.** First-principles study of phase stabilities in $Al_{1-x}Fe_xOOH$ and $Al_{1-x}Cr_xOOH$ metal oxyhydroxides. **D. Pope**, A.E. Clark, M. Prange
- 12:15** **734.** Manipulating magnetic properties via chemical variations in $TlFe_3Te_3$. **R. Compton**, C.M. Thompson

SECTION F

Marriott Marquis San Diego Marina
Marina Ballroom Salon E

Organometallic Chemistry: Catalysis - Late Transition Metals

N. S. Radu, *Organizer*

M. A. Bowring, *Presiding*

- 8:30** **735.** Mechanistic insights of the direct arylation of arylhalides: Density functional theory study. **R. Wei**, P. Miro
- 8:50** **736.** Modeling the reactivity of alkanes toward organometallic electrophiles. **P.J. Perez**, A. Caballero, G. Asensio, M. Etienne, F. Maseras, A. Olmos, R. Gava, M. Besora, K. Jacobs
- 9:10** **737.** Thermodynamic hydricity as a tool for designing catalysts for hydrogenation of ketones and esters. **E.S. Wiedner**, B. Neisen, J.C. Linehan, A.M. Appel
- 9:30** **738.** Highly active ruthenium metathesis catalysts at low temperatures: Unprecedented ring-opening metathesis polymerization of cyclopentadiene. **S. Hong**
- 9:50** **739.** Robust Re(V) alkylidyne catalysts for alkyne metathesis reactions. **M. Cui**, W. Bai, H. Sung, I. Williams, Z. Lin, G. Jia
- 10:10** **740.** Strongly σ -donating ligands with pendant bases for water oxidation catalysis. **A.G. Nash**, B.D. Vincenzini, C.J. Breyer, B.E. Silva, D.B. Grotjahn
- 10:30** **741.** Large isotope effects in organometallic reactions. **M.A. Bowring**, P.T. Truong, E.D. Douma, M.P. Ahmad, Z. Mathe, J. Tsang
- 10:50** **742.** High variance of metal oxidation states in nickel catalysis. A. de Aguirre, I. Funes-Ardoiz, **F. Maseras**
- 11:10** **743.** Reversible CO₂/formate conversion by a homogeneous platinum electrocatalyst. **D.W. Cunningham**, J.Y. Yang

SECTION G

Marriott Marquis San Diego Marina
Marina Ballroom Salon G

Main Group Chemistry

T. Hudnall, *Organizer*

F. Jaekle, E. Lee, *Presiding*

- 8:30** **744.** Reactive phosphonium cations. **R. Dobrovetsky**
- 8:50** **745.** *N*-heterocyclic carbene-functionalized ferrocenes. **E. Lee**
- 9:10** **746.** Lewis pair functionalization of polycyclic aromatic hydrocarbons. K. Liu, M. Vanga, R. Lalancette, **F. Jaekle**
- 9:30** **747.** Lewis adduct formation of sulfones, sulfonate, and sulfate esters with arsenic and antimony pentafluoride. **T.H. Saal**, K.O. Christe, R.M. Haiges
- 9:50** Intermission.
- 10:00** **748.** C₆F₅B-Binolate: Synthesis, structure, Lewis acid–base chemistry and catalytic activity. **S. Garg**, C. Krempner
- 10:20** **749.** Guanidine-based intramolecular frustrated Lewis pairs (FLPs): Synthesis, structure and small molecule activation. **C. Manankandayalage**, C. Krempner
- 10:40** **750.** Reductive elimination at a carbene center. **D.R. Tolentino**, S. Neale, C. Isaac, S. Macgregor, M.K. Whittlesey, R. Jazzar, G. Bertrand
- 11:00** **751.** Carbones and catalysis. **T. Ong**

Nanoscale & Molecular Assemblies: Designing Matter to Control Energy Transport

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THURSDAY AFTERNOON – INOR

Nanoscale & Molecular Assemblies: Designing Matter to Control Energy Transport

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MEDI

DIVISION OF MEDICINAL CHEMISTRY

J. Schwarz, Program Chair

SUNDAY MORNING – MEDI

SECTION A

San Diego Convention Center

Room 6C

Machine Learning in Medicinal Chemistry

S. Patel, J. Stec, Organizers, Presiding

- 8:15** 1. NCATS ASPIRE: Synergizing engineering, synthetic chemistry, machine learning/AI, and biology to advance drug development. **D. Rudnicki**, K. Duncan, D.A. Tagle
- 8:55** 2. Lessons from the world's largest prospective application of machine learning to hit discovery. S. Omlid, K.T. Nguyen, A. Lee, D. Bernard, C. Laggner, A. Stecula, N.M. Henriksen, t. o'brien, J.M. Warrington, M.H. Ahmed, I. Wallach, **A. Heifets**, H. Lim
- 9:35** 3. Machine learning for hit discovery: Recent work in virtual screening and *de novo* drug design. **R.E. Amaro**, C. Parks, Z. Gaieb
- 10:15** Intermission.
- 10:30** 4. Designing for developability: Machine learning in data-driven drug discovery. **J. Karpiak**
- 11:10** 5. Withdrawn
- 11:50** Panel Discussion.

SECTION B

San Diego Convention Center

Room 6D

General Orals

J. B. Schwarz, Organizer

S. K. Cyr, Presiding

- 8:30** 6. Synthesis and evaluation of near-IR boron-dipyrromethene (BODIPY) bioconjugates selectively targeting cancers overexpressing epidermal growth factor receptor (EGFR). **N. Kaufman**, Q. Meng, K.E. Griffin, S.S. Singh, A. Dahal, Z. Zhou, F.R. Fronczek, J.M. Mathis, S. Satyanarayanajois, M. Vicente
- 8:50** 7. Where do recent candidate drugs come from?. **J. Boström**, D.G. Brown

- 9:10** 8. Discovery of lipid prodrugs of tenofovir with improved metabolic properties. **N. Pribut**, E.J. Miller, M. D'Erasmus, M. Dasari, K. Giesler, B. Iskandar, S.K. Sharma, M.B. Kim, A.E. Basson, D. Liotta
- 9:30** 9. Discovery of small molecule antagonists of the toll-like receptors TLR7/8/9 for the treatment of lupus. **A.J. Dyckman**, C.P. Mussari, D. Dodd, M.A. Poss, L. Lombardo, J.E. Macor, R. Sreekantha, L. Pasunoori, S. Posy, A. Tebben, D. Critton, S. Ruepp, D. Harden, D. Shen, M. Cvijic, Q. Zhao, A. Watson, P. Davies, G.L. Schieven, L. Salter-Cid, R. Srivastava, M. Subramanian, D. Tagore, S. Dudhgaonkar, P.H. Carter
- 9:50** 10. Discovery and disclosure of GLPG1205, a first in class GPR84 negative allosteric modulator in phase II clinical trial. F. Labeguere, S. Dupont, R. Brys, **R.L. Gosmini**, L. Saniere, R. Blanque, S. de Vos, L. Nelles
- 10:10** 11. 4,6-Disubstituted quinazolines as MEK5 inhibitors. **P.T. Flaherty**, S. Patel, A. Bhatt, T. Wright, J. Cavanaugh, M.E. Burow
- 10:30** 12. Azetidiny diamides as potent reversible inhibitors of monoacylglycerol lipase (MAGL). **B. Zhu**, P.J. Connolly, Y. Zhang, M. McDonnell, H. Bian, S. Lin, L. Liu, S. Zhang, K. Chevalier, C. Schubert, C. Milligan, C. Flores, M.J. Macielag
- 10:50** 13. Development of a PCAF/GCN5 bromodomain chemical probe/PROTAC toolbox and its utility in target (in)validation. **P. Humphreys**
- 11:10** 14. Selective ARTD8 inhibitors to better the understanding of metastatic cancers. **S.S. Schweiker**, A.L. Tauber, C. Kam, S.M. Levis
- 11:30** 15. Selective class I HDAC inhibitors based on aryl ketone zinc binding induce HIV-1 protein for clearance. **J. Liu**, J. Kelly, W. Yu, D. Clausen, Y. Yu, H. Kim, J.L. Duffy, C.C. Chang, R. Myers, D.J. Klein, J. Fells, K. Holloway, J. Wu, G. Wu, B. Howell, R. Barnard, J.A. Kozlowski
- 11:50** 16. Challenging the sensitivity of HDX/MS with a large heterodimeric protein receptor: Characterization of the binding interactions of new generation integrin $\alpha 4\beta 7$ inhibitors. F. Perez, H. Broughton, J.J. Carrillo, M. Vieth, A.m. Russell, S. Afshar, **A. Espada**

Origins & Future of Metabolite & Small Molecule Identification

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Measuring Protein Conformations & Folding Inside the Cell

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SUNDAY AFTERNOON – MEDI

SECTION A

San Diego Convention Center
Room 6C

General Orals

J. B. Schwarz, *Organizer, Presiding*

- 1:30** 17. Discovery of a series of pyrimidine carboxamides as inhibitors of vanin-1 for the treatment of inflammatory conditions. **A. Casimiro-Garcia**, C.P. Allais, A. Brennan, C. Choi, G. Dower, M. Fleming, R. Frisbie, J. Hall, D. Hepworth, H. Jones, B.D. Hollingshead, J.D. Knafels, S.W. Kortum, F.E. Lovering, S. Mohan, P.M. Morgan, C. Parnig, N. Pullen, F.J. Schlerman, J.W. Strohsbach, F. Vajdos, F. Vincent, H. Wang, S.W. Wright
- 1:55** 18. Discovery and development of novel diazeniumdiolate derivatives as nitric oxide donors. **N. Kauser**, A. Ali, M.D. Weisel, Y.L. Zhong, M.M. Lo, T. Bateman, K. Mitra, Y. Li
- 2:20** 19. Glycopeptide drugs from endogenous peptides violate all of Lipinski's rules and penetrate the BBB. L. Szabo, C. Apostol, W. Alabsi, T. Jaynes, M. Heien, J. Streicher, T. Falk, C. Liu, **R. Polt**
- 2:45** 20. Small molecule inhibitors of IRAK4. **M.C. Bryan**
- 3:10** 21. Novel, potent small-molecule inhibitors modulating immune-oncology targets CD73 and A_{2A}/A_{2B} adenosine receptors discovered via DNA-encoded library screening. **A.J. McRiner**, J.N. Andersen, L.A. Fouser, J. Zhang, K. Certel, J. Cuozzo, B. Chan, R. Chandran, M.A. Clark, D. Gikunju, C.D. Hupp, A.D. Keefe, J. Liu, Y. Liu, M. Monteiro, A. Olszewski, M. Von Rechenberg, D. Resnicow, H.A. Thomson, D.M. Troast, Z. Wang, N. Westlund, Y. Zhang, F. Zhou, X. Zhu, M. Briskin, D. Ezzeddine
- 3:35** 22. Asymmetric synthesis of aromatic lipoxin A_4 analogues with upper chain modifications. **A. Mahon**, P.J. Guiry
- 4:00** 23. Discovery of BMS-211, a self-immolative prodrug as an orally active imidazo[2,1-f][1,2,4] triazinepan-CK2 inhibitor for the treatment of cancer. **A.V. Purandare**, H. Wan, K. Zimmermann, C.M. Tarby, L. He, A.C. Hart, W. Johnson, Y. Zhang, D.

O'Malley, L. Chen, V. Ahuja, G. Zhang, J.A. Inghrim, H. Mastalerz, J.S. Tokarski, A.V. Gavai, G. Vite, B. Rupnow, J.T. Hunt, C. Gao, S. Roy, M. Obermeier, A. Fura, P.A. Elzinga, B. Henley, J. Lippy, J. Fagnoli, A. Hernamdez, Z. Hong, D. Wu, P. Li, N. Raghavan, G. Everlof, F. Lee

- 4:25** 24. Design, synthesis, and evaluation of novel heterocyclic warheads for cysteine targeting covalent inhibitors. **K. McAulay**, J. Kettle, R. Ward, M. Waring

SECTION B

San Diego Convention Center
Room 6D

Disease Modifying Approaches for the Treatment of Neurodegeneration

E. F. DiMauro, *Organizer*

H. Zhang, *Organizer, Presiding*

E. DiMauro, *Presiding*

- 1:30** Introductory Remarks.
- 1:35** 25. Discovery of small molecule inhibitors of neutral sphingomyelinase 2 for the treatment of neurodegenerative diseases. **C. Rojas**, M. Sala, A. Thomas, A. Chaudhuri, S. Yoo, Z. Li, R. Dash, R. Rais, N. Haughey, R. Nencka, B. Slusher
- 2:10** 26. Molecular insights into effects of Alzheimer's disease risk-variant R47H TREM2. **Z. Wang**
- 2:45** 27. Design, synthesis, and identification of novel, orally bioavailable non-covalent NRF2 activators. **B. Ma**, B.S. Lucas, A. Capacci, E. Lin, J. Jones, M. Dechantsreiter, I. Enyedy, G. Xiao, D. Marcotte, B. Li, K. Richter
- 3:20** Intermission.
- 3:35** 28. Discovery and development of potent, selective, and brain-penetrant LRRK2 kinase inhibitors for Parkinson's disease. **J. De Vicente**, M. Dresser, A.A. Estrada, J. Feng, A. Henry, C. Ho, S. Huntwork-Rodriguez, E. Negrou, S. Poda, K. Scarce-Levie, H. Solanoy, Z. Sweeney, G. Tonn, J. He, R. Zhang, M. Xu, B. Wong
- 4:10** 29. CD33: From Alzheimer's disease GWAS to therapeutic target. C. Rillahan, N. Vo, M. Taga, G. Guzman, J.J. Kohler, M. Schenone, W. Elyaman, S. Carr, P. De Jager, **E. Bradshaw**
- 4:45** 30. CoREST complex-selective HDAC inhibitors promote pro-synaptic effects and represent promising therapies for multiple neurodegenerative diseases. **N.O. Fuller**, A. Pirone, B.A. Lynch, M.C. Hewitt, M.S. Quinton, T.D. McKee, M. Ivarsson
- 5:20** Concluding Remarks.

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SUNDAY EVENING – MEDI

SECTION A

San Diego Convention Center
TBD

General Posters

J. B. Schwarz, *Organizer*

7:00 - 9:00

31. Therapeutic potential of the caspase 1 inhibitors for the treatment of inflammatory disease. **K. Kim**, M. Iyer, R. Cinar, G. Kunos
32. Discovery of BCL-X_L degraders as potent and platelet-sparing anticancer agents. **X. Zhang**, D. Thummuri, S. Khan, X. Liu, P. Zhang, D. Zhou, G. Zheng
33. Homology modeling of DNMT isoforms: Towards the identification of selective inhibitors in food chemicals. **A. Gomez García**, B. Hyang-Min, C. Sae-Lee, J. Medina-Franco
34. Discovery and structural optimization of small molecule inhibitors that regulate the wnt signaling pathway. **W. Zhang**
35. Synthesis, cytotoxicity, and apoptosis induction study of new tetrahydroisoquinoline derivatives. **K. Bielawski**, N. Pawlowska, A. Gornowicz, A. Bielawska, Z. Kaluza, A. Szymanowska, R. Czarnomysy
36. Syntheses, characterizations, and a preliminary comparative cytotoxicity study of berenil-platinum complexes. **A. Bielawska**, R. Czarnomysy, K. Bielawski, A. Gornowicz, A. Muszynska
37. Synthesis and anti-endoplasmic reticulum stress activity of 2-arylcarbonylhydrazinecarbothioamides. D. Kim, S. Park, S. Jang, W. Yun, K. Seon, K. Jeong, **T. Nam**
38. Dual CDK4/ARK5 inhibition by ON 123300 for targeting metastatic colorectal cancer. **M. Reddy**, S.C. Cosenza, S.A. Divakar, B. Akula, M.R. Mallireddigari, P. Reddy
39. Optimization of quinazolinone-based covalent inhibitors of KRAS^{G12C} in the discovery of AMG 510. **P. Lopez**, J.R. Allen, J.G. Allen, A.K. Amegadzie, K. Ashton, S. Booker, J.J. Chen, N. Chen, M.J. Frohn, G. Goodman, D.J. Kopecky, L. Liu, J.D. Low, V. Ma, T.T. Nguyen, N. Nishimura, A.J. Pickrell, A.B. Reed, Y. Shin, A. Siegmund, N.A. Tamayo, C. Tegley, M. Walton, H. Wang, R.P. Wurz, M. Xue, K.C. Yang, P.

Achanta, M.D. Bartberger, J. Canon, J.D. McCarter, C. Mohr, K. Rex, A. Saiki, T. San Miguel, L. Volak, K.H. Wang, D. Whittington, J. Lipford, V.J. Cee, B.A. Lanman

40. Synthesis and structure–activity relationships of pyrazine-2-carboxamide derivatives as novel echinoderm microtubule-associated protein-like 4 (EML4)–anaplastic lymphoma kinase (ALK) inhibitors. **K. Iikubo**, K. Kurosawa, T. Matsuya, Y. Kondoh, A. Kamikawa, A. Moritomo, Y. Iwai, H. Tomiyama, I. Shimada
41. Scaffold repurposing of a serotonin 2C agonist led to the discovery of highly selective dopamine D3 antagonists. **L. Tan, J. Cheng**
42. Discovery of BMS-986160 as a second-generation inhibitor of the hepatitis C virus NS3/4A with pan-genotypic antiviral activity. **L. Sun**, E. Mull, S. Kandhasamy, V. Baratam, S. Puttaswamy, N. Pulicharla, S. Vishwakrishnan, S. Reddy, R. Trivedi, S. Sinha, S. Sivaprasad, A. Rao, S. Desai, K. Ghosh, R. Rajamani, Y. Wang, H. Fang, A. Mathur, R. Rampulla, S. Jenkins, N.A. Meanwell, F. McPhee, P.M. Scola
43. Theoretical elucidation of the nucleophosmin enzyme inhibition by synthetic, natural, and designed new ligands: Molecular docking and molecular dynamic. **N. NEDJINI**, A. Ghomri, N. Missoum, S. Bouchentouf, S. Ghalem
44. Synthesis and evaluation of new enantiopure pyridine-based arylaminoalcohols as antimalarial drugs. E. Pair, A. Dassonville-Klimpt, G. Bentzinger, **P. Loupias**, A. Bouchut, C. Mullié, P. Agnamey, P. Sonnet
45. Exploration of *Mycobacterium tuberculosis* RNA polymerase's putative ppGpp binding site as a potential therapeutic target. **K. Guild**, M.A. Stefan, G. Garcia
46. Why is reversed-phase flash chromatography use increasing?. **J.R. Bickler**
47. Thiadiazole analogues as potent, liver selective glucokinase activators. **D.S. Yoon**, S. Wu, R.P. Brigance, S.S. Chen, W. Meng, y. shi, R.A. Smirk, s. tao, Y. Wang, H. Zhang, A. Mathur, S. Kalinowski, A. Wang, H. Fuentes, L. Kunselman, M. Cap, X. Ma, H. Liu, R. Zebo, J. Zalaznick, J. Taylor, B. Zinker, K. O'Malley, L.M. Kopcho, Q. Wang, K. Behnia, C. Xu, S. Spronk, X. Chen, Y. Yang, J. Josephs, E. Janovitz, P. Marathe, J. Whaley, J.C. Barrish, M. Kirby, P.T. Cheng
48. Synthesis and structure–activity relationship (SAR) studies of novel pyrazolopyridine derivatives as inhibitors of enterovirus replication. **Y. Xing**, J. Zuo, P.A. Krogstad, M.E. Jung
49. Synthesis of new FDI-6 derivatives as inhibitors and radiotracers of FOXM1. **C.S. Huerta García**, A.

Hernandez Campos, C.A. Velazquez, R. Castillo-Bocanegra

50. New 2-heteroaryl-4-quinolones as potential antibiotics targeting multi-drug resistant ESKAPEE pathogen communication systems. M. Duplantier, **P. Loupias**, E. Lohou, P. Sonnet

51. Synthesis and study of new aminoquinolinemethanols as potential antibacterial drugs. P. Laumailié, A. Dassonville-Klimpt, F. Peltier, **P. Loupias**, C. Mullié, C. Andréjak, S. Castelain, P. Sonnet

52. Efflux pumps in *Acinetobacter baumannii*: Molecular characterization and study of new 1-(1-naphthylmethyl)-piperazine analogs as potential inhibitors. M. Choquet, **P. Loupias**, E. Lohou, C. Mullié, P. Sonnet

53. Optimization of 4-hydroxy-3-(heteroaryl) pyridine-2-one APJ receptor agonists for potency and oral PK profile. **J.A. Johnson**, S. Kim, J. Jiang, M. Phillips, J.S. Bostwick, P.S. Gargalovic, J.M. Onorato, Y. He, C.E. Luk, C. Generaux, X. Chen, C. Xu, M.A. Galella, T. Wang, R.R. Wexler, H.J. Finlay

54. Design and synthesis of a targeted covalent inhibitor of poly(ADP-ribose) glycohydrolase (PARG). **B.T. Jones**, R. Martinez, L. Cleary, J. Sutton, H. Beck, J. Drummond, S. Perumal, N. Ravindran, T. Cheng, L. Belmont, B. Yao, X. Linghu, Z. Newby, J. Hager, M. Dillion, A. Stowell, C. Burt, A. Clifton

55. “First principle” concept in designing small molecules for targeting RNA expansion repeats. **A. Pushechnikov**, V.M. Kysil, R. Timakhov

56. Design, synthesis, and structure activity relationship of novel pyrazolo-pyrimidine muscarinic 1 positive allosteric modulators (M₁ PAM). **s. gagginapally**, D. Kancharla, M. Dasoju, N. Rao, R. Subramanian, R.V. Nirogi

57. Design, synthesis, and structure activity relationship of novel 1,2,4-triazine-3-one: Derivatives as multimodal compounds intended to treat schizophrenia. **V.R. Middekadi**, B. Narasimha, A.R. Mohammed, D. Sisodaya, V. Mekala, S. Petlu, R. Nirogi

58. Synthesis and biological evaluation of optimized analogues of the NPFF antagonist, MES304. **K. Galal**, C.R. McCurdy

59. Discovery of a bromodomain and extraterminal (BET) inhibitor with a low predicted human dose derived from an encoded library technology hit. **C. Wellaway**, D. Amans, H. Barnett, R. Bit, J. Brown, N. Carlson, C. Chung, A. Cooper, P. Craggs, R. Davis, T. Dean, J. Evans, L. Gordon, I. Harada, D. Hirst, P. Humphreys, K. Jones, T. Lewis, M.J. Lindon, D. Lugo, M. Mahmood, S. McCleary, P. Medeiros, D. Mitchell, M. O’Sullivan, A. Tolson, V. Patel, C. Patten, D. Poole,

R. Shah, J. Smith, K. Stafford, P. Thomas, M. Vimal, I. Wall, R. Watson, N. Wellaway, G. Yao, R. Prinjha

60. Development of novel sphingosine kinase inhibitors through structure-activity relationship study on jaspine B derivatives. **S. Inuki**, T. Miyagawa, S. Oishi, H. Ohno

61. Halogen bond and its application in drug design. Z. Xu, **W. Zhu**

62. Design, synthesis, and pharmacological characterization of novel carboxamides as 5-HT₄ receptor agonists. **R.K. Badange**, P.K. Achanta, V. Reballi, V. Mekala, G. Bhyrapuneni, V. Benade, R.V. Nirogi

63. Design, synthesis, and pharmacological characterization of novel series of 4,5,6,7-tetrahydro-thiazolo[5,4-c]pyridine derivatives as H₃ receptor antagonists. **P.K. Achanta**, S. Saraf, R.K. Badange, R. Subramanian, N.R. Mudanna, P. Jayarajan, R. Nirogi

64. Synthesis and anti-neuroinflammatory activity of N-heterocyclic analogs based on natural biphenyl-neolignan honokiol. **S. Lee**, Y. Yuan, S. Kwon, J. Lee, S. Seo

65. Enantioselective synthesis of homoisoflavanones by asymmetric transfer hydrogenation and their biological evaluation for antiangiogenic activity. **S. Kwon**, M. Heo, B. Lee, S. Lee, J. Lee, S. Seo

66. Enantioselective synthesis and absolute configuration determination of hydroxywilfordic acid in sesquiterpene pyridine alkaloids. **J. Lee**, Y. Yuan, S. Lee, S. Kwon, S. Seo

67. Discovery of an advanced dual chitinase inhibitors OAT-870: New potential therapeutic in therapy of lung diseases. **M.L. Kowalski**, M. Mazur, S. Olejniczak, R. Koralewski, B. Dymek, P. Sklepkiwicz, M. Mlacki, M. Salamon, W. Czestkowski, B. Borek, A. Bartoszewicz, G. Andryianau, K. Matyszewski, E. Pluta, A. Zagodzono, M. Mazurkiewicz, M. Piotrowicz, P. Niedziejko, M.M. Gruza, S. Klossowski, F. Stefaniak, K. Dzwonek, M. Nowotny, M. Kwiecien, A. Napiorkowska, J. Olczak, J. Golab, A. Golebiowski

68. Discovery of small molecule compounds interfering with YKL-40 carbohydrate binding as potential therapeutics for cancer. **L. Krzeminski**, W. Czestkowski, M. Mazur, **A. Bartoszewicz**, S. Olejniczak, A. Siwinska, K. Krysztofiak, A. Belczyk-Ciesielska, R. Koziel, D. Papiernik, M. Salamon, R. Koralewski, G. Andryianau, K. Matyszewski, E. Pluta, M. Piotrowicz, J. Golab, K. Dzwonek, J. Olczak, P. Dobrzanski, A. Golebiowski

69. Discovery of OAT-1441: Highly active, selective, and orally bioavailable inhibitor of

- human AMCase. **G. Andryianau**, M.L. Kowalski, M. Piotrowicz, B. Dymek, M. Salamon, A. Zagodzdon, A. Rymaszewska, M. Mazurkiewicz, S. Klossowski, P. Sklepkiewicz, M. Mazur, S. Olejniczak, R. Koralewski, K. Matyszewski, B. Borek, W. Czestkowski, P. Niedziejko, A. Bartoszewicz, E. Pluta, M.M. Gruza, K. Dzwonek, F. Stefaniak, J. Olczak, A. Golebiowski
- 70.** MOEsaic: Application of matched molecular pair analysis to SAR exploration. **G. Fortin**, A. Ajamian
- 71.** Protocol for validating small-molecule structure assignment using calculated ¹³C NMR chemical shifts with quantum mechanics and MOE. **A. Ajamian**
- 72.** Scaffold replacement and 3D ligand optimization applied to the discovery of tyrosine kinase inhibitors. **A. Ajamian**
- 73.** Structure-based predictions of CYP selectivity, reactivity, and regioselectivity. **A. Ajamian**
- 74.** Synthesis and evaluation of racemic [¹¹C] BLZ945: Candidate radioligand for PET imaging of brain macrophage colony-stimulating factor 1 receptor. **S. Altomonte**, C.L. Morse, J. Liow, R. Gladding, S. Zoghbi, B. Innis, V. Pike
- 75.** Novel glycolysis inhibitor improves the therapeutic regimen for triple negative breast cancer under hyperglycemic condition. **D. Tailor**, V. Kumar, A. Resendez, C. Going, S. Pitteri, **S.V. Malhotra**
- 76.** Examining ligand-HIV protease dissociation: Pathway, energy, flexibility, and comparison with association processes. **J. Sun**, M. Raymundo, Y.M. Huang, C. Chang
- 77.** Novel imidazopyrimidine binders to embryonic ectoderm development (EED) protein that inhibit polycomb repressive complex 2 (PRC2) activity. **A.C. Burns**, N. Arora, T.P. Bobinski, D. Briere, A. Calinisan, J. Christensen, J. Ketcham, M.R. Lee, P. Olson, N. Sudhakar, M.A. Marx
- 78.** Discovery of novel 4-alkylamino-2-(arylpiperazin)methylbenzotrile derivatives as virus entry inhibitors for treatment of HCV infection. X. Jiang, J. Tan, Y. Wang, J. Li, J. Jin, X. Shi, Y. Quan, **Y. Li**, Z. Peng, Z. Li
- 79.** Discovery of carbazole carboxamides as novel ROR α agonists. M. Yu, N. Sun, Y. Huang, Y. Yan, C. Zhu, Q. Xie, **Y. Wang**
- 80.** Focused gradient generation: Easy method development for normal phase preparative chromatography. **J.E. Silver**, R. Lewis, N. Fowler, I. Henderson, M. Xie
- 81.** Design and synthesis of folate receptor targeted self-immolative tris-payload conjugates. **H.K. Santhapuram**, K. Wang, A.E. Felten, J. Vaughn, P.J. Kleindl, C.P. Leamon, I.R. Vlahov
- 82.** Synthesis of targeted small molecule drug conjugates employing a self-immolative disulfide/quaternary ammonium-based linker system. F. You, **P.J. Kleindl**, J. Reddy, M. Vetzal, M. Nelson, C.P. Leamon, I.R. Vlahov
- 83.** Rational design and synthesis of novel inhibitors specific for interleukin-33. **Y. Kim**, J. Han, J. Paek, K. Kim, S. Park, D. Choi, S. Son, S. Son, K. Lee, K. Lee, Y. Jung, Y. Jeon, Y. Byun
- 84.** Discovery of biphenylflavone analogs as novel TSLP Inhibitors. **D. Choi**, B.B. Park, Y. Park, T. Lim, Y. Kim, S. Son, Y. Jung, K. Lee, K. Lee, Y. Jeon, Y. Byun
- 85.** Design and synthesis of non-peptide analogs as novel hepsin inhibitors. **H. Kwon**, H. Ha, S. Nam, S. Son, Y. Byun
- 86.** Design and synthesis of trisubstituted pyridines as AKT inhibitors. **D.L. Prado Romero**, A. Hernandez Campos, R. Castillo-Bocanegra
- 87.** Discovery of small molecules that interact with Rpn-6 and are toxic to hematological cancers. **W. Tian**, D.J. Trader
- 88.** Synthesis and *in vitro* anticancer evaluation of novel 2,4,6-trisubstituted pyridines designed as AKT inhibitors. **J. Miguel**, A. Hernandez Campos, R. Castillo-Bocanegra
- 89.** Pharmacophore-based tailoring of new fused thiophenes for JNK inhibition as potential anticancer agents. **s.A. abdelrahman**, A. Kareem, G. Hassan, A. Maarouf, A.K. Salem
- 90.** Establish cell-based assays for small molecules evaluation toward mucopolysaccharidosis type II. **C. Yu-Hsin**, W. Cheng
- 91.** Synthesis of nucleotide-based inhibitors against bacterial cell wall translocase MraY. **Y. Lin**, W. Cheng
- 92.** Exploring Zafirlukast as a novel West Nile virus NS2B-NS3 protease inhibitor. **S. Nguyen**, N.T. Salzameda
- 93.** Synthesis and initial assessment of 6-aminopyridin-3-ol derivatives against inflammatory bowel disease *in vitro* and *in vivo*. **T. Nam**, S. Park, H. Kim, K. Seon, S. Banskota, B. Jeong, J. Kim
- 94.** Novel synthesis of chiral 2-trifluoromethylmorpholine. **J. Li**, L. Qi
- 95.** Syntheses of 2-fluoropyridines. **G. Yang**, S. Yu, H. Li, M. Yang
- 96.** Improved synthesis of 4,4-disubstituted-2-aminomethyl oxetanes. **H. Lian**, G. Liu, S. Yu, M. Yang
- 97.** Syntheses of 2-fluoromethyl N-containing heterocycles. **J. Xu**, S. Yu, H. Li, M. Yang

- 98.** Natural products as source to find potential inhibitors from methicillin-resistant *Staphylococcus aureus* shikimate kinase: *In silico* based screening. **I.i. Lozano**, A. Téllez Valencia, M. Gómez Palacio, J. Cisneros-Martinez, C.I. Avitia Domínguez
- 99.** Exploration of target space of electrophilic quinazolines. **B. Espinosa**, A. Ekanayake, C. Zhang
- 100.** Synthesis and spectroscopic identification of analgesic prodrugs attached to polyvinyl alcohol or polyvinyl phenol. **K. Mohamoud**, H.D. Tabba
- 101.** Pharmacophore-based virtual screening for finding potential inhibitors of shikimate kinase from methicillin-resistant *Staphylococcus aureus*. **L.I. Rios**, A. Téllez Valencia, C.I. Avitia Domínguez
- 102.** Structural characterization of capillary morphogenesis gene 2 inhibitors. **S. Soleimani**, J.D. Moody
- 103.** New methodology for the synthesis of sirtinol analogues a Sirtuin 2 inhibitor as antichagasic candidates. E.F. Pereira, R.A. Gomes, H.A. Stefani, **G.H. Trossini**
- 104.** *pro*-Pyrrolobenzodiazepine (*pro*-PBD) bioconjugates, part 5: Design and synthesis of *bis-pro*-PBD conjugates containing a self-immolative linkers that release active drug via intramolecular diazepine-ring-closure. I.R. Vlahov, **A.E. Felten**, N. Zou, K. Wang, S. Hahn, J. Vaughn, C.P. Leamon
- 105.** Glycone manipulation as a general strategy of optimizing the drug properties of the phyllanthusmin class of natural products. **B.K. Mize**, A. Huntsman, A. Young, J.L. Woodard, H. Chai, Y. Ren, M.A. Phelps, A.D. Kinghorn, J.E. Burdette, J. Fuchs
- 106.** Carbamate-benzoxaborole compounds as potent and broad-spectrum antifungal agents targeting protein prenylation. T. Liu, L. Whitesell, D. Kim, Y. Zhang, **Y. Zhou**, C. Liu, C. McGregor, M. Aubrey, L. Cowen
- 107.** Novel macrocyclic lipopeptides as serine protease inhibitors targeting *Escherichia coli* type I signal peptidase. **A. Benediktsdottir**, N. Natalia Szalaj, L. Lu, E. Zamaratski, S. Cao, G. Olanders, A. Karlén, M. Erdélyi, D. Hughes, S. Mowbray, P. Brandt
- 108.** Development of a prodrug strategy for CNS delivery of nuclear receptor modulators. **S.J. Ferrara**
- 109.** Synthesis and trypanocidal activity of new N-(1H-benzimidazole-2-yl)benzenesulfonamides. **A. Hernandez Campos**, C.S. Huerta García, C. Nava-Garcia, R. Nieto-Meneses, L. Yépez-Mulia, A. Vazquez-Raygoza, A. Téllez Valencia, R. Castillo-Bocanegra
- 110.** Synthesis and evaluation of a series of analogues to the AT₂R prototype antagonist C38. **J. Lindman**, R. Isaksson, J. Wannberg, J. Sallander, M. Backlund, D. Baraldi, R. Widdop, M. Hallberg, J. Åqvist, H. Gutierrez de Teran, J. Gising, M. Larhed
- 111.** Scaffold hopping: Versatile approach to develop new ligands for Liver X Receptor. **R. Komati**, J. Miller, J. Sridhar, K. Riley
- 112.** Synthesis of 2-aminooxazole inhibitors of kinase STK-16. **R. Schioldager**, A. Manjunath, N. Soderberg, D. Liyanage, **S.C. Eagon**
- 113.** Synthesis of benzoxazole inhibitors of kinase CK2. B.D. Popa, **E. Schwegman**, D. Liyanage, **S.C. Eagon**
- 114.** Synthesis of cathepsin B inhibitors as a treatment targeting anthrax and ebola. **S. Platt**, **I. Hernandez**, H. Wood, J. Gieschen, **S.C. Eagon**
- 115.** Novel boron-enhanced compounds with broad spectrum antifungal activity. C. Liu, T. Liu, Y. Zhang, Y. Zhou, C. McGregor, **M. Aubrey**
- 116.** Withdrawn
- 117.** Discovery of allosteric inhibitors of NF-κB inducing kinase (NIK). **J. Tang**, O. Demir, G. Chan, A. Ayoub, R.E. Amaro, D.A. Harki
- 118.** Structure property relationship of fluorinated carboxylic acid bioisosteres. **T. Alle**, K. Oukoloff, B. Lucero, Z. Owyang, S. Joyasawal, K. Long, T. Paniak, V. Tran, A. Devas, D.M. Huryrn, M. Kozlowski, D. Cahard, C. Ballatore
- 119.** Leveraging atropisomerism to obtain a selective inhibitor of RET kinase with secondary activities towards EGFR mutants. **S. Toenjes**, **V. Garcia**, S.M. Maddox, G. Dawson, M.A. Ortiz, J. Piedrafitra, J.L. Gustafson
- 120.** Benzimidazole derivatives as new potential antibacterial and antifungal agents. **S. Melo Hernandez**, **C. Cabrera**, D. Vargas, J. Diaz, J. Portilla, E. Jimenez
- 121.** IODVA1, a di-pyridine derivative with *in vivo* activity against cancer models. **G. Premnauth**, E.J. Merino, N. Nassar
- 122.** Design, synthesis, and biological evaluation of the inhibitors of fatty acid binding protein 5 (FABP5) as next-generation therapeutics for chronic pain and inflammation. **A. Taouil**, M. Awwa, T. Clement, A. Maharaj, J. Kim, Y. Sun, A. Pepe, H. Li, R.C. Rizzo, M.W. Elmes, M. Kaczocha, I. Ojima
- 123.** Revised synthesis of TC007: Potent lead for SMA treatment. **U. Pandey**, Y.P. Subedi, C.T. Chang
- 124.** Structure-activity relationships of phenypyrimidine compounds as novel candidate treatments for schistosomiasis. **L. Monti**, K. Oukoloff, A. Cornec, S.C. Wang, N. El-Sakkary, D.E. Skinner, K. Brunden, C.R. Caffrey, C. Ballatore
- 125.** Design and synthesis of tri-aryl methyl amine compounds for biological evaluation as anti-

- infective agents. **I. Bal**, W. Hatcher, T. Van Laar, S. Maitra
- 126.** Design, synthesis, and evaluation of GUNW-3 as a brain-targeting agent. **A. Najmi**, S. Wang, Y. Huang, Y. Alqahtani, X. Guan
- 127.** Diversity oriented synthesis encoded by deoxyoligonucleotides. **J. Mason**, L. Hudson, M.V. Westphal, C.J. Gerry, B. Hua, W. Wang, H.L. Osswald, G. Xia, B. Melillo, C. Gampe, S. Bonazzi, N. Smith, R.G. Karki, J. Ottl, F. Berst, F. Zecri, K. Briner, J. Bradner, S.L. Schreiber
- 128.** Synthesis and evaluation of small molecule scaffolds as potential protein-protein interaction inhibitors to prevent gankyrin-MDM2 binding. **S. Yoganathan**, J. Kong, A. Muth
- 129.** Use of neomycin as a side chain for phenanthroline based G-quadruplex binding ligands and telomerase inhibitors. **M. Singh**, R. Hekman, C. Vierra, L. Xue
- 130.** *In silico* screening and synthesis of 2,5,6-trisubstituted benzimidazoles as a new class of antitubercular agents targeting FtsZ. **S. Kim**, K. Haranahalli, A. Panapakides, A. Taouil, M. Awwa, I. Ojima
- 131.** eIF4E mRNA-cap-competitive covalent inhibitors: Design, synthesis and effectiveness. **V.H. Grant**, D.S. Mortensen, L. Nadolny, S. Norris, D. Huang, J. Elsner, J.S. Parnes, L. Tehrani, S.G. Hegde, Z.D. Aron, D. Niu, K. Fultz, J. Apuy, K. Leftheris, B. Pagarigan, S.L. Delker, S. Bahmanyar, K.R. Condroski, J.C. Petter, P. Chamberlain
- 132.** Light-activated, targeted treatment of traumatic brain injury. **C. Black**, E. Zhou, C.M. DeAngelo, I. Asante, S.G. Louie, M.S. Humayun, N.A. Petasis
- 133.** Atropisomerism and PROTACs as strategies towards increased potency and selectivity of analogs of common kinase inhibitors. S. Toenjes, **S. Albright**, **R. Hazin**, S. Vaidya, J.L. Gustafson
- 134.** Design, synthesis and biological evaluation of new anti-*Candida* agents. **K. Rodriguez Villar**, A. Hernandez Campos, M.E. Drago-Serrano, J. Palacios-Espinosa, J. Cortés Benítez, O. Soria-Arteche, J.P. Villanueva
- 135.** Co-crystal structure-based drug design and synthesis of plinabulin derivatives. M. Ma, Z. Ding, S. Wang, L. Ma, Y. Wang, J. Yang, **W. Li**
- 136.** Selective bromodomain inhibition of BRD4-D1 using trisubstituted-imidazoles and triazoles. **A. Divakaran**, H. Cui, S. Henry, A. Carlson
- 137.** Withdrawn
- 138.** Preparation of intermediate of asenapine. **x. tian**, J. Ding, R. Zhang
- 139.** Withdrawn
- 140.** Development of a chemoproteomic platform for identifying cell membrane proteins as drug targets from live cells and tissues using chemical probe. **R. Miyajima**, Y. Otani, K. Sakai, T. Wadatsu, M. Tanaka, T. Hayashi, M. Hayashi, K. Kondo
- 141.** Significance of chirality in drug design and synthesis of bitopic ligands as D₃R selective agonists. **A. Bonifazi**, F. Battiti, S. Cemaj, A.M. Guerrero, A. Shaik, A.H. Newman
- 142.** D₄R-Selective compounds reveal structure-activity relationships that engender agonist efficacy. **C.A. Boateng**, T.M. Keck, R. Free, S.L. Brown, M.S. Maddaluna, A. Bonifazi, A.H. Newman, D.R. Sibley, C. Wu
- 143.** Discovery of pyrrolo[3,2-d]pyrimidine-containing compounds as inhibitors of NIK kinase. **Y. Zhao**, Z. Li, Z. Yan, X. Lv
- 144.** Discovery of 'all-in-one' nitric oxide-donor cephalosporin-3'-diazoniumdiolates with dual-antibacterial and antibiofilm properties. **M.J. Kelso**
- 145.** Targeting cancer fructose metabolism: Development of novel ketohexokinase inhibitors. **X. Liu**, B.R. Wilde, S.K. Thaker, H.R. Christofk, M.E. Jung
- 146.** Ester bioisostere analogues of Astemizole as potential antiplasmodium agents. **D. Mambwe**, K. Chibale
- 147.** Modification of lactoferrin by peroxyinitrite reduces its antibacterial activity and changes protein structure. **A.Y. Alhalwani**, R.L. Davey, N. Kaul, s.A. barbee, J.A. Huffman
- 148.** Synthesis of [¹⁸F]FPFB through radiofluorination of a diarylselenoxide and diarylselenone precursor. **C.F. Lynch**, F.G. Simeon, S. Lu, V. Pike
- 149.** Phosphoramidate derivatives as controlled-release prodrugs of L-Dopa. **F.P. Olatunji**, B.N. Kesic, C.J. Choy, C.E. Berkman
- 150.** Discovery of tetrahydroisoquinoline-containing CXCR4 antagonists with enhanced ADMET properties and evaluation as anti-cancer agents. **E.J. Miller**, E. Jecs, C. Sun, Y.A. Tahirovic, S. Sharma, L.J. Wilson, H.T. Kissick, H.H. Nguyen, R.J. Wilson, M.B. Kim, R. Arnold, J. Petros, D. Liotta
- 151.** Synthesis of PPAR ligands for the control of mesenchymal stem cell differentiation: Novel treatment avenue for osteoporosis. **B.J. Kress**, D. Kim, J.R. Mayo, J.T. Farris, J.G. Sarver, J.A. Trendel, B.E. Heck, P.W. Erhardt
- 152.** Microwave-assisted expeditious and efficient synthesis of novel quinolin-4-ylmethoxychromen-2- and -4-ones catalyzed by YbCl₃ under a solvent free one-pot three component domino reaction and their

antimicrobial activity. **S. Kumar**, A. Patel, N. Ahmed

153. Structure-activity relationship and evaluation of non-electrophilic NRF2 activators in a diabetic mouse model. **B. David**, M. Barakat, P. Lazzara, L. Chen, L. DiPietro, T.W. Moore

154. Modeling drug metabolism identifies intermediate metabolites which precede reactive metabolite formation. **N. Flynn**, M. Ward, S. Swamidass

155. Design of GSK9742, a chemical probe for the TAF1/TAF1L bromodomains. **M. Clegg**, N. Theodoulou, G. Liwicki, R. Prinjha, N. Tomkinson, P. Humphreys

156. Assessing the liability of isoxazole containing compounds to form reactive metabolites. **M. Ward**, R. Farmer, N. Flynn, W.C. Pomerantz, G.P. Miller, S. Swamidass

157. Combatting the opioid and benzodiazepine epidemic by the synthesis of novel safer drugs designed to be functionally selective for $\alpha 5$ - or $\alpha 6$ -containing GABA_A receptors. **D.E. Knutson**, G. Li, T. Prevot, L. Arnold, L. Chiou, M. Ernst, M. Mihovilovic, M. Savic, W. Sieghart, E. Sibille, J.M. Cook

158. Computationally bridging the gap: From fragment hit to lead. **W.S. Wade**, T. Meyer, T.A. Ford-Hutchinson, P.V. Pallai

159. Solvent-free biogels for mechanobiology. **F. Fahimipour**, E. Dashtimoghadam, M. Vantankhah-Varnosfaderani, S. Sheyko

160. Metabolism enhanced multiplexed FDA-approved drug screening for novel antibacterial activities. **W.G. Gutheil**, N.J. Ayon

161. Novel computational strategy for neuroprotection prediction: Identification of novel nicotine-analogs as potential Parkinson therapeutic agents. **F. Rojas**, C. Morantes, R. Cabezas, G. Barreto, A. Pinzón, J. Gonzalez

162. New rhodium(I) NHC complex targeting TrxR inhibits hepatocellular carcinoma *in vivo*. **w. liu**

163. Discovery of potent hits and solving ADME challenges with free energy perturbation and deep learning. **S. Mondal**, J. Greenwood, S. Feng, P. Ghanakota, S. Rafi, B. Kim, Y. Deng, Y. Wu, L. Wang, K. Leswing, C. Wu, E. Harder, R. Abel

164. Structure and ligand-based design of promising small molecule EZH2 inhibitors. **F. Ramilo-Gomes**, S.D. Bryant, T. Langer, R. Martini, L. Sobral, M. Marques, R.C. Guedes

165. Milestone based computational approach to estimate energy barriers in the drug designing, and application to P38-MAP kinase-SB2 system. **H.D. Pandey**, **S. Chen**, **Z. Tang**, **C. Chang**

166. Development of bioactive γ -AA peptides based peptidomimetics to control angiogenesis.

S.A. Abdulkadir, P. Sang, C. Li, J. Cai

167. Preformulation analysis and stability of hydrophobic small molecular echinomycin for injection formulation. **J. Lee**, M. Tran, P. Yuan, G.K. Potti

168. Biological and computational assessment of (-)-Incarvillateine mechanism of action. **M. Awwa**, J. Kim, D.M. Bogdan, M.W. Elmes, S. Yan, J. Che, G. Lee, D.G. Deutsch, R.C. Rizzo, M. Kaczocha, I. Ojima

169. Approaches to demonstrate pharmaceutical equivalence of Ibrutinib cocrystal complex for the follow-on generic drugs. **W. Jiang**, W. Liu, Y. Xu, B. Lim, D. Skanchy, R. Randad

170. Introduction of BBXC (building block exchange): New business model to efficiently access novel monomers. **S. Sakata**, **D. McLeod**, E. Cooper, C.J. Helal, B. Lefker, J. Klug-McLeod, H. Zhu, J. Wasserman, M. Munchhof, L. Meerpoel, C. Krogman, M. Willis, B. Daniel

Biosensing: New Strategies & Latest Development

Sponsored by ANYL, Cosponsored by BIOL, BIOT and MEDI

MONDAY MORNING – MEDI

SECTION A

San Diego Convention Center

Room 6C

Rising Stars: Women in Medicinal Chemistry

Cosponsored by WCC

A. L. Garner, *Organizer, Presiding*

- 8:30** Introductory Remarks.
- 8:35** **171.** Strategies for targeting aberrant microRNA activity in cancer. **A.L. Garner**
- 9:05** **172.** Fragment to lead: Discovery and optimization of a novel bromodomain inhibitor. **A. Adams**
- 9:35** **173.** Chemical targeting of deubiquitinating enzymes. **S. Buhrlage**
- 10:05** Intermission.
- 10:20** **174.** PROTAC™ targeted protein degraders: Exciting modality for drug discovery. **E. Araujo**
- 10:50** **175.** Generating new synthetic transformations and unique heterocycles to drive anti-infective agent discovery and development. **J.E. Golden**
- 11:20** **176.** Enabling medicinal chemistry as a process chemist. **J. McCabe Dunn**
- 11:50** Concluding Remarks.

SECTION B
San Diego Convention Center
Room 6D

Catastrophic Epilepsies: How Medicinal Chemists can Help

Financially supported by Sage Therapeutics
M. Blanco, *Organizer, Presiding*

- 9:00** Introductory Remarks.
- 9:05** **177.** Overview of current drug discovery approaches for childhood epilepsies. **A. Mingorance**
- 9:55** **178.** Phytocannabinoids in the modern treatment of catastrophic epilepsies. **G. Guy**
- 10:40** Intermission.
- 10:55** **179.** Nav1.6 inhibitors: Approach to treat severe childhood epilepsies. **T. Focken**, M.E. Grimwood, V.A. Lofstrand, K. Burford, W. Gong, Q. Jia, A. Hasan, M. Taron, W. Zhang, M. Wilson, P.K. Tari, G. Bankar, S. Singh, K. Nelkenbrecher, K. Khakh, E. Chang, J.B. Li, J. Mezeyova, S. Goodchild, N.G. Shuart, S. Lin, R. Kwan, L. Sojo, C.J. Cohen, N. Weishaupt, S.S. Wesolowski, J.P. Johnson, C.M. Dehnhardt, J.R. Empfield
- 11:30** **180.** Novel synthetic neurosteroids to reduce seizure burden and improve survival in preclinical models of catastrophic epilepsies. **M. Blanco**
- 12:05** Concluding Remarks.

Future of Biomacromolecules at a Crossroads of Polymer Science & Biology
Synthetic Cells

Sponsored by POLY, Cosponsored by BIOL, CARB, CELL, COLL, ENVR, MEDI, PHYS and PMSE

Recent Advances in Kinase Drug Discovery: A Joint Venture Between Medicinal, Biological & Computational Chemists

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2019 ACS International Award for Research in Agrochemicals: Advances in the Physiology & Biochemistry of Insect Control

Sponsored by AGRO, Cosponsored by AGFD, BIOL, MEDI, POLY and PROF

MONDAY AFTERNOON – MEDI

SECTION A
San Diego Convention Center
Room 6C

Optimizing Brain Penetration

A. B. Dounay, *Organizer, Presiding*

- 1:30** **181.** Probabilistic MPO (pMPO) and its application in CNS drug discovery. **H. Gunaydin**
- 2:00** **182.** Harnessing preclinical data as a predictive tool for human brain tissue targeting. **N. Patel**
- 2:30** **183.** BBB organoid platform for modeling therapeutic delivery to the brain. **C. Cho**, J. Wolfe, C.M. Fadzen, D. Calligaris, K. Hornburg, **E. Chiocca**, N. Agar, B.L. Pentelute, S. Lawler
- 3:00** Intermission.
- 3:15** **184.** Use of a CSF cannulated dog model in development of BACE1 inhibitors. **S. Monk**
- 3:45** **185.** Considerations for optimizing CNS penetration and successful programs. **C.W. Lindsley**
- 4:15** **186.** Optimization and identification of brain penetrant, M4 subtype-selective muscarinic receptor positive allosteric modulator (M4 PAM) clinical candidate. **C. Butler**

SECTION B
San Diego Convention Center
Room 6D

No Linker Required: Non-PROTAC Degraders

G. Wang, *Organizer*
J. Liang, *Organizer, Presiding*

- 1:00** **187.** Cyclic peptide ternatin-4 promotes degradation of the translation elongation factor, EF1A. **J.W. Taunton**
- 1:40** **188.** Small-molecule estrogen receptor degraders (SERDs): Chemical exploration and optimisation at AstraZeneca. **J.S. Scott**
- 2:20** **189.** Small molecules that catalyze the degradation of splicing factors. **D. Nijhawan**
- 3:00** **190.** Discovery of CC-92480: CRBN E3 ligase modulating drug (CELMoD) for the treatment of relapsed and refractory multiple myeloma. **J.D. Hansen**, M. Nagy, M. Correa, t. kercher, r. harris, M.D. Alexander, D. Huang, v. plantevin, V.H. Grant, b. whitefield, A. Lopez-Girona, C. Havens, D. Mendy, R. Krishna Narla, Y. Tang, J.R. Piccotti, B.E. Cathers, g. khambatta, I. LeBrun
- 3:40** **191.** ASTX660, a small molecule antagonist and degrader of cellular inhibitor of apoptosis proteins in phase I/II clinical trials. **R. Holvey**

- 4:20** **192.** Discovery and characterization of a novel small molecule BRD4 protein degrader. **P.S. Dragovich**, R.A. Blake, H. Chen, J. Chen, E. Cosino, I. Enquist, K.E. Gascoigne, S.J. Hartman, S. Kaufman, D.S. Kirkpatrick, T. Kleinheinz, C. Li, Y. Lu, J. Murray, T. Pillow, G. del Rosario, C.M. Rose, R.K. Rowntree, L.R. Staben, S.T. Staben, J.S. Wai, I.E. Wertz, C. Wilson, Z. Xu, J. Xue, H. Yao, S. Yu, B. Wei, M. Wong, C. Zhang, D. Zhang, H. Zhou

2019 ACS International Award for Research in Agrochemicals: Advances in the Physiology & Biochemistry of Insect Control

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Future of Biomacromolecules at a Crossroads of Polymer Science & Biology

Tissue Engineering

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Recent Advances in Kinase Drug Discovery: A Joint Venture Between Medicinal, Biological & Computational Chemists

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MONDAY EVENING – MEDI

SECTION A

San Diego Convention Center
TBD

Sci-Mix

J. B. Schwarz, *Organizer*

8:00 - 10:00

39, 45, 58, 72, 77, 87, 92, 99, 102, 107, 108, 109, 111, 114, 115, 117, 124, 132, 134, 140, 142. See Previous Listings.
253, 263, 266, 268, 280, 282, 289, 295, 298, 299, 307. See Subsequent Listings.

TUESDAY MORNING – MEDI

SECTION A

San Diego Convention Center
Room 6AB

MEDI Awards Symposium

J. B. Schwarz, *Organizer*
A. Stamford, *Presiding*

- 9:00** **193.** Translational chemistry. **P.S. Baran**
9:45 **194.** Progress in the discovery of kinase inhibitors for treatment of parasitic diseases. **D.P. Rotella**
10:20 **195.** Joining forces: Discovery of novel biological tools and utilising new therapeutic modalities. **A.T. Plowright**
10:55 **196.** How I spent my summer vacation: Insights from a 30-year career in drug discovery (and molecules that have broken my heart). **J.E. Macor**

SECTION B

San Diego Convention Center
Room 6D

Drug Discovery Beyond the Rule of 5

D. A. DeGoey, *Organizer, Presiding*

- 8:30** Introductory Remarks.
8:35 **197.** Property-based drug design: bRo5. **P.B. Cox**
9:05 **198.** Onward, beyond the rule of 5! Understanding and controlling cell permeability in macrocyclic peptides. **S. Lokey**
9:35 **199.** Approaches to targeting protein-protein interactions. **M.R. Arkin**
10:05 **200.** Breaking the rules to interdiction at a protein-protein interface: Structure-based design of the Mcl-1 inhibitor AMG 176. **S.P. Brown**
10:35 **201.** Design of orally bioavailable proteolysis targeting chimera (PROTAC) small-molecule degraders. **S. Wang**
11:05 **202.** Chemical induced dimerization for targeted protein degradation. **J. Bradner**
11:45 Concluding Remarks.

Recent Developments in Structural Biology

Sponsored by BIOL, Cosponsored by MEDI

2019 ACS International Award for Research in Agrochemicals: Advances in the Physiology & Biochemistry of Insect Control

Sponsored by AGRO, Cosponsored by AGFD, BIOL, MEDI and PROF

Global Health: Biology & Chemistry of Waterborne Diseases

Sponsored by BIOL, Cosponsored by MEDI

Mass Spectrometry of Biomolecular Assemblies

Sponsored by ANYL, Cosponsored by BIOT, BMGT and MEDI

Biostimulants in Agriculture: Chemistry & Regulatory Aspects

Sponsored by AGRO, Cosponsored by BIOL, MEDI and TOXI

Recent Advances in Kinase Drug Discovery: A Joint Venture Between Medicinal, Biological & Computational Chemists

Sponsored by COMP, Cosponsored by MEDI

TUESDAY AFTERNOON – MEDI

SECTION A

San Diego Convention Center
Room 6AB

MEDI Awards Symposium

J. B. Schwarz, *Organizer*
A. Stamford, *Presiding*

- 2:00** **203.** Targeted small molecule degradation of a hypoxia-associated non-coding RNA enhances the selectivity of an RNA targeted small molecule. **M.G. Costales**, B. Suresh, M.D. Disney
- 2:25** **204.** Novel phyllanthusmin derivatives as anticancer agents: Pharmaceutical optimization and mechanistic insight. **A. Huntsman**, B.K. Mize, A. Young, E. Addo, J.L. Woodard, H. Chai, Y. Ren, M.A. Phelps, A.D. Kinghorn, J.E. Burdette, J. Fuchs
- 2:50** **205.** Altering the tumor microenvironment to improve immunotherapy: Molecular imaging of PD-L1 in pancreatic cancer. **K.E. Henry**, M. Davydova, T.R. Dilling, I.L. Fox, J. Lewis
- 3:15** **206.** Encoding all stereoisomers of homologous cyclic α -aryl amino acids. **L. Hudson**, C. Gerry, F. Zecri, K. Briner, S.L. Schreiber
- 3:40** **207.** Adventures in allosteric drug discovery. **C.W. Lindsley**
- 4:20** **208.** Immunopharmacotherapy for the treatment of substance use disorders. **K.D. Janda**

SECTION B

San Diego Convention Center
Room 6D

Privileged & Underprivileged Functional Groups in Drug Design

N. A. Meanwell, P. M. Scola, K. Yeung, *Organizers, Presiding*

- 2:00** Introductory Remarks.
- 2:05** **209.** Natural product derived privileged scaffolds in drug discovery. **M. Brimble**, E. Davison
- 2:35** **210.** Leveraging the necessary nitrogen atom in chemical biology and drug discovery. **L.D. Pennington**
- 3:05** **211.** Geminal diheteroatomic motifs in drug design: Applications of acetals, ketals, and their sulfur and nitrogen homologues in medicinal chemistry. **Y. Wu**, N.A. Meanwell
- 3:35** **212.** Design of ligands targeting carbohydrate binding sites: Galectin 3. **F. Zetterberg**
- 4:05** **213.** Sulfoximines in drug discovery revisited: What has happened since 2013?. **U.T. Luecking**
- 4:35** **214.** Advances in neurosteroid drug discovery: GABA and NMDA modulators. **M. Blanco**

ACS Infectious Diseases Young Investigators Award Symposium

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TUESDAY EVENING – MEDI

Future of Biomacromolecules at a Crossroads of Polymer Science & Biology

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SECTION A

San Diego Convention Center

Room 6AB

First Time Disclosure of Clinical Candidates

E. DiMauro, *Organizer, Presiding*

- 8:15** Introductory Remarks.
- 8:20** **215.** Discovery of MK-8719: Potent O-GlcNAcase inhibitor as a potential treatment for tauopathies. H.G. Selnick, J.F. Hess, X. Wang, L. Zhang, P. Sandhu, J. Lee, D.J. Klein, R. Kaul, T. Li, D.J. Vocadlo, Y. Zhou, Y. Zhu, C. Mu, Y. Wang, Z. Wei, S.M. Smith, A. Struyk, J.L. Duffy, **E.J. McEachern**
- 8:50** **216.** Discovery of SAR439859, an orally bioavailable Selective Estrogen Receptor Degradator (SERD) to treat ER+ breast cancers. **Y. Elahmad**
- 9:20** **217.** Movement to the clinic of soluble epoxide hydrolase inhibitor EC5026 as an analgesic for neuropathic pain and for use as a non-addictive opioid alternative. K.S. Lee, S. Hwang, C. McReynolds, K. Wagner, B. Inceoglu, C. Morisseau, W.K. Schmidt, A. Buckpitt, K. Hashimoto, **B.D. Hammock**
- 9:50** Intermission.
- 10:05** **218.** Discovery of AB928, a potent first-in-class dual A_{2a} and A_{2b} receptor antagonist for cancer immunotherapy. **M.R. Leleti**, J. Jeffrey, E.U. Sharif, B. Rosen, J. Beatty, L. Debien, R. Thomas-Tran, D. Mandal, W.H. Lim, M. Walters, U. Schindler, S. Young, J. Jaen, J. Powers
- 10:35** **219.** Discovery of JNJ-61393215: Selective orexin-1 receptor antagonist. **T. Lebold**, C.F. Gelin, C. Preville, J. Ziff, H. Coate, C.A. Dvorak, P. Bonaventure, T. Koudriakova, B. Lord, D. Nepomuceno, M. Rizzolio, K.J. Coe, A. Ndifor, C. Dugovic, J. Shelton, D.J. Pippel, T.W. Lovenberg, N.I. Carruthers, B.T. Shireman
- 11:05** **220.** Discovery of clinical candidate, BMS-986235/LAR-1219: Selective FPR2 agonist for prevention of heart failure. **N. Wurtz**, Y. Asahina, R. Garcia, Y. Saito, H. Yamada, K. Ohata, K. Fujii, K. Fukuchi, S. Matsushima, J. Ishiyama, T. Yamaoka, K. Arakawa, N. Carson, M. Hsu, B. Ito, E.K. Kick, J. Lupisella, J.C. Ostrowski, D. Search, F. Villarreal, Y. Kohno
- 11:35** **221.** Discovery of potent reversible inhibitors of LSD1. **Y. Chen**, T. Kanouni, C. Severin, J. Xu, J. Del Rosario, L. Shi, C. Lai, J.A. Stafford, J.M. Veal, R.K. Stansfield, R. Cho, N. Yuen
- 12:05** Concluding Remarks.

Emerging Targets for Drug Abuse Therapy

C. R. Hopkins, *Organizer, Presiding*

- 9:00** Introductory Remarks.
- 9:10** **222.** Issues in the evaluation and validation of targets for substance use disorder medication development. **J. Acri**
- 9:40** **223.** Serotonin 5-HT_{2c} receptor-based molecular therapeutics for substance use disorders. **K.A. Cunningham**, N. Anastasio, J. Zhou, S.R. Gilbertson
- 10:10** **224.** Discovery of VMAT2 modulators as potential treatments for methamphetamine use disorders. **G. Zheng**
- 10:40** **225.** Design, synthesis, and preclinical characterization of small molecule group II metabotropic glutamate receptor positive allosteric modulators. **N.D. Cosford**
- 11:10** **226.** Discovery of selective OX₁ antagonist HTL0027772 by structure-based drug design. **S.J. Bucknell**, K.A. Bennett, G.A. Brown, J. Christopher, M. Congreve, R.M. Cooke, G. Cseke, A.S. Doré, J.C. Errey, F.H. Marshall, J.S. Mason, M. Mills, R. Mould, R. Nonoo, J.C. Patel, M. Rappas, N.A. Swain, B.G. Tehan

Future of Biomacromolecules at a Crossroads of Polymer Science & Biology

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SECTION A

San Diego Convention Center
Room 6AB

Pharma Leaders Symposium

K. Briner, *Organizer, Presiding*

- 2:00** **227.** Discovery of CAD-1883: Clinical-stage positive allosteric modulator of the SK channel for the treatment of essential tremor and spinocerebellar ataxia. **G.F. Keaney**, D. Amrutkar, P. Christophersen, M. Curtis, B. Dagher, K. Foster, D. Grayzel, T. Jacobsen, M. Jefson, J. Larsen, J. Morrison, K. Nielsen, T. Piser, J. Resnick, N. von Schoubye, D. Strøbæk
- 2:40** **228.** DNA-encoded libraries at GSK. **K.B. Goodman**
- 3:10** **229.** DOSEDO: Diversity-oriented synthesis encoded by deoxyoligonucleotides. **L. Hudson**, J. Mason, M.V. Westphal, C.J. Gerry, B. Hua, W. Wang, H.L. Osswald, G. Xia, B. Melillo, C. Gampe, S. Bonazzi, N. Smith, R.G. Karki, J. Ottl, F. Berst, F. Zecri, K. Briner, J. Bradner, S.L. Schreiber
- 3:40** **230.** Strain-promoted cycloadditions for DNA-encoded library synthesis. **M.V. Westphal**, L. Hudson, J. Mason, C. Gampe, S. Bonazzi, N. Smith, F. Berst, F. Zecri, K. Briner, S.L. Schreiber
- 4:10** **231.** DNA-encoded chemical space: Widening the scope of DNA compatible chemistry. **F. Berst**, Y. Ruff, R. Martinez

SECTION B

San Diego Convention Center
Room 6D

General Orals

J. B. Schwarz, *Organizer*
M. Lu, *Presiding*

- 1:30** **232.** Structure-based design of an N-terminal bromodomain selective bromodomain and extraterminal (BET) inhibitor retaining an antiproliferative phenotype. **C. Wellaway**, S. Baddeley, P. Bamborough, S. Bernard, C. Chung, P. Craggs, E. Demont, L. Gordon, B. Karamshi, T. Lewis, M.J. Lindon, D. Mitchell, I. Pastor, P. Soden, S. Taylor, R. Watson, R. Willis, J. Witherington, J.M. Woolven, B. Wyspianska, W.J. Kerr, R. Prinjha
- 1:50** **233.** New piperazine-based siderophore-antibiotic conjugates to fight antimicrobial resistance. **P. Loupias**, E. Baudrin, v. pierre, L. Dupont, I. Dechamps, C. Mullié, A. Dassonville-Klimpt, N. Taudon, P. Sonnet

- 2:10** **234.** Experimental identification of protein-ligand interactions in fragment-based drug discovery with high-throughput protein crystallography screening of fragment libraries. **D. Das**
- 2:30** **235.** Structure-based design of potent and selective CGRP receptor antagonists for the treatment of migraine. **I.M. Bell**
- 2:50** **236.** BBB-penetrating delivery to glioma using engineered, size-controlled nano phage. **U. Tsedev**, C. Lin, F.C. Lam, A.M. Belcher
- 3:10** **237.** Discovery of potent, selective, and brain-penetrant apoptosis signal-regulating kinase 1 (ASK1) inhibitors. **F. Gonzalez Lopez de Turiso**, M. Himmelbauer, J. Jones, Z. Xin, R. Gilfillan
- 3:30** **238.** Discovery of novel FoxO1 inhibitors for the treatment of diabetes. **A. Johansson**, M. Petersson, M. Fredenwall, Y. Chen, O. Karlsson, J. Ulander, A. Peric, E. Ericson, C. Wennberg Huldt, M. Hayes, T. Norris, D. Lindén
- 3:50** **239.** Fisetin sensitizes the hypoxia induced chemotherapy resistance in head and neck cancer. **R.P. Singh**, D. Tailor, D. Nambiar, **S.V. Malhotra**
- 4:10** **240.** Identification of a small-molecule agonist for the APJ receptor as a clinical candidate. **S. Kim**, J.A. Johnson, J. Jiang, M.S. Phillips, J.S. Bostwick, P.S. Gargalovic, J.M. Onorato, C.E. Luk, C. Generaux, X. Chen, C. Xu, Y. He, M.A. Galella, T. Wang, R.R. Wexler, H.J. Finlay
- 4:30** **241.** Design of a multi-component reaction scaffold with inhibitory activity on aspartic proteases. **M. Konstantinidou**, F. Magari, F. Sutanto, M. Ünver, V. Jumde, G. Klebe, A. Hirsch, A. Doemling
- 4:50** **242.** Discovery and optimization of a novel series of highly selective JAK1 kinase inhibitors. **N. Grimster**, E. Anderson, M. Alimzhanov, G. Bebernitz, K. Bell, C. Chuaqui, T. Deegan, A. Ferguson, T.W. Gero, A. Harsch, D. Huszar, A. Kawatkar, J. Kettle, P. Lyne, J. Read, C. Rivard Costa, L. Ruston, P. Schroeder, J. Shi, Q. Su, S. Throner, D. Toader, M. Vasbinder, H. Wang, R. Woessner, A. Wu, M. Ye, W. Zheng, M. Zinda
- 5:10** **243.** Discovery of a potent and selective fragment-like inhibitor of SPIN1. **X. Yan**, H. Greschik, C. Johansson, L. Seifert, J. Bacher, K. Park, N. Babault, M. Martini, V. Fagan, F. Li, I. Chau, T. Christott, D. Dilworth, D. Baryte-Lovejoy, M. vedadi, C. Arrowsmith, P. Brennan, o. Fedorov, M. Jung, G. Farnie, J. Liu, U. Oppermann, R. Schüle, J. Jin

Discovery of Therapeutic Agents for Chronic HBV Infection

M. Mish, H. Shen, *Organizers, Presiding*

- 2:00** Introductory Remarks.
- 2:05** **244.** Discovery and development of a novel, class I Core protein Assembly Modulator (CpAM) for the treatment of chronic HBV infection. **W. Zhu**
- 2:35** **245.** Discovery of RG7834 and target identification: First-in-class selective and orally bioavailable small molecule HBV expression inhibitor with a novel mechanism of action. **S. Yang**
- 3:05** **246.** SB 9200 (inargivir), a selective oral immunomodulator for chronic hepatitis B. **R. Iyer**
- 3:35** Intermission.
- 3:50** **247.** Hit to lead optimization of toll-like receptor agonists toward the treatment of hepatitis B virus. **D.C. McGowan**
- 4:20** **248.** Discovery of the selective TLR8 agonist GS-9688 for HBV cure. **M. Mish**, G. Chin, V. Aktoudianakis, S. Metobo, H. Pyun, A. Villasenor, T. Appleby, J.K. Perry, S. Daffis, D. Ramakrishnan, C. Niu, J. Zheng, R. Santos, H. Yu, G. Lee, A. Palazzo, C. Frey, S. Pflanz, W.E. Delaney IV, S.P. Fletcher, R.L. Mackman
- 4:50** Concluding Remarks.

Covalent & Non-Covalent Dimers as Therapeutic Agents in Drug Discovery

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General Posters

J. B. Schwarz, *Organizer*

7:00 - 9:00

- 249.** Hidden bias in the dataset leads to misleading performance of deep learning in structure-based virtual screening. **E. Chen**, A. Cruz, S. Ramsey, V. Hornak, D. Koes, T. Kurtzman
- 250.** Design and synthesis of Janus kinase inhibitors for inhaled delivery and the importance of aldehyde oxidase metabolism in the lung. **C. Wellaway**, I.R. Baldwin, M.A. Bartholomew, D. Barker, D.M. Coe, J. Evans, N.J. Fazakerley, S.P. Keeling, X.Q. Lewell, J. Morley, D. Needham, F. Rianjongdee, C.M. Robertson, P. Rowland, R. Shah, E.B. Sheriff, S. Teague, D.A. Thomas, N. Wellaway, J. Wojno-Picon, J.M. Woolven, A.J. van Oosterhout
- 251.** Discovery of a C-8 hydroxychromene as a potent inhibitor of estrogen receptor alpha with improved rat oral exposure over GDC-0927. **S.S. Labadie**
- 252.** Process development and biological evaluation of antibody drug conjugate (ADC) based on a novel site-specific chemical conjugation platform. **Y. Matsuda**, K. Yamada, T. Seki, Y. Ooba, T. Fujii, T. Narita, A. Nakayama, Y. Kitahara, N. Shikida, K. Shimbo, K. Nakata, Y. Ito, **B. Mendelsohn**, T. Okuzumi
- 253.** Directed *meta* C-H amination of benzyl picolates via FeCl₃-catalysis. R. Anugu, S. Munnuri, **J.R. Falck**
- 254.** Efficient synthetic approach for 3-acetamido phthalides: Complement inhibitor virtual screening hit. **A. Chatterjee**, B.L. Garcia, B.V. Geisbrecht, J.K. Walker
- 255.** Efficacy of 4-oxo-4,5-dihydrothieno[3,2-c]quinoline CDK5 inhibitors as modulators of adipogenic insulin/metabolic pathways. **A. Chatterjee**, S. Mukherjee, M. Chakraborty, A. Chakraborty
- 256.** Dual-acting compounds targeting the adenosine 2A receptor (A2AR) and histone deacetylases (HDACs) for cancer immunotherapy. **W. Yan**, R. Liu, **J. Cheng**
- 257.** HER-2 kinase-targeted cancer therapy: Design, synthesis, and kinase profiling of novel quinazoline derivatives as selective antitumor hits. **T.A. elwaie**, S. Abbas, E. Ali, R.F. George, H. Ali, Z. Abdelmageed, H. Ali

- 258.** Design, synthesis, and evaluation of O5 modified apramycin derivatives. **V. Sarpe**, A. Sonousi, J.C. Quirke, P. Rajasekaran, A. Vasella, E. Böttger, D. Crich
- 259.** Synthesis of a novel enzyme-activated nitric oxide prodrug for antibacterial applications. **H. Hibbard**, M.M. Reynolds
- 260.** Novel pyrrolomycins as potential anticancer agents. Y. Liu, T. McGuire, J. Wang, J. Li, D.W. Coulter, J.G. Sharp, M. Cheng, **R. Li**
- 261.** Synthetic and biological studies of benzazepine derivatives as dopamine receptor ligands. **R. Giri**, W.W. Harding
- 262.** Inhibitors of the KRIT1/HEG1 interaction as potential candidates for cardiovascular disease. **K. Francisco**, M.A. Lopez-Ramirez, K. Oukoloff, L.A. Sklar, A.R. Gingras, C. Ballatore
- 263.** Computational and experimental filtering of potential therapeutics using ADMET properties. **K.D. Hannie**, A.L. Parrill-Baker, D.L. Baker
- 264.** Developing chemical probes against falcilysin, an essential malarial metalloprotease. **N. Maslov**
- 265.** Anti-fatty liver effects of 1-Hydroxy-2-naphthoic acid, a novel chemical chaperone. **T. Nam**, E. Kim, D. Choi, A. Choi, H. Hwang, H. Choi, S. Jeong, Y. Kim
- 266.** Discovery and evaluation of potent orally bioavailable retinoic acid receptor-related orphan receptor-gamma-t (ROR γ t) inhibitors. **Y. Sasaki**, M. Odan, S. Yamamoto, S. Kida, A. Ueyama, M. Shimizu, T. Haruna, A. Watanabe, T. Okuno
- 267.** Synthesis of silibinin analogues targeting amyloid beta. **M. Mizuno**, K. Mori, M. Shibanuma, K. Fukuhara
- 268.** Effect of bridged pyrrolidine rings on SAR and physicochemical properties in a series of Na ν 1.6 selective aryl sulfonamide inhibitors. **A. Zenova**, W. Gong, S. Chowdhury, M. Wilson, K. Burford, J. Andrez, N.G. Shuart, P.K. Tari, R. Kwan, K. Khakh, E. Chang, J.B. Li, S. Lin, M.D. Tandy, L. Sojo, C.J. Cohen, J.P. Johnson, C.M. Dehnhardt, J.R. Empfield, S.S. Wesolowski, T. Focken
- 269.** Novel pyrrolopyrimidine derivative DCBCO1601 as potent AXL kinase inhibitor with *in vitro* and *in vivo* biological activity. **S. Yen**, C. Liao, P. Chen, B. Chen, Y. Pan, S. Chen, S. Ciou, T. Li, Y. Kuo
- 270.** Studies on the design, synthesis, and antibacterial evaluation of new semisynthetic vancomycin derivatives reported. **M. Chunying**
- 271.** Development of novel ecto-5'-nucleotidase inhibitor with non-competitive mechanism. **W. Sun**, Y. Lee, M. Kuo, C. Huang, S. Chen, C. Liu
- 272.** OATD-01: Dual hAMCase and hCHIT inhibitor as a potential therapeutic agent for treatment of pulmonary diseases. **A. Bartoszewicz**, **S. Klossowski**, M. Mazur, S. Olejniczak, R. Koralewski, M. Kowalski, B. Dymek, P. Sklepkiwicz, M. Mlacki, W. Czestkowski, G. Andryianau, E. Pluta, P. Niedziejko, K. Matyszewski, M.M. Gruza, L. Joachimiak, A. Zagodzdzon, M. Salamon, J. Golab, M. Kwiecien, M. Nowotny, A. Napiorkowska, K. Dzwonek, P. Dobrzanski, J. Olczak, A. Golebiowski
- 273.** Planar catechin conjugated with DTPA as a promising antioxidant triggered by Fe $^{3+}$ coordination. **K. Fukuhara**, K. Imai, I. Nakanishi, K. Matsumoto, A. Ohno
- 274.** Drug development and production for cardiovascular diseases & arrest (CDA/CDD) (Oxonitrogenic). **S.N. Olatunji**
- 275.** Structure-activity and structure-metabolic stability relationship study of 1,2,3,4-tetrahydrobenzo[*b*][1,6]naphthyridine and 3,4-dihydro-1*H*-pyrano[4,3-*b*]quinoline phosphodiesterase 5 inhibitors for the treatment of Alzheimer's disease. **J. Fiorito**, E. Zuccarello, S. Deng, D. Landry, O. Arancio
- 276.** Discovery of Praliguat (IW-1973): Novel, once daily, orally bioavailable, stimulator of soluble guanylate cyclase with extensive tissue distribution. **T. Nakai**, T.C. Barden, S.G. Bernier, A. Carvalho, R. Deming, P. Germano, G. Im, K. Iyer, R.R. Iyengar, J. Jia, J. Jung, T. Lee, G. Liu, J. Masferrer, A. Mermerian, J. Moore, N.R. Perl, P.A. Renhowe, G.R. Rennie, J.E. Shepck, E.O. Solberg, J. Tobin, X.Y. Yu, D.P. Zimmer
- 277.** Compound selectivity evaluation in PPAR family using machine learning modelling. **O.B. Scott**, R. Chen Xu, D. Ni, A.E. Chan
- 278.** Cross-link breaking activity and inhibitory effect of *Moringa oleifera* leaf crude extracts on fructose-derived advanced glycation end products. **O.I. Adeniran**, M.A. Mogale
- 279.** Synthesis and evaluation of a cinnoline-core type candidate radiotracer for positron emission tomography of brain macrophage colony-stimulating factor 1 receptor. **S. Altomonte**, C.L. Morse, X. Yan, R. Dick, J. Liow, R. Gladding, S. Zoghbi, B. Innis, V. Pike
- 280.** Metal-binding pharmacophores as scaffolds for the development of potent human arginase-1 inhibitors. **R. Adamek**, S. Cohen
- 281.** Structure-based design and synthesis of novel DYRK1A inhibitors targeting inactive kinase conformation to induce human pancreatic β -cell proliferation. **C. Suebsuwong**, P. Wang, K. Kumar, S. Khamrui, C. Secor, M. Lazarus, R. Sanchez, A.F. Stewart, R.J. DeVita
- 282.** Identification of a new class of proteasome

- inhibitors based on a naphthylcarbonyl-phenyl urea scaffold. D. Allardyce, M. Szalecka, R. Nkwo, S. Asvid, C.D. Zeinalipour-Yazdi, **E. Loizidou**
- 283.** Structure-based design of dual AChE and BACE-1 inhibitors as potential therapeutics for neurodegenerative diseases. **M. Gabr**, M. Abdel-Raziq
- 284.** Amelioration of experimental autoimmune encephalomyelitis and DSS-induced colitis by thiazole derivatives of 6-aminopyridin-3ol through the inhibition of Th1 and Th17 cells differentiation. S. Acharya, M. Tilmilshina, S. Park, H. Kim, K. Seon, B. Jeong, J. Kim, **T. Nam**, J. Chang
- 285.** Identification and SAR studies of RhIR antagonists derived from 4-gingerol. **S. Nam**, S. Ham, S. Moon, H. Kwon, H. Kim, S. Son, H. Park, Y. Byun
- 286.** Amphiphilic kanamycin for treatment and diagnosis of the fungal infection. **Y.P. Subedi**, P. Roberts, M. Grilley, J.Y. Takemoto, C.T. Chang
- 287.** Dopamine D1R-preferring ligands via structural modifications on apomorphine. **A. Karki**, W.W. Harding
- 288.** Discovery of clinical candidate, BMS-986235/LAR-1219: Design and optimization of selective 4-phenylpyrrolidinone FPR2 agonists. **K. Tsuda**, Y. Asahina, Y. Saito, H. Yamada, K. Ohata, K. Fujii, K. Fukuchi, S. Matsushima, J. Ishiyama, T. Yamaoka, K. Arakawa, Y. Kohno
- 289.** Development of novel synthetic TLR4 agonists. **J.K. Khalaf**
- 290.** Synthesis of *N*-cyclopropylbenzamide-benzophenone hybrids as novel and selective p38 mitogen-activated protein kinase inhibitors and their biological evaluation for neuroinflammation. **S. Son**, H. Yoo, M. Gee, K. Inn, J. Lee, N. Kim
- 291.** Design, synthesis, and biological evaluation of sulfamoylbenzamide derivatives as hepatitis B virus capsid inhibitors. **N. Hyogyong**, H. Kim, Y. Jung, S. Han
- 292.** Optimization of (8-quinolyloxymethyl) benzamide derivatives as potent and selective ROR γ inhibitors. J. Amaudrut, M.A. Argiriadi, M.M. Barth, E. Breinlinger, D. Bressac, P. Broqua, D.J. Calderwood, K.P. Cusack, V. Derain, S.B. Gauld, E. Gauthier, F. Guillier, S. Jacquet, E. Jacquier, R.V. Kamath, M.E. Kort, V. Lepais, J. Llacer, J. Luccarini, P. Masson, C. Montalbetti, L. Mounier, **D. Potin**, O. Poupardin, S. Rouaud, L. Spitzer, C.D. Wallace
- 293.** Synthesis of novel bipyridine ligands as potential telomerase inhibitors. E. Smith, N. Sivetz, S. Yan, M.M. Michael, D. Jose, **M. Lamberto**
- 294.** Flexible and integrated collaboration tools to aid, co-ordinate, and inspire medicinal chemistry. **P. Tosco**, S. Sciammetta, T. Cheeseright, M.D. Mackey
- 295.** Toward a selective small-molecule antagonist of hyaluronan binding by CD44. **W. McCue**, S. Maitra, L. Liu, G.I. Georg, J. McCarthy, B. Finzel
- 296.** 3-Dimensional metal complexes as scaffolds for fragment-based drug discovery. **R. Stokes**, C.N. Morrison, A. Cordes, E.K. Kurbanov, C.V. Credille, N. Metzler-Nolte, S. Cohen
- 297.** Identification of a β -hairpin peptide that disrupts growth arrest-specific gene 6 (Gas6)/Axl receptor interaction. **J.X. Qiao**, S. Spronk, J. Hua, C. Mapelli, K. O'Malley, D. Calambur, M.R. Witmer, J. Yang
- 298.** Leveraging academic collaborations and expanding the millimolecular chemistry synthetic toolbox. **J.X. Qiao**, M.A. Poss, G. Chen, Y. Shao, Z. Zhuang, G. Xia, P. Shen, Q. Wu, P. Wang, S. Ni, T. Qin, T. Liu, R. Rampulla, H. Yip, D.Z. Sun, D. Wu, T. Rasam, M. Pitchai, N. Kulahalli, A. Gupta, A.K. Gupta, M. Vetrichelvan, I. Gopikumar, A. Mathur, M.D. Eastgate, P.S. Baran, J. Yu, W.R. Ewing
- 299.** Discovery of APOBEC3B DNA cytosine deaminase ligands by protein observed fluorine NMR screening. **M. Grillo**, W.C. Pomerantz, H. Aihara, D.A. Harki
- 300.** GUNW-3 as a brain-targeting agent to improve the delivery of tamoxifen to the brain. **Y. Huang**, S. Wang, A. Najmi, X. Guan
- 301.** Small molecule-mediated degradation of BRAF-V600E for the treatment of melanoma. X. Han, Y. Wei, L. Huang, W. Yu, C. Zhang, X. Li, Y. Chen, B. Jiao, L. Sun, C. Zhang, Y. Xu, Y. Luo, L. Chen, J. Wang, **M.B. Plewe**
- 302.** Design through computer-aided approach and synthesis of new benzimidazole derivatives as inhibitors of protein tyrosine phosphatase 1B. **M.I. Campos Almazán**, A. Téllez Valencia, A. Hernandez Campos, E. Sierra Campos, M.A. Valdez Solana, C.I. Avitia Domínguez
- 303.** Nucleoside analogue inhibitors of GTP cyclohydrolase I (GCYH-I) as a potential new class of antibiotics. **G. Samaan**, N. Paranagama, R. Murphy, D.A. Hecht, M. Swairjo, B.W. Purse
- 304.** Discovery of IWP-597: Novel carboxylic acid-containing soluble guanylate cyclase stimulator. **G.R. Rennie**, T.C. Barden, A. Carvalho, R. Deming, P. Germano, C. Hudson, G. Im, R.R. Iyengar, J. Jia, J. Jung, E. Kim, T. Lee, A. Mermerian, J. Moore, T. Nakai, N.R. Perl, P.A. Renhowe, J. Tobin, D.P. Zimmer
- 305.** Identification of a potent inhibitor of notch signaling. **J.E. Gomez Galeno**, C. Hurtado, J.R. Cashman, M. Mercola, J. Cheng, C. Yardimci
- 306.** Synthesis and spectroscopic characterization of analgesic drugs esters of poly-acrylic acid. **M.G.**

Nassr, H.D. Tabba

307. Synthesis, evaluation, and computational simulations of novel 1,2,3-triazole analogues of sitagliptin as DPP-4 inhibitors. **K.H. Hong**, D. Vo, H. Park

308. Synthesis and spectroscopy of binary prodrugs. **M.K. Mohamed**, H.D. Tabba

309. Synthesis of new hepatitis C virus translation inhibitors. **K.J. Walsworth**, **A. Simon**, **T. Nelson Hall**, **J. Molina**, **A. Bender**, T. Hermann, M.B. Bergdahl

310. Design and synthesis of novel CDK9-specific PROTACs for the treatment of leukemia. **R.J.**

Tokarski, A. Huntsman, N. Cockroft, B. Carmichael, N. Muthusamy, J.C. Byrd, J. Fuchs

311. Synthesis of three fluoro-containing [¹¹C] ER176 analogs for PET imaging of TSPO in monkey brain. **F.G. Simeon**, J. Lee, C. Morse, I. Stukes, J. Liow, S. Zoghbi, S. Taliani, S. Castellano, f. Da Settimo, B. Innis, V. Pike

312. Novel nanoformulation of Levofloxacin and antimicrobial efficacy. **U. Haroon**, M. Zuberi, a. Tabassum

313. Structure-kinetics relationship study of CDK8 inhibitors with milestone. **S. Chen**, Z. Tang, H.D. Pandey, C. Chang

314. Lewis acid-modified pyrophosphate bond synthesis via an improved phosphoramidite approach. **Z. Xu**, M.S. Fleur-Rema

315. Combinatorial approach for synthesis of novel 1,3,5-triazine-2,4-diamines with potent and selective anti-proliferative activity. **A. Junaid**, C. Lay Hong, A.V. Dolzhenko

316. New approach to preparation of RNA-targeted libraries. **Y. Moroz**, O. Gavrylenko

317. Advantages of fluorinated fragment library in the discovery of novel specific binders and hit to lead optimization. **O. Gavrylenko**, Y. Moroz

318. Designing a compact plasmonic nanoparticle with enhanced fluorescence and potentially safer T1 magnetic imaging contrast. **L. Henderson**, O. Neumann, C. Kaffes, R. Zhang, V. Marangoni, M.K. Ravoori, V. Kundra, J. Bankson, P.J. Nordlander, N.J. Halas

319. Fatty acylated CGKRK conjugated cell-penetrating peptide for targeted delivery of siRNA in tumor. **M.I. Sajid**, N.S. El-Sayed, H.M. Aliabadi, R.K. Tiwari

320. Synthesis and evaluation of bicyclic peptides containing arginine and tryptophan residues as molecular transporters. **S.A. Darwish**, S. Mozaffari,

R.K. Tiwari, K. Parang

321. Synthesis and evaluation of cyclic peptide-dasatinib conjugates as antimelanoma agents. **S.A. Darwish**, S. Fong, S. Yang, R.K. Tiwari, K. Parang

Asymmetric Reactions & Syntheses

Sponsored by ORGN, Cosponsored by MEDI

CH Activation

Sponsored by ORGN, Cosponsored by MEDI

Metal-Mediated Reactions & Syntheses

Sponsored by ORGN, Cosponsored by MEDI

Photoredox Chemistry

Sponsored by ORGN, Cosponsored by MEDI

Total Synthesis of Complex Molecules

Sponsored by ORGN, Cosponsored by MEDI

THURSDAY MORNING – MEDI

Study of Circulating, Cell-Free Biomarkers with Analytical Tools

Sponsored by ANYL, Cosponsored by BIOL, BIOT and MEDI

Development of Novel Vector Control Technologies

Sponsored by AGRO, Cosponsored by MEDI

Biosensing: New Strategies & Latest Development

Sponsored by ANYL, Cosponsored by BIOL, BIOT and MEDI

MPPG

MULTIDISCIPLINARY PROGRAM PLANNING GROUP

E. Fox and C. Avery, *Program Chairs*

SUNDAY MORNING – MPPG

SECTION A

San Diego Convention Center
Room 5A

Chemists Without Borders: Celebrating 15 Years of Scientific/Humanitarian Collaboration

Cosponsored by CEI and ENVR

R. L. Grosse, *Organizer*

R. Grosse, *Presiding*

- 9:00** Introductory Remarks.
- 9:05** **1.** Confronting the largest mass poisoning of a population in history by providing clean water in Bangladesh. **S.D. Chambreau**
- 9:30** **2.** Bangladesh arsenic and climate change projects. **R. Kronquist**
- 9:55** **3.** Emerging sustainable wastewater sludge management innovations for value recovery. E. Musvoto, **A. Mackintosh**
- 10:20** **4.** Providing hands-on science training to teachers in Guatemala. **R.M. Malczewski**
- 10:45** Intermission.
- 10:55** **5.** Lab studies of the ocean-atmosphere system: Disentangling human and natural impacts on our climate. **K.A. Prather**
- 11:20** **6.** Chemistry in Cameroon: Advancing laboratory sciences. **R.R. Hodel**
- 11:45** **7.** Considering fieldwork? Lessons learned in Latin America. **N.D. Leigh**

Nanotechnology & Single Cell Analysis in Biology & Medicine

Nanoscience, Biology & Medicine

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

SUNDAY AFTERNOON – MPPG

SECTION A

San Diego Convention Center
Room 5A

Celebrating Sir Martyn Poliakoff: From Blue Matrix to Green Chemistry & Everything in Between

Cosponsored by CPRC

Financially supported by C&EN

M. W. George, L. K. Wolf, *Organizers*

S. Morrissey, *Organizer, Presiding*

- 1:00** Introductory Remarks.
- 1:10** **8.** NMR goes faster with a pulsed laser and parahydrogen. **R.N. Perutz**
- 1:30** **9.** Challenging computational chemistry with chemical questions. **O.G. Eisenstein**
- 1:50** **10.** From liquid xenon to green chemistry: How Martyn Poliakoff influenced my career. **R.K. Upmacis**
- 2:10** **11.** Photochemistry, spectroscopy and supercritical fluids: Journey from organometallic alkane and noble gas complexes to manufacturing antimalarial compounds. **M.W. George**
- 2:30** Intermission.
- 2:40** **12.** Essential power of story. **P.T. Anastas**
- 3:00** **13.** Green chemistry in China. **Z. Liu, B. Han**
- 3:20** **14.** Taking green chemistry to Ethiopia. **N. Asfaw**
- 3:40** **15.** From flow to endangered elements: God bless Sir Martyn. **D.J. Cole-Hamilton**
- 4:00** **16. Award Address** (James T. Grady–James H. Stack Award for Interpreting Chemistry for the Public sponsored by ACS). From test tube to YouTube. **M. Poliakoff**
- 4:30** Q&A.

SECTION B

San Diego Convention Center
Room 5B

Tiny Solutions to Big Problems: Water Sustainability Through Nanotechnology

C. W. Avery, E. B. Fox, *Organizers*

- 1:00** 17. Water sustainability through Nanotechnology Signature Initiative (Water NSI) overview. **S. Standridge**
- 1:15** 18. Nano-enabled solutions for increasing water availability. **M.S. Mauter**
- 1:35** 19. Nanotechnology for water quality monitoring. **P.J. Vikesland**
- 1:55** 20. Application of liquid-impregnated surfaces to improving process and water transport efficiency. **D. Smith**
- 2:15** Q&A

SECTION C

San Diego Convention Center
Room 6AB

Chemistry & Water: Opening Session

Cosponsored by CEI, ENVR and PRES

C. W. Avery, *Organizer*

E. B. Fox, *Organizer, Presiding*

- 3:00** Introductory Remarks.
- 3:05** 21. Water's effect on chemistry. **V.H. Grassian**
- 3:25** 22. Meeting the challenges of the world's growing dependence on groundwater. **W.M. Alley**
- 3:45** 23. Environmental stewardship and community service: Essential best practices for the clean water utility of the future. **A. Kricun**
- 4:05** 24. Water, water, everywhere, nor any drop to drink. **B. Gerber**
- 4:25** Panel Discussion.
- 4:55** Concluding Remarks.

Nanotechnology & Single Cell Analysis in Biology & Medicine

Nanoscience

Sponsored by ANYL, Cosponsored by COLL, MPPG and PHYS

MONDAY MORNING – MPPG

SECTION A

San Diego Convention Center
Room 5A

Spotlight on the Chemistry of Water in the Journal of the American Chemical Society

E. Mills, *Organizer, Presiding*

- 8:00** Introductory Remarks.
- 8:05** 25. Water window on membrane biochemistry. **S. Roke**
- 8:35** 26. Molecular recognition of ice by proteins: From ice nucleation to antifreeze. **V. Molinero**
- 9:05** 27. Water-based precision nanostructures. **R.K. Oreilly**
- 9:35** 28. Metal-organic frameworks for practical water harvesting from desert air. **O.M. Yaghi**
- 10:05** 29. Sustainable electrolysis of water from first principles. **E.A. Carter**

Nanotechnology & Single Cell Analysis in Biology & Medicine

Nanoscience

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

MONDAY AFTERNOON – MPPG

SECTION A

San Diego Convention Center
Room 5A

Materials Making a Splash – Emerging Trends in Nanoscience, Materials Science & Photonics

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

- 1:00** Introductory Remarks.
- 1:05** 30. Observing the trajectories of artificial atoms joining together to form artificial solids. **P. Alivisatos**
- 1:30** 31. New electrochemical desalination technologies. **D. Nam, M. Lumley, K. Choi**
- 1:55** 32. Reversible assembly of charged macrocycles into high aspect ratio organic nanotubes. **W.R. Dichtel, C. Sun, M.J. Strauss**
- 2:20** 33. Single-molecule microscopy and spectroscopy of plasmon-coupled fluorescence. **J.S. Biteen**
- 2:45** 34. Emerging organ models and organ printing for regenerative medicine. **A. Khademhosseini**

- 3:10 35. Aqueous-phase nanophotonic materials to probe molecular and cellular processes. **J. Dionne**
- 3:35 36. Photo-triggered drug delivery systems. **D.S. Kohane**

SECTION C
San Diego Convention Center
Room 6AB

The Fred Kavli Series

The Kavli Foundation Emerging Leader in Chemistry

B. A. Charpentier, *Organizer*

- 4:00 37. Harnessing the quantum mechanics of the hydrogen bond: From atmospheric science to enzyme catalysis. **T. Markland**

SECTION C
San Diego Convention Center
Room 6AB

The Fred Kavli Series

The Fred Kavli Innovations in Chemistry Lecture

B. A. Charpentier, *Organizer*

- 5:00 38. Innovation by evolution: Bringing new chemistry to life. **F.H. Arnold**

Nanotechnology & Single Cell Analysis in Biology & Medicine

Nanoscience

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

TUESDAY MORNING – MPPG

Water for Two Worlds

Technologies for Tomorrow

Sponsored by COMSCI, Cosponsored by MPPG

TUESDAY AFTERNOON – MPPG

SECTION C
San Diego Convention Center
Room 30D

Environmental Chemistry through the Transformative Power of Film: A Showcase of CEI-ENVR Environmental Film Competition Awardees

Cosponsored by CEI and ENVR
S. O. Obare, *Organizer, Presiding*

- 1:00 39. Environmental chemistry through the transformation power of film: An environmental film competition of CEI & ENVR. **S.O. Obare**

Water for Two Worlds

Lighting the Way to Safe Water

Sponsored by COMSCI, Cosponsored by MPPG

NTS

COMMITTEE ON NOMENCLATURE, TERMINOLOGY AND SYMBOLS

SUNDAY AFTERNOON – NTS

Chemical Nomenclature & Representation: Past, Present & Future

Sponsored by CINF, Cosponsored by HIST and NTS

MONDAY MORNING – NTS

Chemical Nomenclature & Representation: Past, Present & Future

Challenges & Opportunities in Chemical Representation

Sponsored by CINF, Cosponsored by HIST and NTS

MONDAY AFTERNOON – NTS

Chemical Nomenclature & Representation: Past, Present & Future

InChI'ng Forward

Sponsored by CINF, Cosponsored by HIST and NTS

NUCL

DIVISION OF NUCLEAR CHEMISTRY AND TECHNOLOGY

J. Auxier, *Program Chair*

SUNDAY MORNING – NUCL

SECTION A

Marriott Marquis San Diego Marina
Catalina

Molten Salt Reactor Chemistry

Radiation Chemistry in Molten Salts

Cosponsored by I&EC

J. McFarlane, K. G. Myhre, *Organizers, Presiding*

- 8:00** Introductory Remarks.
- 8:05** **1.** Radiation effects in molten salts. **J.A. Laverne**, G.P. Horne, K. Chen-Wiegart, R. Gakhar, S.M. Pimblott, J.F. Wishart
- 8:35** **2.** Liquid fueled molten salt reactor fuel salt composition evolution and implications for operations and performance. **B. Betzler**
- 9:05** **3.** Fundamental study of electrochemically separated uranium in the presence of cerium in molten LiCl-KCl electrolyte. **D. Killinger**, S. Phongikaroon
- 9:35** Intermission.
- 9:55** **4.** Measuring the structure of bulk KCl/MgCl₂ molten salts using X-ray and neutron scattering. **S.M. Mahurin**, A. Ivanov, D. Dolzhenkov, P.W. Halstenberg, S. Gill, M. Topsakal, B. Layne, E. Dooryhee, S. Dai
- 10:25** **5.** Investigating structure and speciation of metals in molten salt system using X-ray absorption fine structure. **S. Gill**, K. Sasaki, M. Topsakal, R. Gakhar, W. Phillips, L. He, S.M. Mahurin, I. Ecker, A. Frenkel
- 10:55** **6.** Spectroscopic and electrochemical investigation of f-elements and optical materials in molten salt. **S.D. Branch**, H. Felmy, J.M. Wislon, A. Lines, G.J. Lumetta, S.A. Bryan
- 11:25** **7.** Application of electrochemical and laser spectroscopic methods for composition measurements of UCl₃-MgCl₂-GdCl₃ in LiCl-KCl molten salt. **H. Andrews**, S. Phongikaroon
- 11:55** Concluding Remarks.

SUNDAY AFTERNOON – NUCL

SECTION A

Marriott Marquis San Diego Marina
Catalina

Molten Salt Reactor Chemistry

Salt Redox Chemistry & Thermodynamics

Cosponsored by I&EC

J. McFarlane, K. G. Myhre, *Organizers, Presiding*

- 1:00** Introductory Remarks.
- 1:05** **8.** Modeling Cr dissolution in molten KCl-MgCl₂. **J.W. McMurray**, S. Utlak, S. Raiman
- 1:35** **9.** Surface segregation behavior in molten salt facing Ni-Cr alloys: First principles investigation. **J. Startt**, S. Raiman, C. Deo
- 2:05** **10.** Measurement of molten KCl-MgCl₂ salt penetration depth in nickel alloys using LIBS. **W. Ponder**, K.G. Myhre, S. Zinkle, S. Raiman
- 2:35** Intermission.
- 2:55** **11.** Analysis and modeling of the equilibrium behaviors of U and Pu in molten LiCl-KCl/Cd system at 500°C. **G. Fredrickson**, T. Yoo
- 3:25** **12.** Measurement and analysis of equilibrium potentials of Ag/AgCl reference with respect to Cl₂/Cl⁻ in LiCl-KCl eutectic salt. **S. Phongikaroon**, D. Yoon
- 3:55** **13.** Thermophysical properties of CaCl₂-KCl-MgCl₂ eutectic salt. **M. Woods**, A. Baggett, S. Phongikaroon
- 4:25** **14.** First principles molecular dynamics simulations of U(III) and U(IV) in molten chlorides. **D. Jiang**
- 4:55** **15.** Zn-doped, graphene-like carbon nitride for uranium extraction with high capacity. **L. Shuang**, Y. Lu, G. Wei
- 5:25** Concluding Remarks.

SUNDAY EVENING – NUCL

SECTION A

San Diego Convention Center
TBD

Computational Methods for Lanthanides & Actinides: Theory & Applications

Cosponsored by COMP

D. A. Penchoff, C. Peterson, *Organizers*

6:30 - 8:30

16. Synthesis, radiolabeling, and characterization of phenoxyphenyl acetamide or pyrazolopyrimidine derivatives for imaging the TSPO kDa with PET. **M. Alam**, S. Lee

17. Morphological and chemical evolution of Ni and Ni-20Cr microwires in molten KCl:MgCl₂. **A. Ronne**, L. He, D. Dolzhenkov, M. Ge, X. Xiao, W. Lee, S.M. Mahurin, K. Chen-Wiegart

MONDAY MORNING – NUCL

SECTION A

Marriott Marquis San Diego Marina
Catalina

Molten Salt Reactor Chemistry

Industrial Perspectives & Safety Considerations

Cosponsored by I&EC

J. McFarlane, K. G. Myhre, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 **18.** Molten salt reactor off-gas monitoring using laser induced breakdown spectroscopy. **K.G. Myhre**, J. McFarlane, G. Del Cul, N. Bull Ezell, H. Andrews

8:35 **19.** Iodide in fluoride salts: Its behaviors and iodine ion separation. **J. Zhang**

9:05 **20.** Fission product volatility in molten salt reactors. **J. McFarlane**, J.W. McMurray, C.F. Weber

9:35 Intermission.

9:55 Panel Discussion.

10:55 Concluding Remarks.

MONDAY AFTERNOON – NUCL

SECTION A

Marriott Marquis San Diego Marina
Catalina

Computational Methods for Lanthanides & Actinides: Theory & Applications

Cosponsored by PHYS

D. A. Penchoff, C. Peterson, *Organizers, Presiding*

A. Ta, *Presiding*

2:30 Introductory Remarks.

2:35 **23.** Computational protocol for binding selectivity of lanthanide and actinide systems. **C.C. Peterson**, D.A. Penchoff

3:05 **24.** Predicting the properties of actinide complexes in the gas phase and in solution. **D.A. Dixon**

3:35 Intermission.

3:45 **25.** *De novo* design of ligands for selective trivalent f-elements complexation. **A. Mitrofanov**, B. Sattarov, S. Kalmykov, **V. Tkachenko**

4:15 **26.** How calculations unite with synthesis to tackle novel actinide chemistry. J. DeJesus, R. Kerr, C. Peterson, D.A. Penchoff, P.L. Arnold, **D.M. Jenkins**

4:45 Concluding Remarks.

SECTION A

San Diego Convention Center
TBD

Molten Salt Reactor Chemistry

Poster Session

Cosponsored by I&EC

J. McFarlane, K. G. Myhre, *Organizers*

12:15 - 2:15

21. Electrochemical study in molten salts: Assembly and characterization of micro-reference electrodes. **H. Felmy**, S.D. Branch, J.M. Wislon, A. Lines, G.J. Lumetta, S.A. Bryan

22. *In-situ* spectroelectrochemistry of transition metal and lanthanide chlorides in molten chloride salts. **W.C. Phillips**, M. Shaltry, S. Frank, R. Gakhar

TUESDAY MORNING – NUCL

SECTION A

Marriott Marquis San Diego Marina
Catalina

Computational Methods for Lanthanides & Actinides: Theory & Applications

Cosponsored by PHYS

D. A. Penchoff, C. Peterson, *Organizers, Presiding*

A. Ta, *Presiding*

- 8:00 Introductory Remarks.
- 8:05 **27.** First principles molecular dynamics simulations of UCl_n -NaCl ($n=3, 4$) molten salts. **B. Li**, S. Dai, D. Jiang
- 8:25 **28.** Modeling highly asymmetric mixtures in the warm dense plasma regime: From enhancement factors to transport. **A.J. White**, C. Ticknor, J.D. Kress, L. Collins, J. Clerouin, P. Arnault, N. Desbiens
- 8:45 Intermission.
- 8:55 **29.** Probing the electronic structure and chemical bonding of actinide organometallic compounds. **J. Su**, C. Goodwin, A. Gaunt, E.R. Batista, P. Yang
- 9:15 **30.** Examination of the sensitivity of computational models to hyperparameter selection. **J.R. Powers-Luhn**, C. Peterson, H.L. Hall
- 9:35 Concluding Remarks.

SECTION A

Marriott Marquis San Diego Marina
Catalina

Celebration of the Centennial of Rutherford's First Nuclear Reaction

T. A. Bredeweg, D. R. Porterfield, *Organizers, Presiding*

- 9:50 Introductory Remarks.
- 9:55 **31.** Marking the 80th anniversary of the discovery of nuclear fission by chemists. **W.B. Walters**
- 10:20 **32.** Energy dependence of fission product yields for ^{235}U , ^{238}U , and ^{239}Pu with monoenergetic neutrons between thermal and 14.8 MeV. **M. Gooden**, T.A. Bredeweg, M.M. Fowler, J. Wilhelmy, A. Tonchev, J. Silano, M.A. Stoyer, S. Finch, W. Tornow
- 10:45 **33.** Iridium: Important neutron flux monitor. **R.S. Rundberg**
- 11:10 Intermission.
- 11:30 **34.** Nuclear reaction studies with GODDESS. **J.A. Cizewski**, S.D. Pain, A. Ratkiewicz

- 11:55 **35.** Validation of an indirect method for constraining neutron-capture cross sections. **K.L. Childers**, S.N. Liddick, A. Spyrou, A. Larsen, M. Guttormsen, D.L. Bleuel, L.C. Campo, B.P. Crider, A. Couture, A. Dombos, R. Lewis, S. Mosby, F. Naqvi, G. Perdikakis, C.J. Prokop, S. Siem, T. Renstrom, S. Quinn
- 12:20 **36.** Constraining neutron-capture reactions through the surrogate reactions method. **A. Ratkiewicz**, J.A. Cizewski, J.E. Escher, G. Potel

Molten Salt Chemistry

Reactivity in Molten Salts

Sponsored by I&EC, Cosponsored by NUCL

TUESDAY AFTERNOON – NUCL

SECTION A

Marriott Marquis San Diego Marina
Catalina

Celebration of the Centennial of Rutherford's First Nuclear Reaction

T. A. Bredeweg, D. R. Porterfield, *Organizers, Presiding*

- 1:30 Introductory Remarks.
- 1:35 **37.** Shapes and transition rates in nuclear structure, the case of ^{78}Ge . **W.B. Walters**
- 2:00 **38.** Advances in nuclear astrophysics measurements in the FRIB era. **S.D. Pain**
- 2:25 Intermission.
- 2:45 **39.** $^4\text{He} + ^{14}\text{N} \rightarrow ^{18}\text{F}^*$: What comes next?. **P.J. Karol**
- 3:10 **40.** Measurement of neutron-capture cross sections of copper isotopes with DANCE for constraining s-process nucleosynthesis. **C.J. Prokop**, A. Couture, S. Jones, S. Mosby, G. Rusev, J.L. Ullmann, M. Krticka
- 3:35 **41.** Production of heavy actinides for support of superheavy element discovery. **S. Hogle**, R.A. Boll, J. Ezold, K.M. Bennett

Molten Salt Chemistry

Structure & Properties of Molten Salts

Sponsored by I&EC, Cosponsored by NUCL

SECTION A

Marriott Marquis San Diego Marina
Catalina

Nuclear Forensics

J. D. Auxier, G. Bull, N. A. Vanagas, *Organizers, Presiding*

- 8:00** 42. Laser-induced breakdown spectroscopy for nuclear forensics: Current trends, advancements, and challenges. **M. Shattan**
- 8:20** 43. Handheld LIBS analysis of post-detonation synthetic nuclear melt glass. **J. Bishop**, J.D. Auxier, N. Xu
- 8:40** 44. Production and characterization of uranium-containing particles for nuclear safeguard applications. A. Baldwin, M.G. Bronikowski, M.A. DeVore, L. Inabinet, W. Kuhne, R. Smith, T. Tenner, T. Williamson, **M.S. Wellons**
- 9:00** Intermission.
- 9:10** 45. Optimizing ligand design for selective binding to lanthanides and actinides. **D.A. Penchoff**, C. Peterson, J.D. Auxier, G.K. Schweitzer, D.M. Jenkins, R. Harrison, H.L. Hall
- 9:30** 46. Dynamic separation of Eu³⁺ and Nd³⁺ using bis-(2-ethylhexyl) phosphoric acid functionalized ordered mesoporous carbon nanoparticles. **E.R. Bertelsen**, G. Deodhar, K. Kluherz, M.R. Davidson, M. Adams, B.G. Trewyn, J. Shafer
- 9:50** 47. Functionalized polymer thin films for plutonium capture and isotopic screening from aqueous sources. **J.C. Foster**, S. Starstrom, T.A. Devol, B.A. Powell, S.M. Husson
- 10:10** Intermission.
- 10:20** 48. Potential strategies for uranium chronometry using nuclear counting techniques. **D.R. Porterfield**, J.D. Auxier
- 10:40** 49. Characterization of chemical signatures from ADU and AUC materials. **J.M. Dorhout**, G.L. Wagner, C. Anderson-Cook, K. Sentz, A. Ross, B. Scott, M.P. Wilkerson

Molten Salt Chemistry

Materials Compatibility & Interfacial Phenomena

Sponsored by I&EC, Cosponsored by NUCL

SECTION A

Marriott Marquis San Diego Marina
Catalina

General Topics in Radiochemistry

J. Shafer, *Organizer*R. G. Surbella, *Organizer, Presiding*

- 12:20** 50. Selective separation of americium from europium using 2,9-diamide-1,10-phenanthroline in ionic liquids. **Y. Li**, C. Xu
- 12:40** 51. Structural and thermodynamic factors underlying the Ln(III)/An(III) selectivity by Di-2,4,4-trimethylpentyl dithiophosphinic acid. **C. Xu**
- 1:00** 52. Separation of transplutonium elements as part of the ORNL californium campaigns. **L.H. Delmau**, E. Collins, J. Ezold, J. Dryman, C. Nevius, B. Tinker
- 1:20** 53. Density functional theory analysis of the adsorption and surface chemistry of inorganic iodine species on graphite. **A.M. Ritzmann**, M.J. Sassi, N.J. Henson
- 1:40** 54. Radiation-resistant, ultra-microporous materials for efficient removal of krypton from nuclear reprocessing facilities. **S.K. Elsaidi**, M.H. Mohamed, D. Hopkinson, A.S. Helal, J. Li, P.K. Thallapally
- 2:00** Intermission.
- 2:20** 55. New strategies in nuclear human decorporation using macromolecular systems. F. Lahrouch, L. Leost, B. Siberchicot, A. Van Der Meeren, J. Aupiais, C. Hennig, C. Di Giorgio, **c. den auwer**
- 2:40** 56. Differential ability of leachate produced from leaf litter of different plant species to solubilize U from stable mineral forms. **N. Edayilam**, B.A. Powell, N. Tharayil
- 3:00** 57. Leveraging radioanalytical and mass-spectrometry based technologies to investigate iron assimilation and allocation in rhizobacteria-associated maize. **A.F. Bauer**, G. Powell, A. Anstaett, A. Gerheart, S. Scott, M. Benoit, J. Guthrie, B. Higgins, S. Wilder, M. Schueller, R. Ferrieri
- 3:20** 58. Analysis of actinides other than uranium and plutonium by thermal ionization mass spectrometry. **R.B. Thomas**, R.M. Achey, M.A. Bernard
- 3:40** 59. Single-pass flow-through studies of simulated Hanford low-activity waste glass in varying pH, temperature, and presence of cement-contacted groundwater. **K.K. Sockwell**, R.M. Asmussen, Y. Katsenovich

SECTION A

Marriott Marquis San Diego Marina
Catalina

Water Behavior in Concentrated Electrolytes

Cosponsored by PHYS

S. B. Clark, *Organizer*A. E. Clark, *Organizer, Presiding*

- 8:30** **60.** Dynamics of organic molecule-ion and water-ion complexes in concentrated aqueous salt solutions: 2D IR chemical exchange spectroscopy. **M.D. Fayer**
- 9:15** **61.** Oxyanion aqueous solvation structure and alkali ion pair interactions in concentrated electrolytes. **E. Martinez Baez**, M. Pouvreau, C. Pearce, G.K. Schenter, A.E. Clark
- 9:50** **62.** Towards a realistic modeling of ion hydration, one molecule at a time. M. Riera, P. Bajaj, D. Zhuang, C. Egan, B. Bizzarro, **F. Paesani**
- 10:35** Intermission.
- 10:50** **63.** Nonlinear optical studies of cooperative adsorption to lipid films: Role of buffers. **R.A. Walker**, K.A. Link, G.N. Spurzem
- 11:25** **64.** X-ray emission spectroscopy at X-ray free electron lasers: Limits to observation of unperturbed electronic structures. **S. Jensen**, B. Sullivan, Y. Pushkar

SECTION A

Marriott Marquis San Diego Marina
Catalina

Water Behavior in Concentrated Electrolytes

A. E. Clark, *Organizer*S. B. Clark, *Organizer, Presiding*

- 1:15** **65.** Coarse-grained modeling of ion transport in complex fluids. **S. Sankaranarayanan**
- 2:00** **66.** Investigations of the role of water for promoting hydride transfer during catalytic hydrogenation of CO₂. **E.S. Wiedner**, S.A. Burgess, S.J. Connelly, S.E. Flowers, J.C. Linehan, A.M. Appel
- 2:35** **67.** Salt solubilities in aqueous solutions of NaNO₃, NaNO₂, NaCl, and NaOH: Hofmeister-like series for understanding alkaline nuclear waste. **J. Reynolds**
- 3:20** Intermission.
- 3:35** **68.** Sorption behavior of Nd³⁺, Th⁴⁺, and UO₂²⁺ to dolomite in high ionic strength systems and the effect of EDTA. **K.K. Sockwell**, F. Zengotita, A. Vento, T.M. Dittrich, D.T. Reed, Y. Katsenovich, H. Emerson
- 4:10** **69.** Exploring the role of electrolyte concentration in aluminate dimerization. **M. Pouvreau**, E. Martinez Baez, M. Dembowski, R. Gorniak, A. Wildman, C. Pearce, K. Russo, G. Schenter, A.E. Clark

ORGN

DIVISION OF ORGANIC CHEMISTRY

S. Silverman and E. McLaughlin, *Program Chairs*

SUNDAY MORNING – ORGN

SECTION A

San Diego Convention Center
Room 7B

New Reactions & Methodology

S. M. Silverman, *Organizer*

G. Alachouzos, *Presiding*

- 8:00** 1. Cyclization strategies for the synthesis of complex halocyclopentenes. **G. Alachouzos**, A.J. Frontier
- 8:20** 2. Chemoselective reductive N-alkylation of amines with carboxylic acids under hydrosilylation conditions and direct functionalization. **P. Trillo**, H. Adolfsson
- 8:40** 3. Turning waste into value: New trifluoromethylation reactions with fluoroform-derived CuCF_3 . **G. Tsui**
- 9:00** 4. Application of bond cleavage reactions for removal of directing groups. **H. XIN**, T. Deguchi, W. Akkad, H. Morimoto, T. Ohshima
- 9:20** 5. Diastereoselective iridium catalyzed amination of biosourced isohexides through borrowing hydrogen methodology. M. Jacolot, S. Moebs, **F. Popowycz**
- 9:40** 6. Development of catalytic aza-Nazarov cyclization reactions. **Y.E. Turkmen**
- 10:00** 7. Iterative Csp^3 bond formation: Second-generation automated synthesizer. S. Chitti, D. Kostyra, S.G. Ballmer, R. Hansen, **D.J. Blair**, M.D. Burke
- 10:20** 8. Halogen bond organocatalysis. **P.H. Toy**
- 10:40** 9. Domino stereoselective synthesis of β,γ -unsaturated ketones from alkenylboronic acids and tosylhydrazone-tethered nitriles. **L. Florentino**, C. Valdés
- 11:00** 10. Olefin-accelerated C-N cross-coupling in the solid-state. **K. Kubota**, T. Seo, K. Koide, Y. Hasegawa, H. Ito
- 11:20** 11. Catalytic aerobic oxidations of alcohols and aldehydes. **S. Ma**

- 11:40** 12. ^{18}F -deoxyfluorination of phenols via Ru π -complexes for the synthesis of positron emission tomography (PET) tracers. **M. Beyzavi**, D. Mandal, M. Strebl, C. N. Neuman, E. D'AMATO, J. Chen, J. M. Hooker, T. Ritter

SECTION B

San Diego Convention Center
Room 10

Asymmetric Reactions & Syntheses

S. M. Silverman, *Organizer*

T. Benkovics, *Presiding*

- 8:00** 13. Asymmetric nucleophilic fluorination under hydrogen bonding phase-transfer catalysis. **G. Pupo**, F. Ibba, D. Ascough, A. Vicini, J.M. Brown, R.S. Paton, V. Gouverneur
- 8:20** 14. Stereospecific nickel-catalyzed cross-coupling and cross-electrophile couplings of sulfonamides. **K.A. Hewitt**, E. Lucas, E.R. Jarvo
- 8:40** 15. Chiral derivatization of sulfinamides for ^1H NMR enantiomeric excess determination and chiral resolution. **R. Groleau**, T.D. James, S.D. Bull
- 9:00** 16. Accelerated asymmetric reaction screening and sensing of chiral compounds using small molecular probes. **F.Y. Thanzeel**, C. Wolf
- 9:20** 17. Iridium-catalyzed asymmetric allylic fluoroalkylation reactions. **T.W. Butcher**, J.L. Yang, J.F. Hartwig
- 9:40** 18. Stereodivergent synthesis of β -amino alkylboronic acids by diastereocontrolled mono-protodeboronation of *gem*-diboryl precursors. X. Li, **D.G. Hall**
- 10:00** 19. Catalytic asymmetric [3+2] annulation with allenylsilanes for the synthesis of spirocyclopentene oxindoles with vinylsilane functionality. **A. Cobos**, A.K. Franz
- 10:20** 20. Enantioselective carbene insertion into silanes: Access to chiral benzhydryl silanes. **J. Jagannathan**, A.K. Franz
- 10:40** 21. Catalytic asymmetric heteroatom Diels–Alder reactions catalyzed by VANOL-derived chiral borate catalysts. **L. Zheng**, X. Yin, W.D. Wulff

- 11:00** **22.** Computer-assisted design of asymmetric copper-catalyzed borylation of terminal aliphatic alkenes. **H. Iwamoto, T. Imamoto, H. Ito**
- 11:20** **23.** Iterative synthesis of Csp³ rich small molecules by using bifunctional carbenoid-boronate building blocks. **S. Chitti, D. Kostyra, D. Blair, M.D. Burke**
- 11:40** **24.** Ketoreductase enabled synthetic strategy to chiral bicyclic piperidine building blocks. **T. Benkovics, J. McIntosh, A.J. Neel, D. Lehnher, C.E. Suh**

SECTION C

San Diego Convention Center
Room 9

CH Activation

S. M. Silverman, *Organizer*
G. Hughes, *Presiding*

- 8:00** **25.** Using two diarylacetylenes as an implicit benzofulvene for benzofulvenation of *o*-arylanilines through palladium-catalyzed C–H bond activation. **S. Chuang**
- 8:20** **26.** Regio- and stereoselective palladium-catalyzed C(sp³)–H arylation of pyrrolidines and piperidines with C(3) directing groups. **D. Antermite, J.A. Bull**
- 8:40** **27.** Weakly coordinating, ketone-directed cobalt(III)-catalyzed C–H allylation, alkenylation, and vinylation: Easy access to the simple and useful structural motifs. **M. Sk, M. Maji**
- 9:00** **28.** -C–H activation of oxygen-containing heterocycles using organolithium reagents. **K. Kasten, N. Seling, A. Kwong, M. Atobe, P. O'Brien**
- 9:20** **29.** Designing of templates to reach the distal C–H bond. **D. Maiti**
- 9:40** **30.** Explaining the regioselectivity of rhodium(II)-catalyzed C–H functionalization of strained bicyclo[1.1.1]pentanes. **J.N. Sanders, Z.J. Garlets, H.M. Davies, K.N. Houk**
- 10:00** **31.** Iridium-catalysed hydrogen isotope exchange of amino acid and peptide molecules. **A. Queen, W.J. Kerr, D. Hesk, D.M. Lindsay, H. Yang**
- 10:20** **32.** Directed C–H activation using cobalt or iridium: Applications in medicinal chemistry. **M.J. Johansson, L. Ackermann, B. Martin-Matute, S.D. Friis, E. Weis**
- 10:40** **33.** Iridium-catalyzed monoselective C–H iodination of benzoic acids: Development and mechanistic investigation. **E. Weis, M.J. Johansson, B. Martin-Matute**
- 11:00** **34.** Heterocycle synthesis via C–H functionalization. **M. Shea, D. Nagib, A. Prusinowski**

- 11:20** **35.** Site-selective C–H functionalization via palladium/norbornene catalysis. **J. Wang, G. Dong**
- 11:40** **36.** Mechanistic insights and method development of selective photochemical fluorination of polycyclic terpenoid derivatives. **F. Ghorbani, S.A. Harry, T. Lectka**

SECTION D

San Diego Convention Center
Room 8

Copper-Catalyzed C-Element Bond Cross-Coupling with Arylboronic Acids: Twentieth Anniversary of Chan-Lam Reaction Discovery

Y. Du, A. J. Watson, *Organizers, Presiding*

- 8:30** Introductory Remarks.
- 8:35** **37.** Twentieth anniversary of Chan–Lam reaction. **P.Y. Lam**
- 8:55** **38.** Copper-catalyzed *N*-arylation: From method development to discovery chemistry. **P. Das**
- 9:25** **39.** Ionising cross-coupling inspired by the Chan-Lam mechanism. **A.J. Watson**
- 9:55** **40.** Oxidative carbon-carbon bond forming processes inspired by the Chan-Lam reaction. **R. Lundgren**
- 10:25** **41.** Chan–Lam couplings with tridentate sulfonate ligands: Small steps toward more general catalysts. **V. Hardouin Duparc, F. Schaper**
- 10:55** **42.** Deaminative cross-couplings via C–N bond activation. **M.P. Watson**
- 11:25** **43.** Drug discovery in academia: Success stories. **M.E. Jung**

SECTION E

San Diego Convention Center
Room 7A

Young Investigator Symposium

J. Aube, *Organizer, Presiding*

- 8:00** **44.** Designing for bias: Computational methods to drive rational design of G-protein biased agonists. **R. Torella**
- 8:30** **45.** Asymmetric atropisinduction. **C.A. Lewis**
- 9:00** **46.** Rationally designed, conformationally constrained inverse agonists of ROR γ t: Identification of a potent, selective series with biologic-like *in vivo* efficacy. **D. Marcoux, J. Duan, Q. Shi, R.J. Cherney, A. Srivastava, L. Cornelius, D.G. Batt, Q. Liu, M. Beaudoin-Bertrand, C. Weigelt, P. Khandelwal, S. Vishwakrishnan, S. Kumaravel, A. Karmakar, A.K. Gupta, M. Basha, S. Ramlingam, N. Kulahalli, S. Vanteru, S. Karmakar, N. Rao, M.**

Vetrichelvan, A. Gupta, R. Rampulla, A. Mathur, H. Yip, P. Li, D. Wu, M. Ruzanov, J. Sack, J. Wang, M. Yarde, M. Cvijic, S. Li, D. Shuster, V. Borowski, J. Xie, K. McIntyre, M. Obermeier, A. Fura, K. Stefanski, G. Cornelius, J. Hynes, J.A. Tino, J.E. Macor, L. Salter-Cid, R. Denton, Q. Zhao, P.H. Carter, M. Dhar

9:30 47. High-throughput experimentation in flow: From screening to compound production. **J.W. Tucker**

10:00 48. High-throughput reaction screening enabled by small scale solid dispensing. **A.W. Dombrowski**

10:30 49. Investigation of small molecule inhibitors of PLD for the treatment of ALS. **T. May-Dracka**

11:00 50. Robust catalytic transformations: Value of mechanistic studies in process chemistry. **S.R. Wisniewski**

SECTION F

San Diego Convention Center
Ballroom 20A

Organometallics Distinguished Author Award

P. J. Chirik, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 51. Co-catalyzed hydroacylation. **V.M. Dong**

9:05 52. Transition-metal-catalyzed asymmetric direct transformations of aromatic compounds. **S. You**

9:35 Intermission.

9:45 53. Development of Ni-catalyzed enantioselective reductive cross-coupling reactions. **S.E. Reisman**

10:15 54. Ti-catalyzed nitrene transfer reactions: Harnessing the Ti^{II}/Ti^{IV} redox couple for new transformations. **I. Tonks**

2:00 58. Computationally study of ligand effects using ligand substrate interaction model: Design of ligands that significantly improve the efficiency of CuH-catalyzed hydroamination reactions. **A.A. Thomas, K. Speck, I. Kevlishvili, Z. Lu, P. Liu, S.L. Buchwald**

2:20 59. Nickel-catalyzed cross-electrophile coupling reactions of sulfonamides for diastereoselective cyclopropane synthesis. **E. Lucas, K.A. Hewitt, E.R. Jarvo**

2:40 60. Efficient synthesis of 3-benzoyl benzo[*b*] thiophenes and raloxifene via mercury(II)-catalyzed cyclization of 2-alkylphenyl alkyl sulfoxides. **M. Wu, S. Wen, C. Lin, C. Chen**

3:00 61. Palladium-catalyzed transfer hydrogenation of alkenes using tetrahydroxydiborane as the H atom donor. **M. Yaghoubi, J. Ochoa, W. Spaller, H. Do, I. Gonzalez, B.J. Stokes**

3:20 62. Enantioselective synthesis of MK-8591 from benzalacetone via asymmetric ketone alkynylation and ozonolysis. **H.C. Johnson, N. Patel, A.M. Whittaker**

3:40 63. Bifunctional palladium complexes bearing masked protic NHC ligands as highly active catalysts for sustainable cross-coupling reactions. **V. Lindsay, J. Zhu**

4:00 64. Chromium-triggered cyclization and selective hydrogenation of conjugated dienes. **H. Steger, J.M. O'Connor**

4:20 65. Chemo- and regioselective ruthenium-catalyzed cycloaromatization of conjugated dienes. **P. Qin, J.M. O'Connor, D.M. Hitt, H. Steger, K.K. Baldrige**

4:40 66. Transition metal-catalyzed cycloaromatization of conjugated trienes. **P. Qin, J.M. O'Connor, L. Wang, Y. Li, K.M. Veccharelli, K.K. Baldrige, J. Chen, B. Tufekci**

SUNDAY AFTERNOON – ORGN

SECTION A

San Diego Convention Center
Room 7B

Metal-Mediated Reactions & Syntheses

S. M. Silverman, *Organizer*

H. C. Johnson, *Presiding*

1:00 55. Potential safety hazards associated with the Pd-catalyzed cross-coupling reactions. **Q. Yang, N. Babij, S. Good**

1:20 56. Mesoporous nanoparticle supported nickel boron composite for the catalytic reduction of nitroarenes. **G. Amberchan, J.L. Hauser, R. Manley, M. Tso, K. Bustillo, J. Cooper, J.H. Golden, B. Singaram, S. Oliver**

1:40 57. Efficient synthesis of chiral drugs facilitated by ligand design. **W. Tang**

SECTION B

San Diego Convention Center
Room 10

Chemistry & Water

S. M. Silverman, *Organizer*

A. M. Hyde, *Presiding*

1:00 67. Role of chalcogenide containing fluorescence in the analysis of reactive oxygen species (ROS) as neurodegenerative disease factor. **Y. Tesla, D.G. Churchill**

1:20 68. First catalytic asymmetric total synthesis of the 6a-hydroxypterocarpan glyceollin I. **P. Ciesielski, P. Metz**

1:40 69. Micellar gold catalysis: Three-component spirocyclization in bulk water. **N. Krause**

- 2:00 70. Synthesis, characterization and evaluation of novel heterocyclic thiosemicarbazones against MRSA. **A. Delpe Acharige**, A.M. Almeida, S.H. Bossmann
- 2:20 71. Towards the enantioselective synthesis of the sesquiterpenoid dehydrocostus lactone. **S. Nowotni**, P. Metz
- 2:40 72. Enantioselective approach to (–)-dehydrocostus lactone by a domino ring-closing-metathesis strategy. **F. Kaden**, P. Metz
- 3:00 73. Withdrawn
- 3:20 74. Estimation of polyamide interfacial polymerization reactivity ratios via solution-phase model studies. **M.J. Jansma**, T.M. Bechtel, S. Rosenberg, J.D. Wilbur
- 3:40 75. Rhodamine–Hoechst positional isomers for highly efficient staining of heterochromatin. **J. Bucevičius**, J. Keller-Findeisen, T. Gilat, S.W. Hell, G. Lukinavicius
- 4:00 76. Reductive etherification. **L. Whitaker**, K. Wheelhouse, W.J. Kerr, M. Reid
- 4:20 77. Specific ion effects in organic chemistry: Improve your liquid-liquid extractions and reactions in water. **A.M. Hyde**

SECTION C

San Diego Convention Center
Room 9

Total Synthesis of Complex Molecules

S. M. Silverman, *Organizer*
T. Davis, *Presiding*

- 1:00 78. Towards the total synthesis of agariblazeispirol. **C. R. Chung**, W.J. Kerr, T.A. Clohessy
- 1:20 79. Synthesis of melokhanine E. **A. Cholewczynski**, P. Williams, J.G. Pierce
- 1:40 80. Generation of dithianyl and dioxolanyl radicals exploiting photoredox catalysis: Application in the total synthesis of spiroketal natural products. **Y. Deng**, A.B. Smith
- 2:00 81. Asymmetric synthesis of esketamine. **C. Chen**
- 2:20 82. Total synthesis of alvaradoins E and F, uveoside, and 10-epi-uveoside. **K. Ng**, T.G. Minehan
- 2:40 83. Total syntheses of sarpagine alkaloids and non-natural derivatives. **H. Rebmann**, T. Gaich
- 3:00 84. Synthesis of polycyclic guanidinium alkaloids. **Y. Lin**, A. Ribaucourt, Y. Moazami, J.G. Pierce
- 3:20 85. Enantioselective total synthesis of (+)-dihydro- β -erythroidine. **S. Clementson**, M. Jessing, J. Langgaard Kristensen, P. Vital
- 3:40 86. Total synthesis of axially-chiral cannabinoids. **A.J. Grenning**
- 4:00 87. Stereocontrolled and practical synthesis of conserved arylomycin macrocyclic core. **N. Wong**, X. Linghu, I. Young, F. Gosselin

- 4:20 88. Uprifosbuvir: Innovating on the critical path. **P. Maligres**
- 4:40 89. Commercial route development toward merck HCV NS5b inhibitor MK-3682. **T. Davis**

SECTION D

San Diego Convention Center
Room 8

First-Generation Academic Faculty: Research Talks & Panel Discussion

S. Zultanski, *Organizer, Presiding*

- 1:15 Introductory Remarks.
- 1:20 90. Reactive vapor deposition of conjugated polymers for textile electronics. **T.L. Andrew**
- 2:00 91. Catalyst-controlled selectivity in iridium-catalyzed alkyl ether cleavage. **N.D. Schley**
- 2:40 92. Synthesis of microbial fake IDs. **S.D. Townsend**
- 3:20 93. Harnessing negative photochromic materials for synthesis of smart materials. **J. Read De Alaniz**
- 4:00 Panel Discussion.

SECTION E

San Diego Convention Center
Room 7A

Young Investigator Symposium

J. Aube, S. M. Silverman, *Organizers*
A. J. Grenning, *Presiding*

- 1:00 94. New insights into acetylation & oncometabolism from chemoproteomics. **J.L. Meier**
- 1:30 95. Process development in the pharmaceutical industry. **B. Sherry**
- 2:00 96. Synthesis of bioactive flavagline analogues as inhibitors of cap-dependent translation: Discovery of eFT226. **T. Michels**
- 2:30 97. Application of under-utilized transformations to the synthesis of pharmaceutically relevant molecules. **I. Young**
- 3:00 98. Want to improve your (bio)performance? Take a closer look at the physical properties. **J.L. Terebetski**
- 3:30 99. Polyolefin catalysts for the production of ethylene-based fluids. **B. Bailey**
- 4:00 100. Impacting the pipeline through discovery synthesis groups: Cystic fibrosis, HCV, and immunology. **S.N. Greszler**
- 4:30 101. Universal chromatographic methods and fit for purpose workflows in the research and development of new pharmaceuticals. **E. Regalado**, I. Haidar Ahmad, R. \. Bennett, V. D'Atri, A.A. Makarov, G.R. Humphrey, I.K. Mangion, D. Guillaume

SECTION F
San Diego Convention Center
Ballroom 20A

JOC/OL Lectureship

E. M. Carreira, S. J. Miller, *Presiding*

- 1:00** **102.** Enantioselective and remote C–H activation reactions. **J. Yu**
- 1:30** **103.** Bioorthogonal cyclopropanones for targeting and activating cellular proteins. **J.A. Prescher**
- 2:00** **104.** Building bridges: Strategies for the synthesis of polycyclic natural products. **S.E. Reisman**
- 2:30** **105.** Chemoenzymatic synthesis of sialidase inhibitors. **X. Chen**
- 3:00** Introduction of Awardee.
- 3:05** **106.** TCFH-NMI: Direct access to n-acyl imidazoliums for challenging amide bond formations. **G. Beutner**, I. Young, M.L. Davies, M.R. Hickey, H. Park, J.M. Stevens, Q. Ye
- 3:45** **107.** Nature's medicine chest: Opportunities for synthesis and drug discovery. **M. Brimble**
- 4:15** Introduction of Awardee.
- 4:20** **108.** Recent advances in the preparative and mechanistic aspects of synthetic methods. **S.E. Denmark**

SUNDAY EVENING – ORGN

SECTION A
San Diego Convention Center
TBD

Biologically-Related Molecules & Processes

E. C. McLaughlin, *Organizer*

5:30 - 7:30

- 109.** Human vault nanoparticle targeted delivery of antiretroviral drugs to inhibit human immunodeficiency virus type 1 infection. **K. Tamshen**, A. Wollenberg, J. Fulcher, V. Kickhoefer, J. Mrazek, J. Elliot, F. Ibarra, P. Anton, L.H. Rome, H.D. Maynard, T.J. Deming, O. Yang
- 110.** Withdrawn
- 111.** Design and synthesis of novel androstenedione-acridinium esters (AO-AEs) and their application in the ADVIA Centaur® androstenedione assay. Z. Zhao, P. Donovan, L. Parker, J. Driscoll, C. Higgins, M. Stranz, K. Garvey, J. Lyons, **Y. Zheng**
- 112.** Development of small molecules for the selective inhibition of the polysaccharide metabolism in human gut microbes. **K.C. Rees**, A.D. Santilli, K.J. Whitehead, D.C. Whitehead

- 113.** Efficient, microwave-assisted synthesis of N'-aryl/(alkyl)-substituted N-(4-hydroxy-6-phenylpyrimidin-2-yl)guanidines: Scope and limitations. **J. Singleton**, P. Machicao, R.K. Christensen, N.B. Lohner, M.A. Peterson
- 114.** Microwave-assisted synthesis of 3,6-disubstituted pyrazolo[1,5-a]-pyrimidines and progress toward discovery of anticancer activities. **J. Singleton**, **R. Dass**, M.A. Peterson
- 115.** Total synthesis and evaluating bioactivity of violaceoids A, B and their analogs. **T. Murata**, T. Kuboki, R. Ishikawa, T. Saitoh, S. Taguchi, K. Takeuchi, M. Shimonaka, I. Shiina
- 116.** Efficient syntheses of phenolic oxabicyclo[3.3.1]non-7-ene scaffolds for optimization of selectivity towards estrogen receptor targets. **T.A. Saxon**, R. Chinnasamy, J.B. Arterburn
- 117.** Trash-to-treasure transformation: Industrially and medicinally privileged compounds from Spanish moss, a neglected botanical. **D. Bandyopadhyay**, Z. Castillo, D. Gonzalez
- 118.** Highly efficient transition metal-free green synthesis of 4-aryl-2,4-dihydropyranopyrazoles. **D. Bandyopadhyay**, J. Escamilla, S. Wadekar, O. Castillo
- 119.** Withdrawn
- 120.** DNA-compatible nitro reduction and multistep synthesis of benzimidazoles and oxadiazoles. **H. Du**, N. Simmons, M. Bangs, J. Faver, Z. Yu, M. Palaniappan, K. Riehle, M.M. Matzuk
- 121.** Optimization of guanidinylation of amines for the synthesis of protease-focused DNA-encoded chemical library. **S. Dawadi**, N. Simmons, M.M. Matzuk
- 122.** Withdrawn
- 123.** Synthesis of novel rearranged stemodane diterpenoids and their biotransformation by *Exophiala jeanselmei* var. *lecanii-corni*. **R.K. Pryce**, P.B. Reese
- 124.** Adaptation of ring-closing olefin metathesis and palladium-catalyzed hydroxycarbonylation reactions to a DNA-encoded chemical library platform. **N. Simmons**, J. Li, O. Monty, M.M. Matzuk
- 125.** Development of an efficient route to beta-lactamase inhibitor relebactam (MK-7655). **J.Y. Chung**, D. Meng, F. Xu, M. Shevlin, Q. Chen, A. Dumas, J.P. Scott
- 126.** Discovery of a novel, boron-containing macrolide as a mosquito-specific toxin for insecticide development. **J.M. Macho**, P. Fu, K. Vian, A. Khadiikar, J. Abrams, J. MacMillan
- 127.** Withdrawn
- 128.** Broadening the activity of ribocil-C through application of the eNTRY rules. **S. Motika**

- 129.** Pd-catalyzed C–N cross coupling between on-DNA aromatic halides and amines. **Y. Chen**, N. Simmons, M.M. Matzuk
- 130.** Catalytic promiscuity vs. stereochemical fidelity: Toward an enzymatic dynamic reductive kinetic resolution (DYRKR) entry into valuable chiral synthons and a model for the structural basis for enantio- and facial selectivity. **G.P. Kudalkar**, V.K. Tiwari, P. Madzalan, M.A. Wilson, D.B. Berkowitz
- 131.** Total synthesis of DHA-derived epoxides and their tissue regenerative sulfido-conjugates. **T.F. Lam**, R. Nshimiyimana, N.A. Petasis
- 132.** Bioluminescence and triplet excited states. N. DeHowitt, Z. Han, **R. Stanton**, N. Villasenor, M.C. Pirrung
- 133.** Synthesis and studies of porphyrin based bifunctional theranostic agents for magnetic resonance imaging and photodynamic therapy. **S. Singh**, A. Aggarwal, C.M. Drain
- 134.** Targeting BACE1 selectivity by spiro-1,3-oxazines and 1,4-oxazines. **C. Hsiao**, A. Peschiulli, F. Rombouts, H. Gijzen
- 135.** Antibacterial activity of multiflora Jamaican propolis. **S.B. Simpson**, A. Nawaz, D. Williams, O.E. Christian
- 136.** Synthesis of isotopically labeled guanosine diphosphate- α -D-[UL]- $^{13}\text{C}_6$ -mannopyranose. **A. Das**, J.P. Malerich
- 137.** Hydrolysis of salicylaldehyde imines by arylboronic acid catalysts. **C.C. Clement**, S. Zakia, M. Philipp

SECTION A

San Diego Convention Center
TBD

Chemistry & Water

E. C. McLaughlin, *Organizer*

5:30 - 7:30

- 138.** Exploration of *cis*-diamine-based conformationally locked chiral ligands in asymmetric synthesis. **C. van Beek**, V.V. Samoshin
- 139.** Mechanistic insights on the on-water Diels–Alder and Claisen rearrangement reactions. **M. Ibrahim**, T. Nizami, W. Cole, R.J. Saykally, H. Mishra
- 140.** Novel nanoprecipitation-based formulation technology to enhance catalytic activity of known catalysts in aqueous media. **D. Budai**, T. Bihari, F. Somodi, F. Darvas
- 141.** Sustainable drug discovery and development: SUDDEN Project. S. Karlsson, S. Kauppi, R. Kärkkäinen, M. Lundström, J. Martikainen, M. Miettinen, M. Mänttari, T. Sikanen, M. Sokero, H.

Xhaard, **J.T. Yli-Kauhaluoma**

- 142.** Polymer fibers from reversibly cross-linked polysaccharide networks in water. **C. Chu**, A. Joseph, R. Langer, D.G. Anderson
- 143.** From detection to complexation: Detecting and removing aluminum from aqueous solutions. J.P. Rickett, **M.W. Fultz**

SECTION A

San Diego Convention Center
TBD

Chemistry of Fullerenes, Carbon Nanotubes & Graphene

E. C. McLaughlin, *Organizer*

5:30 - 7:30

- 144.** Fjord-edge nitrogen doped graphene nanoribbons. **Y.L. Li**, V. Basile, M. Flores, C. Zee, M. Muni, J.B. Lin, K.N. Houk, R.B. Kaner, S.H. Tolbert, Y.F. Rubin
- 145.** Synthesis and characterization of a red to near-IR absorbing donor-acceptor styrl-BODIPY conjugates. **A.D. Benitz**, F. D'Souza, M. Thomas

SECTION A

San Diego Convention Center
TBD

Flow Chemistry & Continuous Processes

E. C. McLaughlin, *Organizer*

5:30 - 7:30

- 146.** Multistep continuous flow synthesis of imatinib. **J. Szeto**, K. Rucker, D. Stout, J. Lim, S. Mallya, J.D. White, J.P. Malerich, N. Collins
- 147.** Continuous flow *N*-Boc deprotection of amines using solid acid catalysts. **J. Wu**, C. Zeng, B. Li, J. Hawkins, S.L. Scott
- 148.** Improving multiphase catalytic microreactor productivity using a tube-in-tube membrane contactor. **M. Burkholder**, S. Gilliland, A. Luxon, C. Tang, F. Gupton

SECTION A

San Diego Convention Center
TBD

Materials, Devices & Switches

E. C. McLaughlin, *Organizer*

5:30 - 7:30

- 149.** Organic thin film transistor characteristics by using biosynthesized biosemiconductor named as *melanindigo*. **Y. Kim**, H. Park, P. Lee, K. Woo, K. Choi, H. Lee

- 150.** Thienopyrroledione-based photosensitizers as strong photoinduced oxidants: Oxidation of $\text{Fe}(\text{bpy})_3^{2+}$ in a >1.3 V dye-sensitized solar cell. **R.R. Rodrigues**, A. Peddapuram, J.H. Delcamp
- 151.** Unique degradable guanidine derivatives and their polymers. **T. An**, Y. Lee
- 152.** Building a cocrystal via supramolecular synthons for pressure-accelerated heteromolecular azide-alkyne cycloaddition. **Y. Ma**
- 153.** Universal engineering of small organic dyes into fluorescent crystals by hierarchical assembly. C. Benson, L. Kacenauskaite, **K. VanDenburgh**, W. Zhao, B. Qiao, T. Sadhukhan, M. Pink, J. Chen, S. Borgi, C. Chen, K. Raghavachari, B. Laursen, A.H. Flood
- 154.** Thermosolient amphidynamic crystals: Effects of a phase transition on the motion at the molecular and macroscopic scales. **M.J. Jellen**, A. Colin-Molina, D. Karothu, R. Toscano, M.A. Garcia-Garibay, P. Naumov, B.V. Rodriguez-Molina
- 155.** Fabrication of black electrochromic device using a small molecule electroactive dye. **M. Baczkowski**, M. Li, O. Yassin, G. Sotzing
- 156.** Aziridine-based photochromic monomers for conductive polymers. **C. Udumulle Gedara**, M.C. Stefan, M.C. Biewer
- 157.** Development of highly soluble cyclopropenium salts leading to highly concentrated non-aqueous flow battery. **Y. Yan**, S.G. Robinson, K. Hendriks, M.S. Sigman, M.S. Sanford

SECTION A

San Diego Convention Center
TBD

Molecular Recognition & Self-Assembly

E. C. McLaughlin, *Organizer*

5:30 - 7:30

- 158.** Insights into supramolecular organization of cellulose nanocrystals in chiral nematic films. **O.V. Kulikov**, N. Wojtania, B.M. Novak
- 159.** Counter ion effect on the high-affinity binding of pyrophosphate by resorcinarene tetra-salt receptors. **J. Feder**, K. Twum, N. Schileru, M. Taimoory, S. Taimoory, J.F. Trant, N.K. Beyeh
- 160.** Allosteric control of photofoldamers for selecting between anion regulation and double-to-single helix switching. **F.C. Parks**, Y. Liu, S. Debnath, S. Stutsman, K. Raghavachari, A.H. Flood
- 161.** Free amino acid recognition: Bisbinaphthyl-based fluorescent probe with high enantioselectivity. **X. Wu**, Y. Zhu, S. Gu, L. Pu
- 162.** Using electron-transfer-induced proton transfer to control binding strength in a H-bond dimer. **H. Choi**, D.K. Smith

- 163.** Electrochemically controlled dimerization in ferrocene ureidopyrimidone derivatives: Effect of ferrocene position. **V. Mikhaylova**, **S. Murillo**, D.K. Smith
- 164.** Comparison of redox dependent H-bonding in simple electroactive ureas containing either ferrocene or phenylenediamine redox couples: Similar results with different mechanisms. D.K. Smith, **K. Logan**, **A. Elashmawy**
- 165.** Perturbation of ureidopyrimidinone polymerization via electrochemical oxidation of a ferrocene-substituted ureidopyrimidone. **M.R. Cedano**, K. Vuong, D.K. Smith
- 166.** Use of a redox-responsive 4 H-bond ureidopyrimidone (UPy) array to control polymerization in a UPy-Based supramolecular polymer. **K. Vuong**, M.R. Cedano, D.K. Smith
- 167.** Electrostatic control of macrocyclization reactions in water-soluble supramolecular capsules. **X. Cai**, B.C. Gibb

SECTION A

San Diego Convention Center
TBD

Peptides, Proteins & Amino Acids

E. C. McLaughlin, *Organizer*

5:30 - 7:30

- 168.** Silylated tag assisted peptide synthesis (STAG-PS): Greener and continuous peptide synthesis for the congested amino acids. **H. Kubota**, S. Yano, T. Mori
- 169.** C18AQ flash column and its application in the purification of strong polar peptides. **B. Xu**, W. Qiu, A. Couture
- 170.** Fully automated optimized synthesis of linaclotide using orthogonally protected cysteine residues and on-resin oxidation chemistry. **E. Denton**, J.R. Bickler
- 171.** Contribution of bulky- α , β -dehydroamino acids to the proteolytic stability of 310-helices. **G. Damstedt**, M. Lee, J. Singh, S.L. Castle
- 172.** Responses of fluorescent probes to amyloid-beta peptides. **C. Chen**, S. Benavides, S. Mattei, J. Debrow, A. Hughes, O. Mantussova, S. Sahloul
- 173.** Synthesis and structural determination of chiral asymmetric ureas as α , β -dipeptide derivatives. **S. García**, R. Guzmán-Mejía, J.A. Aviña-Verduzco
- 174.** Determining the susceptibility of various α , β -dehydroamino acids to conjugate additions. **M. Lee**, J. Singh, G. Damstedt, S.L. Castle

- 175.** Design and synthesis of a peptide-aldoxorubicin conjugate to target triple negative breast cancer. **A. Saghaidehkordi**
- 176.** Peptide-doxorubicin conjugate for specific uptake by triple negative breast cancer cells. **e. ziaei**
- 177.** Challenges in the synthesis of peptidic macrocyclic biaryl ethers. **M.G. Gotz**, R. Dorn
- 178.** Peptide stapling by Lewis base-Brønsted acid catalyzed sulfenylation of tryptophan. **Z. Brown**, M.A. Saputra, H. Henriksen, I.W. Bell, J.J. Provost, J.L. Gustafson
- 179.** Structural studies of charged heptapeptides with point mutations using solution state two-dimensional NMR spectroscopy. **T. Bentley**, A. Xiong, C. Robinson, I. Fuson, K.V. Krishnan, K. Maitra

SECTION A

San Diego Convention Center

TBD

Physical Organic Chemistry: Calculations, Mechanisms, Photochemistry & High-Energy Species

E. C. McLaughlin, *Organizer*

5:30 - 7:30

- 180.** pH and temperature effects on process-scale degradation of clavulanic acid. **J.B. Washington**, M. Reid, S. Baillie
- 181.** Theoretical conformational studies of symmetric diesters including solvent effects. **S. Niwayama**, K. Osada, M. Yoshida, S. Matsushima
- 182.** Photooxidation of *o*-alkynylaryl oximes: Intramolecular cyclization reaction. **V.M. Espinoza Castro**, A. Council, E. Armenta, M. Ko, W.S. Kim, A.M. Abiad, A.S. Petit, P. De Lijser
- 183.** Mechanism of cinchona-alkaloid catalyzed asymmetric chloro-functionalization of alkenes. **A. Sarkar**, T. Kakeshpour, D. Steigerwald, S. Bedford, B. Soltanzadeh, R. Yousefi, B. Borhan, J.E. Jackson
- 184.** Withdrawn
- 185.** Unusual KIE for ring-opening of short-lived intermediate formed by PCET reaction. **S. Alvi**, D.A. Singleton, H. Kurouchi
- 186.** Computational investigations of polymeric NHCs as catalysts for benzoin condensation. **K. Melancon**, T. Cundari

New Reactions & Methodology

S. M. Silverman, *Organizer*A. Sanford, *Presiding*

- 8:00** **187.** Palladium-catalyzed oxidative homocoupling of pyrazole boronic esters to access bipyrazoles for metal-organic frameworks. **M.K. Taylor**, M. Juhl, D. Hwang, G. Hadaf, E. Velasquez, J. Oktawiec, J.B. Lefton, T. Runcevski, J.R. Long, J. Lee
- 8:20** **188.** Quaternary carbon synthesis by acid-catalyzed intermolecular hydroarylation of electron-deficient α -methylstyrenes. **J. Alvarenga**, A. Keshavarz, B.J. Stokes
- 8:40** **189.** Synthesis of novel renewable monomers from abundant monoterpenes. **S. Smith**, R. Stockman, S.M. Howdle
- 9:00** **190.** Diisobutylaluminum borohydride (snelling salt): A versatile and efficient reducing agent. **G. Amberchan**, B. Singaram, E. Moya, M. Landi, K. Lutz
- 9:20** **191.** Inquest for better selectivity and activity: Nucleophilic organocatalysts based on branched/dendritic design. **M. Portnoy**, N. Ashush, R. Fallek, A. Fallek, M. Weiss-Shtofman
- 9:40** **192.** Nickel-catalyzed arylation of aldehydes to form secondary alcohols. **K.J. Garcia**, M.M. Gilbert, D.J. Weix
- 10:00** **193.** I(I)/I(III) catalyzed *vicinal* dichlorination of alkenes. **J.C. Sarie**, J. Neufeld, C.G. Daniliuc, R. Gilmour
- 10:20** **194.** Synthesis of pyrrolidines from sulfinamide azomethine ylide precursors. **D. O'Connor**, R.A. Stockman
- 10:40** **195.** Single-electron reduction of iminium ions via ion pair charge-transfer. **K. Kohara**, M. Gaunt
- 11:00** **196.** Nickel-catalyzed cross-electrophile coupling reactions of diol derivatives. **A. Sanford**, T.A. Thane, E.R. Jarvo
- 11:20** **197.** Synthesis of sulfoximines and sulfonimidamides by highly chemoselective NH and O transfer. **J.A. Bull**, R. Luisi
- 11:40** **198.** Copper-mediated stereospecific intramolecular deoxyfluorination using CuF_2 . **D.E. Sood**, D.M. Dawson, Y.G. Andreev, S. Chabbra, B.E. Bode, A.J. Watson

SECTION B
San Diego Convention Center
Room 10

Peptides, Proteins & Amino Acids

S. M. Silverman, *Organizer*
S. Tower, *Presiding*

- 8:00** **199.** Synthesis of (*R*)- α -methylselenocysteine and its application as a glutathione peroxidase mimic. **R.J. Wehrle**, E. Ste.Marie, R.J. Hondal, D.S. Masterson
- 8:20** **200.** Bioorthogonal modification of dehydroalanine residues in RiPPS via Diels-Alder cycloadditions. **R. de Vries**, R. Oudshoorn, G. Roelfes
- 8:40** **201.** Antimicrobial stapled peptide-drug conjugates. **J. Gynord**, J. Parker, M. Welch, D.R. Spring
- 9:00** **202.** Progress towards the total synthesis of yaku'amide A and analogues. **D. Joaquin**, C. Lo, D. Moya, A. Ramos, S. White, S.L. Castle
- 9:20** **203.** Conformational analysis of lantibiotic peptides. **R. Dickman**, E.R. Danelius, M. Erdélyi, A.B. Tabor
- 9:40** **204.** Developing a novel chemical approach for arginine modification. **M. Xu**
- 10:00** **205.** Sulfatase-cleavable linkers for antibody-drug conjugates (ADCs). **J. Bargh**, S. Walsh, A. Isidro-Llobet, D.R. Spring
- 10:20** **206.** Selective modification of proteins with fluoroalkyl radical precursors. **M. Imiolek**, B.G. Davis
- 10:40** **207.** Chemical biology approaches to understanding the structure and function of Protoxin-II. **S. McCarthy**, J. Robinson, F. Reyes, S. Sanchez-Martinez, T. Gonen, M. Topf, K. Thalassinou, A.B. Tabor
- 11:00** **208.** Preventing Huntington's disease using protein-like polymers. **W. Choi**, Y. Shang, X. Qi, N.C. Gianneschi
- 11:20** **209.** Electron transfer reagents for selective photo-bioconjugation of proteins. **M. Taylor**
- 11:40** **210.** Site-selective modification of tryptophan residues in peptides and proteins using redox active pyridinium salts and light. **S. Tower**, W. Hetcher, T. Myers, M. Taylor

SECTION C
San Diego Convention Center
Room 9

Materials, Devices & Switches

S. M. Silverman, *Organizer*
R. L. Greenaway, *Presiding*

- 8:00** **211.** Observation of conformational transition of perfluorophenyl substituted benzanilide derivative. **R. Yamasaki**, M. Harada, R. Nagata, A. Ito, K. Fukuda, I. Okamoto
- 8:20** **212.** Discotic liquid crystals: From quinoxalinophenanthrophenazine to isoindigo discotics. **B.R. Kaafarani**, S.H. Eichhorn
- 8:40** **213.** High-voltage molecular engineered organic sensitizer-iron redox shuttle pair: 1.4 V DSC and 3.3 V SSM-DSC devices. **R.R. Rodrigues**, H. Cheema, J.H. Delcamp
- 9:00** **214.** Understanding the diverse solution reactivity of N-DMBI-H with organic semiconductor molecules. **S. Jhulki**, H. Un, C. Risko, J. Pei, S. Barlow, S.R. Marder
- 9:20** **215.** Hybrid discovery workflow for organic materials and supramolecular self-assemblies. **R.L. Greenaway**, V. Santolini, E. Berardo, M. Bennison, B. Alston, M. Little, R. Kearsley, M. Miklitz, K. Jelfs, A.I. Cooper
- 9:40** **216.** Effect of thiol substitution on the thiol-ene polymerization: Kinetics and mechanical properties. **K. Long**, M. Olin, A. Ortega, S. Huang, C. Bowman
- 10:00** **217.** Photoswitch generation using mechanical force. **X. Hu**, M.E. McFadden, R. Barber, M.J. Robb
- 10:20** **218.** Photoinduced electron transfer in meso donor carrying bis styryl BODIPY bound to fullerene using "two point" self assembly strategy. **S. Shao**, H.B. Gobeze, P.A. Karr, F. D'Souza
- 10:40** **219.** Enhanced purification of carbon nanomaterials. **V. Gangoli**, B. Brinson, A.R. Barron
- 11:00** **220.** Synthesis of nanographenes via alkyne benzannulation reactions. **P. S**
- 11:20** **221.** Atomically precise graphene nanoribbons: Bottom-up synthesis, characterization, and applications. **A. Sinitskii**

SECTION D
San Diego Convention Center
Room 8

Organic Chemistry at Self-Assembling & Biological Interfaces

S. M. Silverman, *Organizer*
D. Bong, *Organizer, Presiding*

- 8:00** **222.** Targeting structurally and functionally diverse nucleic acids with druglike small molecules. **J. Schneekloth**
- 8:30** **223.** Isomorphous and isofunctional fluorescent nucleosides. **Y. Tor**

- 9:00 **224.** Single chain polymeric nanoparticles containing transition metals as artificial metalloenzymes. **S.C. Zimmerman**, J. Chen, T. Xiong, E.S. Gracia Ramirez, Y. Xu
- 9:30 **225.** Applications of a synthetic base-triple motif in nucleic acid structure-function, diagnostics, and delivery. **D. Bong**
- 10:00 **226.** PNA-based sensors for disease-relevant miRNAs. **A.J. Kennan**, M. Schenkel, C. Henry
- 10:30 **227.** Modulating noncovalent interactions at cellular interfaces. **K. Kumar**
- 11:00 **228.** Exploring the human smORFeome. **A. Saghatelian**
- 11:30 **229.** Toward novel therapeutics via directed remodeling of the gut microbiome. P. Chen, A. Black, P. Mukherjee, Y. Zhao, A.L. Sobel, B. Molparia, G.R. Aleman Muench, J. Wu, W. Chen, A. F. M. Pinto, B.E. Maryanoff, A. Saghatelian, P. Soroosh, A. Torkamani, L.J. Leman, **M.R. Ghadiri**

SECTION E

San Diego Convention Center
Room 7A

Young Investigator Symposium

J. Aube, *Organizer*
H. Xu, *Presiding*

- 8:00 **230.** Shifting the oxidation pathways of polyethylene to provide carbonaceous species in high yield. **B.E. Barton**
- 8:30 **231.** Discovery and evolution of potent and selective heme-displacing IDO1 inhibitors. **M. McGowan**
- 9:00 **232.** Design and development of catalytic processes for the synthesis of antiviral agents EFda (MK-8591) and vaniprevir (MK-7009). **J. Kong**
- 9:30 **233.** Convergent synthesis of the NS5B inhibitor GSK8175 enabled by transition metal catalysis. **I.I. Strambeanu**
- 10:00 **234.** Organic molecules as forensic fuel markers. **R. Wright**
- 10:30 **235.** Rational design of organic materials for advanced microlithography. **J.A. Kaitz**
- 11:00 **236.** Development of PMC friendly approaches to the construction of synthetically challenging cyclopropane motifs. **M. Harris**
- 11:30 **237.** Discovery of MK-8153: ROMK inhibitor as new mechanism diuretic for hypertension and heart failure. **S. Dong**

SECTION F

San Diego Convention Center
Ballroom 20A

Tetrahedron Prize

Financially supported by Elsevier
S. M. Silverman, *Organizer*
S. F. Martin, *Organizer, Presiding*

- 8:00 Introductory Remarks.
- 8:05 **238.** Control of polymer chain growth with external stimuli. **B.P. Fors**
- 8:55 **239.** Using synthetic chemical tools to understand how toxic chemicals and drugs interfere with DNA replication and transcription. **S.J. Sturla**
- 9:45 **240.** Synthesis and applications of complex natural products. **T.J. Maimone**
- 10:35 Introduction of Awardee.
- 10:45 **241.** Palladium-induced carbon-heteroatom bond-forming reactions for the functionalization of molecules big and small. **S.L. Buchwald**
- 11:45 Concluding Remarks.

Frontiers in Interdisciplinary Research: New Paradigms for Integration of Theory & Experiment

Sponsored by BIOL, Cosponsored by COMP, ORGN and PHYS

Identification & Design of Catalytic Sites in Electrochemical Reactions

Sponsored by ANYL, Cosponsored by ORGN

MONDAY AFTERNOON – ORGN

SECTION A

San Diego Convention Center
Room 7B

Physical Organic Chemistry: Calculations, Mechanisms, Photochemistry & High-Energy Species

S. M. Silverman, *Organizer*
C. J. Hall, *Presiding*

- 1:00 **242.** Mechanism, selectivity, and orbital symmetry of CF₃-Py ligand couplings at pentacoordinate phosphorous. **J. Alegre Requena**, R.S. Paton
- 1:25 **249.** Withdrawn
- 1:50 **243.** Computational investigation of the thermal stability and temperature-dependent electronic properties of highly energetic material TKX-50. **J. Scher**, A. Chakraborty

- 2:15 244.** Contra thermodynamic, photocatalytic *E* to *Z* isomerization of alkenyl organoborons: Vectors to facilitate exploration of two dimensional chemical space. **J. Molloy**, J. Metternich, A.J. Watson, R. Gilmour
- 2:40 245.** Mechanistic analysis of trimethylanilinium salts: Implications for methylation and cross-coupling chemistry. **J.B. Washington**, M. Reid, S. Baillie
- 3:05 246.** Unique photochemistry of new strongly alkaline heterocyclic amine-based donor- π -acceptor photoacids. **R. Bhide**, E. Schwartz, D. Fishman, S. Ardo
- 3:30 247.** Solvent-assisted, visible light RAFT polymerization. **M.D. Thum**, D. Falvey
- 3:55 248.** Investigation of the photochemistry of chlorinated flavins and flavinium cations. **B. Etz**, J. DuClos, J. Bingham, S. Vyas
- 4:20 250.** Investigation of the photochemistry and reactivity of diazidobenzene. **J.T. Bingham**, B. Etz, S. Vyas

SECTION B

San Diego Convention Center
Room 10

Heterocycles & Aromatics

S. M. Silverman, *Organizer*

S. P. Mulcahy, *Presiding*

- 1:00 251.** Synthesis and functionalization of [*b*]-fused pyridine compounds. **F. Popowycz**, H. Lavrard
- 1:20 252.** Fascinating dynamic behavior of rare diazacyclobutenes. **C.J. Narangoda**, A. Kitaygorodskiy, C.D. McMillen, J.E. Jackson, D.C. Whitehead
- 1:40 253.** Trapping of *N*-acyliminium ions with enamides: Approach to medium-sized diaza-heterocycles. **L. Andna**, L. Miesch
- 2:00 254.** Parallel synthesis of benzimidazoles via oxidative cyclization. **D. Schmitt**, E. Arnold, P.K. Mondal
- 2:20 255.** Brønsted acid catalyzed one-pot benzannulation of 2-alkenylindoles under aerial oxidation: Route to carbazoles and indolo[2,3-*a*] carbazole-alkaloids. **S. SAHA**, M. Maji
- 2:40 256.** From late-stage oxidation to heterocyclic synthesis: New methodology for drug discovery. **E.P. Talbot**
- 3:00 257.** Synthesis and applications of the MR1 ligand precursor 5-amino-6-D-ribitylamouracil (5-A-RU). **J. Aube**
- 3:20 258.** Tandem transition metal catalysis in the synthesis of carboline heterocycles. **S.P. Mulcahy**

- 3:40 259.** Use of microwaves for synthesis of propargylic ethers as precursors of 1,2,3-triazoles in click reactions. **L.C. García Sanchez**, M.A. García Eleno, E. Cuevas Yañez, **A.F. Becerra Buitrago**, J.A. García Ortiz
- 4:00 260.** Readily accessible sp^3 -rich cyclic hydrazine frameworks exploiting nitrogen fluxionality. **C.L. Dean**, R. Sundaram, G.J. Clarkson, M. Jones, M. Wills, M. Shipman
- 4:20 261.** Tetrazole and oxadiazole heterocycles via multi-component reaction schemes. **M. Konstantinidou**, S. Kurhade, F. Sutanto, K. Kurpiewska, J. Kalinowska, A. Doemling
- 4:40 262.** Practical synthesis of 1-bromocodeine derivatives and the first synthesis of bismorphine. **A. S. Mansouri**, A. Ali, J. Desaulniers, Y. Bolshan

SECTION C

San Diego Convention Center
Room 9

Materials, Devices & Switches

S. M. Silverman, *Organizer*

D. Tilly, *Presiding*

- 1:00 263.** Stimuli responsive discotic semiconductors: From materials to devices. **B. Gomez-Lor**, A. Benito, M. Echeverri
- 1:20 264.** Donor-acceptor molecular switches as novel mechano-responsive chromophores. **Y. Liu**, A. Halmes, Q. Wu, J.S. Moore
- 1:40 265.** Macroscopic photon-powered actuators based on organized photomechanical nanocrystals. **F. Tong**, X. Dong, C.J. Bardeen
- 2:00 266.** Ligand induced polarity switch of dynamic ethylene-bridged non classical oligoureas. **D. Tilly**, D.T. Morris, J. Clayden
- 2:20 267.** Extending the bay-area: Synthesis, characterization, and application (OLED, OFET) of novel azaborinine-substituted coronene diimides. **J. Hoffmann**, M. Hissler, A. Staubitz
- 2:40 268.** Self-assembled azobenzene functionalized molecules for all-optical control of integrated photonics. **J. He**, A. Kovach, A.M. Armani
- 3:00 269.** Design and synthesis of electroactive chromophore for achieving black in electrochromic devices. **O. Yassin**, M. Baczkowski, G. Sotzing
- 3:20 270.** Tuning properties of a hydroquinone chromophore. **H. Arslan**
- 3:40 271.** Synthesis and characterization of dicyanomethyl aryl radicals. **R. Zhang**

- 4:00 **272.** Tale of redox-active organic radical polypeptides as electrode materials: From full organic batteries to electron-transfer kinetics. **T. Nguyen**, A. Easley, N. Kang, C.H. Komatsu, C. Yu, J. Fan, R.A. Letteri, X. He, L. Su, J.L. Lutkenhaus, K.L. Wooley

SECTION D

San Diego Convention Center
Room 8

Artificial Intelligence in Organic Synthesis

A. A. Shah, V. W. Shurtleff, *Organizers, Presiding*

- 1:00 Introductory Remarks.
1:05 **273.** (Un)supervised learning for the screening and classification of homogeneous catalysts. **C. Corminboeuf**, B. Meyer, B. Sawatlon, M.D. Wodrich
1:50 **274.** Machine learning for organic chemistry reaction prediction and retrosynthesis. C.W. Coley, T.J. Struble, H. Gao, X. Wang, W. Lin, R. Barzilay, T. Jaakkola, W.H. Green, **K.F. Jensen**
2:35 Intermission.
2:40 **275.** Towards AI-based synthesis at scale. **M. Waller**
3:25 **276.** Synthia™ (Chematica) retrosynthetic software for practicing chemists: Novel and efficient *in silico* pathway design validated at the bench. **S. Trice**
4:10 **277.** Chemical reaction data reuse: Preparing ELN data for analytics and prediction. **S. Harrison**
4:55 Concluding Remarks.

SECTION E

San Diego Convention Center
Room 7A

Organic Chemistry for Next-Generation Therapeutics

R. M. Franzini, *Organizer, Presiding*

- 1:00 Introductory Remarks.
1:05 **278.** Click and release: Unique approach to prodrugs of gasotransmitters. **B. Wang**
1:35 **279.** Bioconjugation via zwitterionic boron-nitrogen heterocycles. T. Chio, H. Gu, K. Mukherjee, L. Tumey, **S.L. Bane**
2:05 **280.** Click-cleavable antibody-drug conjugates (ADCs). **R. Rossin**
2:35 Intermission.
2:45 **281.** Controlled activation of RNA-based therapeutics. **M. Royzen**, M.V. Yigit
3:15 **282.** SQ3370: Enhancing safety and efficacy of systemic cytotoxic prodrugs using bioorthogonal chemistry-driven local drug activation. S. Srinivasan, N.A. Yee, M. Royzen, **J. Mejia Oneto**

- 3:45 **283.** Bioorthogonal reactions between isonitriles and tetrazines. **J. Tu**, R.M. Franzini
4:15 **284.** Nucleophile-triggered cleavable linkage chemistry: Fundamentals and applications. **M. Finn**, S. Tekkam, L. DePascalis, C. Higginson, M. Yau
4:45 Concluding Remarks.

SECTION F

San Diego Convention Center
Ballroom 20A

Tetrahedron Prize

Financially supported by Elsevier

S. M. Silverman, *Organizer*

S. F. Martin, *Organizer, Presiding*

- 1:00 Introductory Remarks.
1:05 **285.** Break-it-to-make-it strategies for complex molecule synthesis. **R. Sarpong**
1:55 **286.** Rh-catalyzed hydroacylation. **V.M. Dong**
2:45 **287.** Multimetallic catalysis with palladium and nickel. **D.J. Weix**
3:35 Introduction of Awardee.
3:45 **288.** Catalytic substitution and C-H bond functionalization reactions. **J.F. Hartwig**
4:45 Concluding Remarks.

Frontiers in Interdisciplinary Research: New Paradigms for Integration of Theory & Experiment

Sponsored by BIOL, Cosponsored by COMP, ORGN and PHYS

Identification & Design of Catalytic Sites in Electrochemical Reactions

Sponsored by ANYL, Cosponsored by ENFL and ORGN

MONDAY EVENING – ORGN

SECTION A

San Diego Convention Center
TBD

Sci-Mix

E. C. McLaughlin, *Organizer*

8:00 - 10:00

116, 119, 124, 125, 132, 135, 139, 140, 141, 142, 145, 146, 150, 153, 157, 158, 161, 166, 170, 171, 177, 185, 186. See Previous Listings.
389, 390, 397, 398, 400, 407, 409, 414, 428, 444, 448, 449, 451, 452, 458, 459, 460, 461, 464, 467,

471, 476, 478, 481, 484, 597, 600, 607, 611, 612, 616, 617, 620, 622, 624, 633, 635, 636, 641, 645, 648, 655, 656, 669, 673, 675, 676. See Subsequent Listings.

Biologically-Related Molecules & Processes

S. M. Silverman, *Organizer*
Y. L. Zhong, *Presiding*

- 8:00 301. Shape-selective recognition of the major groove of DNA: Synthesis and DNA binding profile of monomeric, dimeric, and trimeric derivatives of crystal violet. **T.G. Minehan**, O. Nunez, R. Shaktah, B. Chavez
- 8:20 302. Optical control of lipid metabolism and signaling. **J. Morstein**, A. Novak, D. Trauner
- 8:40 303. Silicon polymethine fluorophores for the near-infrared and shortwave infrared. **M. Pengshung**, E.M. Sletten
- 9:00 304. X-ray crystallographic investigations and molecular dynamics simulation studies with phospholipase A2 of some Leonard linker pyrazolo[3,4-d]pyrimidine compounds. **U. Yadava**
- 9:20 305. From free radical chemistry to novel classes of bioactive molecules. Y. Guindon, M. Nemer, **M. Prévost**, S. Dostie, P. Mochirian, W. Maharsy, G. Kanaan
- 9:40 306. Safe and high yielding synthesis of diazeniumdiolates and the application for synthesis of MK-8150. **Y. Zhong**, M.D. Weisel, G.R. Humphrey, D.J. Muzzio, L. Zhang, M.A. Huffman, W. Zhong, K.M. Maloney, K.R. Campos
- 10:00 307. Design and stereospecific synthesis of atypical C1, C5, and C6-substituted carbapenem antibiotics. **M. Alqurafi**, T.Q. Nguyen, N.M. Al-Kharji, W. Chai, N. Nformi, M. Pan, J. Kim, A. He, S. Solanki, B. Meshram, C. Varner, K. Wong Wirth, S. Salinas Garcia, L. Newman, Y. Samadzada, J.D. Buynak
- 10:20 308. Convergent synthesis of PI3K inhibitor GDC-0908 featuring palladium-catalyzed direct C-H arylation toward dihydrobenzothienooxepines. **H. Zhang**
- 10:40 309. Near-infrared chemiluminescence probes for detection and imaging. **O. Green**, D. Shabat
- 11:00 310. Flavylium polymethine fluorophores for multiplexed *in vivo* imaging with shortwave infrared light. **E.D. Cosco**, A.L. Spearman, S. Ramakrishnan, J.G. Lingg, M. Pengshung, M. Saccomano, S. Glasl, M. Warmer, R.R. McLaughlin, O.T. Bruns, E.M. Sletten
- 11:20 311. Withdrawn
- 11:40 312. Synthesis of small molecule inhibitors to study fatty acid recycling. **K. Jaremko**, M. Currie, J. Beld

TUESDAY MORNING – ORGN

SECTION A San Diego Convention Center Room 7B

New Reactions & Methodology

S. M. Silverman, *Organizer*
E. Corcoran, *Presiding*

- 8:00 289. Dealkylative *N*-arylation of sulfonamides. **M. West**, B.J. Thomson, A.J. Watson
- 8:20 290. Advancing the original cope rearrangement: Fundamental studies and applications in complex molecule synthesis. **A.J. Grenning**
- 8:40 291. Decarboxylative amination of redox-active esters using diazirines. **P. Chandrachud**
- 9:00 292. Diboron-mediated semireduction of terminal allenes. **A. Gates**, W.L. Santos
- 9:20 293. Pd-Cu mediated decarboxylative *ortho*-halogenation of aryl carboxylic acids. **H. Cai**, Z. Fu, Y. Jiang, **G. Mei**, S. Wang
- 9:40 294. Optimized semi-industrial electrochemical preparation of cyclic encarbamates and its application for the MedChem relevant building blocks synthesis. O.D. Tereshchenko, I.V. Knysh, M.Y. Perebinyis, O.V. Vasylets, A.A. Sorochenko, A. Borisov, S. Ryabukhin, **D.M. Volochnyuk**
- 10:00 295. Scalable synthesis of MedChem relevant (1s) oxazole based building blocks. B.A. Chalyk, E.Y. Slobodyanyuk, O. Grygorenko, S. Ryabukhin, **D.M. Volochnyuk**
- 10:20 296. Fascinating adventures in development of a drug from conception to commercialization: Personal perspective. **M. Chorghade**
- 10:40 297. Visible-light-induced nickel-catalysed cross-coupling with alkylzirconocenes from unactivated alkenes. **C. Jiang**, X. Qi, Y. Gao, C. Yang
- 11:00 298. New frontiers in Castagnoli–Cushman reaction. **S. Ryabukhin**, M. Adamovskiy, O. Grygorenko, D.M. Volochnyuk
- 11:20 299. Stimuli responsive additives: Transforming the future. **C. Roy**, C. Hayes, D. Saccomando, W. Barton
- 11:40 300. Straightforward synthesis of all isomeric cyclo- and fluoro-alkylpiperidines. **S. Ryabukhin**, A. Subota, A. Lutsenko, O. Grygorenko, D.M. Volochnyuk

SECTION C
San Diego Convention Center
Room 9

Molecular Recognition & Self-Assembly

S. M. Silverman, *Organizer, Presiding*

- 8:00** **313.** Controlling chloride affinity swings of photofoldamers with arylazopyrazoles. **F.C. Parks**, S. Stutsman, Y. Liu, S. Debnath, K. VanDenburgh, X. Gao, K. Raghavachari, A.H. Flood
- 8:20** **314.** Orthogonal metal templation strategy for the synthesis of unimolecular linear oligocatenanes. **N.D. Colley**, M. Nosiglia, C. Chang, L. Li, F. Solangi, J.C. Barnes
- 8:40** **315.** Novel multicomponent fluorescent sensors for detection of glycolipids. **M. Xu**, T.E. Glass
- 9:00** **316.** Small structural variations have large effects on the assembly properties and spin-state of room-temperature, high-spin Fe(II) iminopyridine cages. **T. Miller**, L.R. Holloway, R.J. Hooley
- 9:20** **317.** Squaraine lasso peptides: New family of self-threaded fluorescent molecular probes. **C. Zhai**, C. Schreiber, S. Padilla, B.D. Smith
- 9:40** **318.** Advances in porous liquids formed using porous organic cages. **R.L. Greenaway**, R. Kearsley, B. Egleston, M. Brand, A. Kai, A.I. Cooper
- 10:00** **319.** Self-assembly of biohybrid materials with macrocyclic receptors. **N.K. Beyeh**
- 10:20** **320.** Systematic construction of ternary assemblies through weak interactions. R. Puttreddy, M.D. Pour, M. Taimoory, **K. Twum**, F. Pan, K.T. Rissanen, J.F. Trant, N.K. Beyeh

SECTION D
San Diego Convention Center
Room 8

Remarkable Women in Organic Chemistry

Cosponsored by WCC

N. C. Goodwin, R. Ruck, *Organizers, Presiding*

- 8:00** Introductory Remarks.
- 8:10** **321.** Navigating the chemical space of amide activation to drug discovery. **E. Baker-Tripp**
- 8:30** **322.** Innovative strategies toward complex molecule synthesis: Development of a fully biocatalytic manufacturing route for MK-8591. **N. Patel**
- 9:00** **323.** Anion-catalyzed silicon Lewis acid activation of carbonyls. **M. Tekle-Smith**, K.S. Williamson, I. Hughes, J.L. Leighton
- 9:20** **324.** Leaving their mark: From precision electrophile signaling to covalent ligand evolution. **Y. Aye**

- 9:55** Intermission.
- 10:05** **325.** Quest for enantioselective hydroamination reactions: Silver, gold, and serendipity. **A.G. Wenzel**
- 10:35** **326.** Make it or break it with metal-hydrides. **V.M. Dong**
- 11:10** **327.** Academic drug discovery: Playing to the strengths to address challenging targets and unmet medical needs in cancer and acute kidney injury. **D.M. Huryn**

SECTION E
San Diego Convention Center
Room 7A

Young Academic Investigator Symposium

H. M. Davies, L. McElwee-White, *Organizers, Presiding*

- 8:20** Introductory Remarks.
- 8:25** **328.** Development of novel chemical tools for accessing unexplored chemical spaces. **M. Ngai**
- 8:50** **329.** C–H and C–O functionalization via radical chaperones. **D. Nagib**
- 9:15** **330.** Alcohol and amine derivatives guide position-selective C–H functionalization reactions. **J.L. Roizen**
- 9:40** **331.** Catalytic strategies to selectively manipulate aryl radicals and strong C–F bonds. **N. Jui**
- 10:05** Intermission.
- 10:15** **332.** Enantioselective chemical synthesis methods via cooperative catalysis. **T.N. Snaddon**
- 10:40** **333.** Development of high-valent aerobic oxidation catalysis. **D.C. Powers**
- 11:05** **334.** Selective functionalization of pyridines, diazines, and pharmaceuticals via heterocyclic phosphonium salts. **A. McNally**
- 11:30** **335.** Semiconducting polymer blends: Bringing the best of both worlds for organic electronics. **J. Mei**

SECTION F
San Diego Convention Center
Ballroom 20A

Cope Award Symposium

J. Aube, L. A. Marcaurelle, *Organizers*
L. Marcaurelle, *Presiding*

- 8:00** Introductory Remarks.
- 8:10** **336. Award Address** (Arthur C. Cope Late Career Scholars Award sponsored by the Arthur C. Cope Fund). Organic chemistry in harsh reaction environments. **R.J. McMahon**
- 8:45** **337. Award Address** (Arthur C. Cope Mid-Career Scholars Award sponsored by the Arthur C. Cope Fund). Organic & organometallic catalysts and Lewis pairs for polymer synthesis and biorefining. **E.Y. Chen**

- 9:20 338. Award Address** (Arthur C. Cope Late Career Scholars Award sponsored by the Arthur C. Cope Fund). Synthetic reactions driven by energy of photons. **M. Murakami**
- 9:55** Intermission.
- 10:10 339. Award Address** (Arthur C. Cope Early Career Scholars Award sponsored by the Arthur C. Cope Fund). Design and synthesis of topologically controlled polymer networks. **J.A. Johnson**
- 10:45 340. Award Address** (Arthur C. Cope Late Career Scholars Award sponsored by the Arthur C. Cope Fund). Elements of marine bioorganic chemistry: From vanadium to iron. **A. Butler**
- 11:20 341. Award Address** (Arthur C. Cope Late Career Scholars Award sponsored by the Arthur C. Cope Fund). Assembly line synthesis. **V.K. Aggarwal**

Identification & Design of Catalytic Sites in Electrochemical Reactions

Sponsored by ANYL, Cosponsored by ENFL and ORGN

TUESDAY AFTERNOON – ORGN

SECTION A

San Diego Convention Center
Room 7B

Flow Chemistry & Continuous Processes

S. M. Silverman, *Organizer*
V. Vu, *Presiding*

- 1:15 342.** Scale-up of a continuous extraction process for driving an equilibrium-limited reaction to completion. **M.T. Tudesco**, E.G. Moschetta, E.A. Voight
- 1:40 343.** Centre for rapid online analysis of reactions (ROAR): Flow chemistry facility for the Dial-a-Molecule community. **B. Deadman**, P. Ferrini, M. Hii
- 2:05 344.** Development of a safe and high-throughput continuous manufacturing approach to N-(2-hydroxyethyl)thiomorpholine dioxide. **Y. Tan**, N. Strotman, M.C. Soumeillant, S.W. Leung, K. Powers
- 2:30 345.** Data-driven exploration of the catalytic reductive amination reaction. **P. Ferrini**, B. Deadman, M. Hii
- 2:55 346.** Diversity oriented synthesis of highly substituted heteroarenes using photochemistry and flow technology. **G. Sipos**, G. Ignacz, B. Fodi, T. Noel
- 3:20 347.** Tunable chiroptical induction and photolysis in flow. **A.C. Evans**
- 3:45 348.** Studies toward a general strategy for scaling photochemical reactions in flow. **E. Corcoran**, F. Levesque, J. McMullen, J.R. Naber

- 4:10 349.** Continuous synthesis of three nucleoside antivirals in one day on an automated flow chemistry system. **V. Vu**, J. Szeto, K. Rucker, D. Stout, J. Lim, J.P. Malerich, J.D. White, N. Collins

SECTION B

San Diego Convention Center
Room 10

Biologically-Related Molecules & Processes

S. M. Silverman, *Organizer*
D. Bandyopadhyay, *Presiding*

- 1:00 350.** Functionalized nitrodibenzofuran-based protecting groups for biological applications. **M. Hammers**, F. Xu, S. Fang, A. Fenton, M. Hodny, A.T. Healy, D.A. Blank, **M.D. Distefano**
- 1:20 351.** Development of a reversible and repeatable thiol-ene reaction for controlled presentation of signaling proteins in hydrogels. **J.C. Grim**, B.A. Aguado, T. Brown, K.S. Anseth
- 1:40 352.** Synthesis of selective JAK3 inhibitor PF-06651600: Discovery to early clinical supplies. **J.I. Trujillo**, Y. Tao, N. Sach, S. Liang, K.E. Wiglesworth, T.M. Makowski, B. Samas, K. Girard, J.G. Mustakis, P.R. Rose, J.C. McWilliams, R. Mehta, A. Casimiro-Garcia, A. Thorarensen, J. Telliez, M.F. Brown, A.M. Gilbert, M.M. Hayward, J. Langille, J.I. Montgomery, R. Unwalla, F.F. Vajdos
- 2:00 353.** Turning PET on and off to sense amines with BODIPY fluorescence. **K. VanDenburgh**, A.H. Flood
- 2:20 354.** Synthesis and evaluation of 4-oxazolidinones as *Staphylococcus aureus* biofilm modulating agents. **B. Frohock**, J.G. Pierce
- 2:40 355.** Optimizing tetrazine amino acid size and reactivity for efficient protein labeling. **S. jana**
- 3:00 356.** Spontaneously blinking dyes and their utility in super-resolution microscopy. **F.M. Jradi**, T. Vu, T.A. Brown, J. Aaron, C. Galbraith, E. Jorgensen, L.D. Lavis
- 3:20 357.** Synthesis and mechanistic investigation of phospholipid-mimicking small molecules as synthetic modulators for liver receptor homologue-1. **A.R. Flynn**, N. Jui
- 3:40 358.** Imidazotetrazines for the treatment of glioblastoma and as synthetic diazoalkane precursors. **R. Svec**, P.J. Hergenrother
- 4:00 359.** Synthesis of an ideal selective estrogen receptor modulator. **R. LaLonde**
- 4:20 360.** Total synthesis of protectin and resolvin epoxide precursors and their tissue regenerative sulfidoconjugates. **R. Nshimiyimana**, T.F. Lam, N.A. Petasis
- 4:40 361.** Late-stage tailoring of natural product-like macrocycles: Structure and properties of functionalized [13]-macrolactones. **C. Chen**

SECTION C
San Diego Convention Center
Room 9

Molecular Recognition & Self-Assembly

S. M. Silverman, *Organizer*
J. Meisel, *Presiding*

- 1:00** **362.** Facile synthesis of a diverse library of mono-3-substituted β -cyclodextrin analogues and their applications. **K. Kellett**, M.K. Gilson
- 1:20** **363.** Near-infrared rotaxane probes for fluorescence imaging and photothermal heating. **H.H. McGarraugh**, W. Liu, C. Schreiber, B.P. Matthews, B.D. Smith
- 1:40** **364.** Micelle-encapsulated fluorescent probe: Chemoselective and enantioselective recognition of lysine in aqueous solution. **G. Du**
- 2:00** **365.** Complexation thermodynamics between cyclodextrins and fatty acids. **X. Yao**, M. Bonizzoni, L. Kong
- 2:20** **366.** Conversion of a weak DAD-ADA H-bond dimer to a much stronger DDD-AAA dimer via proton-coupled electron transfer. **D.K. Smith**, H. Choi
- 2:40** **367.** Interaction of diazaperylenium guest with cucurbit[n]uril host. **A. Thangavel**, M. Macias, S. Tsumaki
- 3:00** **368.** Rational control of geometry in pentacene macrocycles. **H.M. Bergman**, G.R. Kiel, R. Witzke, Y. Liu, T. Tilley
- 3:20** **369.** Calix[5]arene-derived self-folding cavitand receptor for polycyclic aromatic hydrocarbons. **A. Lledo Ponsati**, D. Lozano, R. Álvarez-Yebra, R. López-Coll
- 3:40** **370.** Heterofunctionalized proteomimetic foldamer libraries for biomolecular recognition. **J. Meisel**, A. Hamilton

SECTION D
San Diego Convention Center
Room 8

Remarkable Women in Organic Chemistry

Cosponsored by WCC
N. C. Goodwin, R. Ruck, *Organizers, Presiding*

- 1:30** Introductory Remarks.
- 1:35** **371.** Selective carbohydrate functionalization reactions. **A.E. Wendlandt**
- 2:05** **372.** Design and synthesis of organic electronic materials. **M. Jeffries-El**, A.A. Burney-Allen, R. Chavez, D.L. Wheeler
- 2:40** **373.** Owning your career: Personal reflections on creating a rewarding and successful career in industry. **E. Guidry**

- 3:10** Intermission.
- 3:20** **374.** Necessity is the mother of invention: Natural products and the chemistry they inspire. **S.E. Reisman**
- 3:55** **375.** Career in medicinal chemistry: Transforming challenges into opportunities. **K.B. Goodman**
- 4:25** **376.** Remarkable women in organic chemistry. **M. Faul**

SECTION E
San Diego Convention Center
Room 7A

Young Academic Investigator Symposium

H. M. Davies, L. McElwee-White, *Organizers, Presiding*

- 1:30** **377.** Stereoselective carbene annulations for assembling molecular complexity. **I. Sharma**
- 1:55** **378.** Harnessing the indole heterocycle to rapidly access complex and diverse compounds from indole alkaloids. **R. Huigens**
- 2:20** **379.** New methods and strategies in the synthesis of natural products. **S. Pronin**
- 2:45** **380.** Biocatalysis and complex molecule synthesis. **A.R. Narayan**
- 3:10** **381.** Flavylium polymethine fluorophores for imaging in the shortwave infrared region. **E.M. Sletten**
- 3:35** **382.** Chemical tools that IMPACT lipid signaling. **J.M. Baskin**
- 4:00** Concluding Remarks.

SECTION F
San Diego Convention Center
Ballroom 20A

Cope Award Symposium

L. A. Marcaurrelle, *Organizer*
J. Aube, *Organizer, Presiding*

- 1:35** **383. Award Address** (Arthur C. Cope Early Career Scholars Award sponsored by the Arthur C. Cope Fund). Synthesis of complex terpenes from simple precursors. **T.J. Maimone**
- 2:10** **384. Award Address** (Arthur C. Cope Mid-Career Scholars Award sponsored by the Arthur C. Cope Fund). Metal catalysts, clusters, and surfaces: Catalytic preparation of chiral bio-molecules and carbon-based self assembled monolayers. **C.M. Crudden**
- 2:45** Intermission.
- 2:55** **385. Award Address** (Arthur C. Cope Mid-Career Scholars Award sponsored by the Arthur C. Cope Fund). Versatile oxidative coupling reactions for site-selective protein modification. **M.B. Francis**

- 3:30** **386. Award Address** (Arthur C. Cope Mid-Career Scholars Award sponsored by the Arthur C. Cope Fund). Stereocontrol in photochemical synthesis. **T.P. Yoon**
- 4:05** Introduction of Awardee.
- 4:15** **387. Award Address** (Arthur C. Cope Award sponsored by the Arthur C. Cope Fund). Research: A magical mystery tour. **D. Seebach**

Identification & Design of Catalytic Sites in Electrochemical Reactions

Sponsored by ANYL, Cosponsored by ENFL and ORGN

TUESDAY EVENING – ORGN

SECTION A

San Diego Convention Center
TBD

Heterocycles & Aromatics

E. C. McLaughlin, *Organizer*

5:30 - 7:30

- 388.** First total synthesis of natural pyridocoumarins, goniotaline A and B. J. Jung, T. Lee, Y. Seo, **Y. Han**
- 389.** BODIPYs in the blue: New molecular design. **Z. Wu**, H. Fujita, N. Magdaong, J. Diers, D. Hood, S. Allu, D.M. Niedwiedzki, C.R. Kirmaier, D.F. Bocian, D. Holten, J.S. Lindsey
- 390.** Fluorocyclization of *N*-propargyl carboxamides by iodine(III) catalysts bearing coordinating substituents. **A. Saito**, S. Takahashi, Y. Umakoshi, A. Yoshimura, V.V. Zhdankin
- 391.** Withdrawn
- 392.** Gold redox catalysis for cyclization/arylation of allylic oximes: Synthesis of isoxazoline derivatives. **A.A. Jimoh**, X. Shi
- 393.** Synthesis of 5-aromatic substituted tetrazoles: Modified catalytic approach. **S.C. Sarngadharan**, M. Malone, J. Faris, P. Pollet, C.L. Liotta
- 394.** Methodology to furnish imidazo[1,2,a]pyrimidines via the annulation of β -alkoxy acrylamides and activated aminoimidazoles. **K. Clagg**, N. White, L. Sirois, H. Zhang, F. Gosselin
- 395.** Vitamin catalysis: Photocatalytic synthesis of benzocoumarins via (–)-riboflavin-mediated electron transfer. **T. Morack**, J. Metternich, R. Gilmour
- 396.** Exploring the synthesis of oxazoles starting from amino acids treated with oxalyl chloride. **V.O. Cesare**, F. Guo, M. Fitzsimmons, D. Werner
- 397.** Synthesis of novel triazine-based aromatic boronic acids with potential for both antibacterial and flame-retardant applications. **B. Cromwell**, M. Levine
- 398.** Acid-mediated ring expansion of 2,2-disubstituted azetidine carbamates to 6,6-disubstituted 1,3-oxazinan-2-ones. **A.J. Boddy**, C. Cordier, K. Goldberg, A. Madin, A.C. Spivey, J.A. Bull
- 399.** 3,3-Diaryloxetanes: New opportunities for drug discovery. **M. Dubois**, J.J. Mousseau, C. Choi, J.A. Bull
- 400.** C(sp³)–H functionalization of saturated heterocycles at unactivated positions: Exploring 3D vectors for fragment growth. **D. Antermite**, D. Affron, O.A. Davis, J.A. Bull
- 401.** Copper-mediated cyclization of 1,2-dibromohomoallylic alcohols to versatile 3-bromodihydrofurans. **J. An**, J. Intano, M. Rhinehart, A.R. Howell
- 402.** Novel domino N₂-extrusion/cyclization approaches for the synthesis of indoloquinolines and carbocycle-fused quinolines. **B. Akkachairin**, J. Tummatorn, N. Khamsuwan, C. Thongsornkleeb, S. Ruchirawat
- 403.** Synthesis and characterization of squaraine-containing macrocycles. **J. Pantano**, M. Levine
- 404.** Short strategy for the diastereoselective synthesis of 2,3-diaryl- γ -butyrolactones: Total synthesis of cinnassin A₁. **A.Y. Nuriye**, C. Craescu
- 405.** Practical preparation of a 1,3,5-trisubstituted pyridazin-4(1*H*)-one using selective C₁ unit insertion and cyclization. **A. Suzuki**, N. Fukuda, T. Kajiwara, T. Ikemoto
- 406.** Combinatorial synthesis of imidazo[2,1-*b*]thiazole acyl derivatives. **A.S. Bunev**
- 407.** 5-Cyano-2,4-diaminopyrimidine derivatives: Approaches to preparative synthesis. **A.S. Bunev**
- 408.** Synthesis of *bis*(thiazol-2-yl)amines. **A.S. Bunev**
- 409.** Sequential anionic intramolecular cyclization of bis-alkynylarene amides toward polycyclic isoindolo-isoquinolines and -benzazepines: Regioselectivity study. **G. Infante**
- 410.** Chemical explorations of the manzamenones from the tropical marine sponge, *Plakortis* sp. **H. Lee**, Y. Lee, J. Lee, J. Lee
- 411.** Pentacene-fused porphyrin dimer exhibiting high stability and solubility. **Y. Hu**, H. Wang
- 412.** Phenoxazine polymers for biosensor applications. **M.N. Almtiri**, C. Scott
- 413.** Suzuki catalyzed one-step access to photoluminescent D-A type diarylmaleimides. **J. Price**, E. Albright, B. Balonova, B. Blight, S. Eisler

- 414.** Synthesis of fluorinated 1,5-3*H*-benzodiazepines from substituted *o*-phenylenediamines and 2-fluoroalk-3-yn-1-ones. **T.L. Olson**, A. Kaspi-Kaneti, A. Walsh, R. Dembinski
- 415.** Design and synthesis of evodiamine and rutaecarpine analogues for biological evaluation. Y. Huang, **V. Sammeta**, R. Alshehry, S. Rasapalli
- 416.** Facile access to C-ring aromatic substituted luotonins and vasicinones for Topo I inhibition via intramolecular aza-Michael reactions (IMAMRs) of quinazolinonyl chalcones. **V. Sammeta**, Z. Murphy, J. Golen, S. Rasapalli
- 417.** Design and synthesis of 4(3*H*)-quinazolinonyl chalcones and their derivatives for antibacterial and antibiofilm activity. Z. Murphy, **V. Sammeta**, S. Rasapalli
- 418.** Design and synthesis of 2-pyrazolyl quinazolinones as celecoxib analogs. G. vicente, V. Sammeta, Z. Murphy, **S. Rasapalli**
- 419.** Efficient approach to pyrroloquinazolinone alkaloids: Vasicinone and luotonin A. **V. Sammeta**, Y. Huang, S. Rasapalli
- 420.** Transition metal catalyzed synthesis of unsymmetrically substituted triazolium salts. **S. Hutchinson**
- 421.** Synthesis of C7-substituted-phenyl-[13]-macrolactones, principal component analysis (PCA), and antiproliferation assays. **C. Chen**, M.W. Peczu
- 422.** Quantification of hydrogen bond accepting ability of medicinally relevant N-heterocycles and alkaloid compounds using ³¹P NMR spectroscopy. **M. Milic**, K. Targos, J. Jennings, A.K. Franz
- 423.** Efficient routes to oxazolines through activation of aromatic amides. **H. Thompson**, M. Musa, S. Alhashim, **A. Dubrovskiy**

SECTION A

San Diego Convention Center
TBD

New Reactions & Methodology

E. C. McLaughlin, *Organizer*

5:30 - 7:30

- 424.** Fluorosulfonic anhydride: Another powerful reagent for the sulfur(VI) fluoride exchange (SuFEx) chemistry. **G. Li**
- 425.** Catalytic application of Eu(II)/Eu(III) redox cycles and photoluminescence tracking. S. Kim, **M. Kim**
- 426.** Facile synthesis of flavanones *via* Pd(II)-catalyzed β-arylation of chromanones with arylboronic acids. **H. Yoo**, N. Kim

- 427.** New strategies towards fine chemicals from HMF and GMF. W. Fan, C. Verrier, L. Wang, E. Dokmak, m. Ahmar, S. Moebs, **F. Popowycz**, Y. Queneau
- 428.** Mechanochemical iridium-catalyzed C-H borylation. **Y. Pang**, T. Ishiyama, K. Kubota, H. Ito
- 429.** Olefin-accelerated C–C cross-coupling reaction in solid-state. **T. Seo**, T. Ishiyama, K. Kubota, H. Ito
- 430.** Catalytic cascade dehydrogenative cross-coupling: One-pot process to break two B–H, one C–H, one X–H and construct new B–C and B–X (X = O, N) bonds. **Y. Au**, Y. Quan, Z. Xie
- 431.** Concise synthesis of potassium acyltrifluoroborates from aldehydes by borylation and oxidation. **T. Takeuchi**, J. Taguchi, R. Takahashi, F. Masero, H. Ito
- 432.** Formation of aryl(1-cyano-4-(dialkylamino)butadienyl)ketones from pyridines. **H. Gim**, M.E. Jung
- 433.** New polyallylsilane-based carbon-carbon bond forming reactions. **E.D. Tan**, **L.K. Baker**, G.W. O’Neil
- 434.** Reactivity enhancement in branched catalysts for phosphorylation reactions: Electronic and steric effects. **A. Fallek**, M. Portnoy
- 435.** Influence of bases and catalysts on substrate-selectivity in a model acylation reaction. **R. Fallek**, M. Portnoy
- 436.** Preparation, structure, and reactivity of phenolic aryliodonium salts. **A. Yoshimura**, G. Rohde, V.V. Zhdankin, M. Yusubov, A. Saito
- 437.** *Ips*o-nitration of arylsilanes. **F. Fu**, S.B. Munoz, T. Mathew, S.G. Prakash
- 438.** Preparation of fluorinated selenium- and sulfur-containing compounds via reactions of selenols, diselenides, and disulfides with *in situ*-generated difluorocarbene and their potential uses for chalcogeno-fluorofunctionalization. **C. Barrett**, V. Krishnamurti, S.G. Prakash
- 439.** Synthesis of novel substituted dihydropyridines with potential pharmaceutical activity. **A.K. Ahmed**, **U. Siddika**, M. Shkoor
- 440.** Siladifluoromethylation and deoxy-trifluoromethylation of P^V–H compounds with TMSCF₃: Route to P^V–CF₂[–] transfer reagents and P–CF₃ compounds. **V. Krishnamurti**, C. Barrett, S.G. Prakash
- 441.** Direct access to acyl fluorides and perfluoroalkyl carbonyl compounds from carboxylic acids using a phosphine-based deoxygenative reagent system. **X. Ispizua**, H. Dang, S.B. Munoz, T. Mathew, S.G. Prakash
- 442.** Withdrawn

- 443.** Vinyl cations as cyclopentenone precursors via C–H insertion and alkene addition reactions. **M. Hensinger**, S. Cleary, M. Brewer
- 444.** Transition metal free selective N^2 -arylation of 1,2,3-triazoles. **S. Roshandel**, M.J. Lunn, S.C. Suri, S.G. Prakash
- 445.** Tuning of regioselectivity by steric hindrance in Suzuki–Miyaura cross coupling reactions. **Y. Kwon**, W. Kim
- 446.** Cu(I)-catalyzed pentafluoroethylation of aryl iodides in the presence of tetrafluoroethylene and CsF. **N. Ishida**, K. Ando, Y. Hashimoto, A. Shigaki, K. Kikushima, M. Ohashi, S. Ogoshi
- 447.** Phosphorylation of carbon-oxygen bond mediated by *N*-phosphine oxide-substituted imidazolylidenes. **T. Asada**, Y. Hoshimoto, S. Ogoshi
- 448.** Exploring the reactivity of sulfur(VI) via sulfonimide intermediates. **O. Goodrich**, R.A. Stockman
- 449.** 3-Aryloxetane-3-carboxylic acids: Two step process towards novel versatile building blocks for drug discovery programs. **M. Dubois**, J.J. Mousseau, C. Choi, J.A. Bull
- 450.** Diastereoselective nucleophilic substitution reactions of acyclic acetals. **A. Ramdular**, K.A. Woerpel
- 451.** Formation of strained rings through a nickel-catalyzed cross-electrophile coupling. **T. McGinnis**, A. Sanford, T.A. Thane, E.R. Jarvo
- 452.** Metal-free cyclopropanation of electrophilic olefins. **G.M. Batista**, P.P. Castro, A.G. Carpanez, B. Horta, G.W. Amarante
- 453.** 4,5,6,7-Tetrahydropyrazolo[1,5-*a*]pyrazine: Lead-oriented scaffold with three diversity points. V.I. Bozhanov, O.V. Zaremba, A. Borisov, S. Ryabukhin, **D.M. Volochnyuk**
- 454.** Isoxazole and 1,2,4-oxadiazole-derived phosphonates via [3+2] cycloaddition. B.A. Chalyk, O. Grygorenko, S. Ryabukhin, **D.M. Volochnyuk**
- 455.** Synthesis of gem-difluorocycloheptanes building blocks. K.P. Melnykov, S. Ryabukhin, **D.M. Volochnyuk**
- 456.** Cu-catalyzed amination of (hetero)arylamines to disubstituted olefins. **S. Park**
- 457.** Synthesis of β -amino sulfones through copper-catalyzed hydroamination of allylic sulfones. **K. Kim**, S. Park
- 458.** Ni-catalyzed oxidative esterification of allylic sp^3 -carbon followed by *in situ* reduction. **D. Moustafa**, **C. Sweet**, P. Kaur
- 459.** 18F deoxyfluorination of phenols via Ru π complexes. **D. Mandal**, M. Beyzavi, M. G. Streb, C. N. Neuman, J. Chen, J. M. Hooker, T. Ritter
- 460.** Copper catalyzed S_N2' functionalization of fluoroalkylated alkenes. **J.L. Yang**, T.W. Butcher, J.F. Hartwig
- 461.** Alkyl-extended pinacol rearrangement. **N. Dao**, J. Sader, J. Wulff
- 462.** Synthesis of allylic amines through Cu-catalyzed aza-Michael addition of heterocycles to dienes. **H. Lee**, S. Park
- 463.** Studies directed toward the total synthesis of saxitoxin: Addition of 1,3-dihydro-2H-imidazol-2-one to aldehydes. **J. Lee**, M. Ryu, H. Lee, Y. Lee, J. Lee
- 464.** Efficient synthesis of L-ribonolactol derivative and their L-nucleoside analogs from D-ribose. **J. Cho**, **Y. Nam**, S. Choi, J. Kim, D. Jung, J. Song, J. Park
- 465.** Synthesis of homoallylic alcohols through addition of allylic aluminum reagents to carbonyls via Cu-catalyzed hydride addition to allenes. **S. Lee**, S. Lee
- 466.** Stereocontrolled multicomponent synthesis of amino acids and peptidomimetics in water. **K.M. Kossick**, N.A. Petasis
- 467.** Ion pair reactions in the high speed ball mill. **L.N. Trankina**, J. Crain, C. Williams III, J. Mack
- 468.** NMR quantification of halogen-bonding ability to evaluate catalyst activity. **Y. Chang**, **T. Tang**, J. Jagannathan, N. Hirbawi, S. Sun, A.K. Franz
- 469.** H_2 -mediated C–C bond formation via ruthenium-ketenimate intermediates. **M.M. Sikes**, L.V. Hale, N.K. Szymczak
- 470.** Hydroboration of carbodiimides using a carbodiphosphorane catalyst. **D. Chang**, A.L. Liberman-Martin
- 471.** One-step synthesis of sulfonamides from tosylhydrazones. A. Tsai, J.M. Curto, A. Dechert Schmitt, **G. Ingle**, V. Mascitti
- 472.** Survey and mechanism of the reductive cleavage of lignin-relevant aryl ethers by small molecule thiols. **G.E. Klinger**, J.E. Jackson, E.L. Hegg
- 473.** New α -thioalkyl phosphonium salts as Wittig substrates for vinyl sulfide synthesis. **S. Dharavath**, J. Deobald, J. Magolan
- 474.** Process development of (S)-2-methylproline synthesis via microreactor. **M. Yu**, D. Zhang, I. Yu, **B. Zhang**
- 475.** Investigation of the 1,3-diaza-Claisen rearrangements in ring expansion of vinyl *N*-heterocycles. **T. Watanabe**
- 476.** Development of new difluoromethylation reactions. **C. Brigham**, C. Malapit, M. Sanford
- 477.** Improved synthesis of *p*-SCN-Bn-HOPO for ^{89}Zr chelation. **N. Bhupathiraju**, A. Younus, J. Ali, M. Cao, S. Ponnala, H. Cicek, L.C. Francesconi, J. Lewis, J. Babich, C.M. Drain
- 478.** *In situ* enzymatic screening (ISES) approach to catalyst screening: Toward a new entry into

halovinyl amino acids. **S.M. Ramos De Dios**, R.A. Dhokale, D.L. Graham, D.B. Berkowitz

479. Stereoretentive Suzuki–Miyaura reaction enabling the synthesis of 1,3-disubstituted-cyclobutane. **T. Piou**

480. Catalytic oxidative reactions of arylalkenes by *tert*-Butyl hydroperoxide: Mechanistic assessment. **L. De Angelis**, Y. Su, M.P. Doyle

481. Biomimetic synthesis of kallosin. **V. Gharat**, P. Scesa, L. West

482. Tailoring chemoenzymatic oxidation via *in situ* peracids. **R. Re**, J. Proessdorf, J.J. La Clair, M. Subileau, M.D. Burkart

483. C–H functionalization of alcohols via radical-polar crossover. **R.K. Twumasi**, A. Prusinowski, E. Wappes

484. Transition-metal catalyzed alkyne coupling reactions. **S. Acharya**, P. Zhao

485. Hybrid synthetic-computational study of versatile approach to curcuminoids. **A. Guerrero**, J. Christensen, J. Cook, K. Wolmutt, V.A. Stepanova

486. SuFEx click chemistry enabled late-stage drug functionalization. **Z. Liu**, J. Li, S. Li, G. Li, K.B. Sharpless, P. Wu

487. Selective methylation of α -methylene ketones. **S. Ryabukhin**, A. Frolov, E. Ostapchuk, D.M. Volochnyuk

488. Synthesis and reactivity of N-difluorocyclopropyl-substituted pyrazoles. **S. Ryabukhin**, P. Nosik, M. Pashko, A. Poturai, K.P. Melnykov, O. Grygorenko, D.M. Volochnyuk

489. Synthesis and properties of monoalkylsubstituted difluorocyclopropenes. **S. Ryabukhin**, P. Nosik, M. Pashko, D.M. Volochnyuk

490. Expanding of the scope of Castagnoli–Cushman reaction: Anhydrides of cyclic 1,2-dicarboxylic acids. **S. Ryabukhin**, M. Adamovskyi, O. Smyrnov, D.M. Volochnyuk

491. Expanding of the scope of Castagnoli–Cushman reaction: Trifluoroacetaldehyde monohydrate. **S. Ryabukhin**, M. Adamovskyi, D.M. Volochnyuk

WEDNESDAY MORNING – ORGN

SECTION A

San Diego Convention Center
Room 7B

New Reactions & Methodology

S. M. Silverman, *Organizer*
M. Jouffroy, *Presiding*

8:00 **492.** Quaternary centers via dual-catalytic alkene hydroarylation. **S.A. Green**, R.A. Shenvi

8:20 **493.** Condensation-driven assembly of bis(heteroaryl) motifs using a linchpin reagent. **C. Apte**, D. Diaz, A.K. Yudin

8:40 **494.** Exploiting enzymes from (hyper)thermophiles for *in situ* enzymatic screening (ISES) at elevated temperature: Toward a catalytic, asymmetric entry into quaternary, α -vinyl amino acids. **V.K. Tiwari**, G. Malik, J.A. Friest, R.A. Swyka, D.B. Berkowitz

9:00 **495.** Distal control of aryne capture regioselectivity by an *in situ* formed boronate. **M. Hribersek**, C. Sollert, M. Ahlquist, L.T. Pilarski

9:20 **496.** Calcium-catalyzed formal [5+2] cycloaddition of alkylidene β -ketoesters with substituted olefins: Chemodivergent synthesis of highly functionalized cyclohepta[b]indoles. **A.N. Parker**, M.C. Martin, R. Shenje, S.A. France

9:40 **497.** Development of an electrocatalytic ruthenium-catalyzed C–H hydroxylation of amine derivatives. **S.G. Robinson**, J. Mack, J. Du Bois, M.S. Sigman

10:00 **498.** Radical mediated S-atom transfer enabled strategies for chemical synthesis. **J. Lopp**

10:20 **499.** Organocatalytic Mukaiyama Mannich reactions of 2,5-bis(trimethylsilyloxy)furan. **S.Y. Howard**, S.W. Laws, R. Mato, J.T. Shaw

10:40 **500.** Selective hydrodefluorination and defluoroalkylation of a diverse range of trifluoromethyl arenes. **D. Vogt**, H. Wang, N. Jui

11:00 **501.** Chemoselective nickel-catalyzed hydrogenation: Synthesis of highly substituted aromatic amines. **M. Tom**, P. Miller, R.L. Grange, D. Esau, G. Jerkiewicz, P. Evans

11:20 **502.** Vinyl sulfides: New preparations and reactions. **J. Magolan**

11:40 **503.** Direct C–H carbamoylation of nitrogen containing heterocycles. **M. Jouffroy**

SECTION B

San Diego Convention Center
Room 10

Heterocycles & Aromatics

S. M. Silverman, *Organizer*
S. Malhotra, *Presiding*

8:00 **504.** Synthesis of pyrene-pyrazole pharmacophores via copper-catalyzed C–N dehydrogenative cross-coupling and structure-activity studies for tubulin polymerization. **D. Sar**, I. Srivastava, D. Pan

8:20 **505.** Selective intermolecular couplings of aryl radical species with olefins. **A.J. Boyington**, N. Jui

- 8:40 506.** Synthesis of 5-fluorocytosine from acyclic precursors: Improving global access to emtricitabine. **B. Derstine**, E. Crawford, J. Dietz, P. Moore, C. Peck, A.J. Arduengo, T. Opatz, T. McQuade, F. Gupton
- 9:00 507.** Carboxyboronate: An unusual C1 building block. **A.E. Holownia**, C. Tien, D. Diaz, R. Larson, A. Yudin
- 9:20 508.** Selectivity in the synthesis of 1-substituted and 1,8-disubstituted fluorenones by directed metalation. **S. Cope**, J.K. Pagano, B. Scott, L.A. Silks, J.L. Kiplinger
- 9:40 509.** Linking cyclopenta-fused polycyclic aromatic hydrocarbons via five-to-five connections. **K.N. Plunkett**
- 10:00 510.** Magnesium-catalyzed regioselective alkylation of 3-substituted pyrazoles. **D. Xu**
- 10:20 511.** Development of two simple building blocks for the biocatalytic synthesis of MK-8591. **C.M. Hong**
- 10:40 512.** Enabling the manufacturing process development of GPR40 MK-8666 through the highly efficient synthesis of the 6-5-3 fused heterocyclic ring system. **Z. Liu**, A.M. Hyde, A. Klapars, G.X. Zhou, J.Y. Chung, N. Yasuda, J. Limanto, K.R. Campos
- 11:00 513.** Withdrawn
- 11:20 514.** Highly chemoselective functionalization of dihaloareomatics. **S. Malhotra**

SECTION C

San Diego Convention Center
Room 9

Photoredox Chemistry

S. M. Silverman, *Organizer*
C. Plummer, *Presiding*

- 8:20 515.** Difunctionalization of *N*-alkyl cyclobutyl and cyclopropyl amines via photoredox catalysis. **Q. Wang**, N. Zheng
- 8:40 516.** Mechanism and optimization of redox-mediated Ni-catalyzed cross coupling. **R. Sun**, Y. Qin, S. Ruccolo, C. Schnedermann, C. Costentin, D.G. Nocera
- 9:00 517.** Benzylic functionalization via visible-light induced photoredox catalysis. **Y. Xing**
- 9:20 518.** Computational characterization of photocatalytic processes with DFT-based methods. **F. Maseras**
- 9:40 519.** Arene cyanation via cation radical accelerated nucleophilic aromatic substitution. **N. Holmberg-Douglas**, D.A. Nicewicz
- 10:00 520.** Radical Stetter reaction enabled by merger of ion-pair photocatalysis with radical umpolung. **T. Morack**, C. Mück-Lichtenfeld, R. Gilmour

- 10:20 521.** Photocatalytic birch-like arylation via C–F functionalization. **J.D. Weaver**
- 10:40 522.** Contra-thermodynamic photocatalysis; Progress towards the synthesis of a hexaprismane. **J.D. Weaver**
- 11:00 523.** Stereoselective glycosides via copper-catalyzed cross couplings of anomeric sp³ carbons with alkyl alcohols induced by visible light. **H.M. Nguyen**, F. Yu, R. Schaugaard, H.B. Schlegel

SECTION D

San Diego Convention Center
Room 8

Sustainable Catalysis: Discovery through Application

S. M. Silverman, *Organizer*
D. K. Leahy, *Organizer, Presiding*

- 8:00 524.** Development of regioselective hydro- and oxidative amination reactions. **K.L. Hull**
- 8:45 525.** Radical biocatalysis: Using light to reveal new enzyme functions. **T. Hyster**
- 9:30 526.** Development of reductive aminases: Useful tool for efficient chiral amine synthesis. **G. Hughes**
- 10:00 527.** Synthesis of enantiomerically enriched diaryl alkanes through a stereoconvergent Suzuki-Miyaura cross coupling reaction catalyzed by iron-based complexes. **J.A. Byers**, C.R. Tyrol, N. Yone
- 10:45 528.** Identifying novel ligand scaffolds for Cu-catalyzed C–O and C–N cross-coupling through library screening. **E. Swift**
- 11:15 529.** Developing practical catalysis for C–H activation reactions. **J. Yu**

SECTION E

San Diego Convention Center
Room 7A

From Lab to Commercial Scale: The Challenges to Scaling Up Flow Chemistry in the Pharmaceutical Industry

K. M. Maloney, *Organizer*
J. R. Naber, *Presiding*

- 8:00** Introductory Remarks.
- 8:05 530.** Continuous manufacturing innovation journey: Lessons from Lilly. **S. O’Keeffe**
- 8:45 531.** Formylation with ethyl formate in flow: Reduction of process mass intensity (PMI) and CO generated. **D.A. Otte**
- 9:25 532.** Scaling photochemical reactions in flow using visible light. **E. Moschetta**
- 10:05** Intermission.

- 10:15 533.** From R&D to commercialization: Successful integration of flow chemistry into manufacturing of API's and intermediates. **M.A. Gonzalez**
- 10:55 534.** Flowing away from batch: Continuous processing for metalation reactions. **S. Opalka**

SECTION F

San Diego Convention Center
Ballroom 20A

Technical Achievements in Organic Chemistry

T. Braden, J. Calvin, *Organizers, Presiding*

- 8:40** Introductory Remarks.
- 8:45 535.** Process chemistry impacts at the interface of discovery and development. **A. Nolting**
- 9:15 536.** Novel technology platform developments to accelerate drug discovery. **N. Tu**
- 9:45 537.** Case studies in the use of machine learning models applied to small molecule therapeutic targets. **I. Aliagas**
- 10:15** Intermission.
- 10:30 538.** Evolution of long and short acting pan-AMPK activators as exercise mimetics. **J. Apgar**, R. Wilkening, J. Hicks, D. Feng, L. Wei, K.J. Leavitt, J. Dropinski, L. Chu, X. Qian, A. Kekec, A. Kassick, A. Kim, H. Lu, G. Dong, H. Guan, K. Lu, X. Yang, J. Gorski, G. Eiermann, A. Gollapudi, M. Kurtz, M. Trujillo, R. Myers, D. Kemp, M. Hu, S. Xu, I.K. Sebhat
- 11:00 539.** Brief history of... a few good molecules. **J. Magano**
- 11:30 540.** Discovery of ambiphilic reagents for the synthesis of chiral pyrrolidines. **Q. Shi**, N.S. Greenwood, M.C. meehan, J. Coombs, W.P. Gallagher, C.A. Guerrero, J. Hynes, M. Dhar, F. Gonzalez Bobes, D. Marcoux

Interface between Experiments & Modeling in Unraveling the Physical & Chemical Properties of Charged Droplets

Sponsored by ANYL, Cosponsored by COMP, ORGN and PHYS

WEDNESDAY AFTERNOON – ORGN

SECTION A

San Diego Convention Center
Room 7B

New Reactions & Methodology

S. M. Silverman, *Organizer*
Z. Liu, *Presiding*

- 1:00 541.** Synthesis inspires design: Importance of synthetic innovations in drug discovery and development. **T. Lyons**
- 1:20 542.** Extraction reaction mechanism determination of powder river basin (PRB) coal in the supercritical CO₂-ethanol system by ¹H, ²H and ¹³C nuclear magnetic resonance (NMR) spectroscopy. **X. He**, T. Wang, W. Lu, K. Sun, M. Fan
- 1:40 543.** SciFinderⁿ in the age of computer-aided synthesis design. **O.Y. Ravitz**, J.W. Taylor
- 2:00 544.** New strategies for catalytic fluorination methods. **C. Brigham**, C. Malapit, M. Sanford
- 2:20 545.** BPh₃ catalyzed [2+3] cycloaddition of Ph₃P=C=C=O with nitrones to 4-triphenylphosphoranylidene-5-isoxazolidinones. **A. Brar**, D. Unruh, C. Krempner
- 2:40 546.** Radical mediated hydroamination using N-hydroxyphthalimide. **S. Lardy**, V.A. Schmidt
- 3:00 547.** Copper mediated photochemical cycloadditions for the synthesis of small heterocycles. **D. Flores**, V.A. Schmidt
- 3:20 548.** Ligand-controlled chemodivergent Suzuki cross coupling using palladium-N-heterocyclic carbene catalysts. **E. Reeves**, S. Neufeldt
- 3:40 549.** Radical-chaperone mediated β,γ-difunctionalization of alcohols. **R.K. Twumasi**, A. Prusinowski, E. Wappes
- 4:00 550.** Systematic chemical diversity: Synthesis of fused Csp²-Csp³ hybrid pyrano/furano pyridines for fragment based lead discovery. **S. Chamakuri**
- 4:20 551.** Synthesis of Cannabigerol derivatives via direct *ortho*-allylation of phenols. **N. Jentsch**, X. Zhang, J. Magolan
- 4:40 552.** Ligand-free rhodium-catalyzed regio- and diastereoselective allylic benzylation using unstabilized nucleophiles. **D. Pal**, T.B. Wright, P. Evans

SECTION B

San Diego Convention Center
Room 10

Asymmetric Reactions & Syntheses

S. M. Silverman, *Organizer*
C. M. Hong, *Presiding*

- 1:00 553.** Asymmetric synthesis of *P*-stereogenic compounds via thulium (III)-catalyzed desymmetrization of dialkynylphosphine oxides. **Y. Zhang**, X. Liu, X. Feng
- 1:20 554.** Nickel(II)-catalyzed asymmetric propargyl [2,3]-Wittig rearrangement of oxindole derivatives: Chiral amplification effect. **X. Xu**, X. Feng

- 1:40 555.** Asymmetric synthesis of 3-aminodihydrocoumarins via the chiral guanidine catalyzed cascade reaction of azlactones. **S. Ruan**, X. Liu, X. Feng
- 2:00 556.** Asymmetric synthesis of α,β -epoxy- γ -lactams by enantioselective Darzens/ring-closure reaction. **b. shen**, X. Liu, X. Feng
- 2:20 557.** Energy decomposition analyses reveal the origins of catalyst and nucleophile effects on regioselectivity in nucleopalladation of alkenes. **X. Qi**, P. Liu
- 2:40 558.** *De novo* synthetic study towards 11-deoxylandomycins. **J. Lee**, Y. Rhee
- 3:00 559.** Development of an asymmetric synthesis of ergoline derivatives. **R. Connon**, P.J. Guiry
- 3:20 560.** Development of a metal-catalysed asymmetric carboxylation. **B. Roche**, P.J. Guiry
- 3:40 561.** Enantioselective synthesis of tricyclic steroidal analogs. **D. Townsend**, A.A. Cobb
- 4:00 562.** Improved generations of catalysts for asymmetric synthesis and stereoselective reactions. **M. Diéguez**, P. Norrby, F. Maseras, M.A. Pericas, O. Pamies
- 4:20 563.** Chemosynthetic livers: Predict, prepare and prove the structure, activity and toxicity of drug metabolites. **M. Chorghade**
- 4:40 564.** Synthesis and application of a novel family of modular ferrocenyl catalysts for asymmetric organocatalysis. **L. Cunningham**, C. Nottingham, P. Guiry

SECTION C

San Diego Convention Center
Room 9

Photoredox Chemistry

S. M. Silverman, *Organizer*
J. D. Weaver, *Presiding*

- 1:20 565.** Synthesis and photochemical behavior of photoconversion-resistant triarylmethane fluorophores. **A.N. Butkevich**, M.L. Bossi, G. Lukinavicius, S.W. Hell
- 1:40 566.** Decarboxylative photoredox/nickel-catalyzed conversion of aryl halides to aryl amino oxetanes. **J.A. Terrett**, K. Kolahdouzan, R. Khalaf, J.M. Grandner, Y. Chen, M.P. Huestis
- 2:00 567.** Electron-catalyzed Diels-Alder reactions by TiO₂ photocatalysis. **Y. Okada**, K. Nakayama, N. Maeta, G. Horiguchi, H. Kamiya
- 2:20 568.** Radical conjugate addition of N-heterocycles and tertiary amines. **A. Aycok**, **H. Wang**, C.J. Pratt, D.B. Vogt, N.T. Jui
- 2:40 569.** Radical anions as reactive intermediates for the synthesis of complex molecules. **C. Seath**, N. Jui

- 3:00 570.** Facile preparation of spirolactones by an alkoxy carbonyl radical 5-*exo* cyclization cross-coupling cascade. **N.A. Weires**, Y. Slutskyy, L.E. Overman
- 3:20 571.** Visible light mediated alkene aminoarylation with benzenesulfonyl acetamides. **A.R. Allen**, R. McAtee, C. Stephenson
- 3:40 572.** Amine and heterocycle synthesis enabled by photoredox catalysis. **A.F. Garrido-Castro**, M. Maestro, J. Alemán

SECTION D

San Diego Convention Center
Room 8

Development of New Strategies for the Synthesis & Functionalization of Strained Rings for Applications as Bioisosteres in Biologically Active Compounds

S. M. Silverman, *Organizer*
J. Mousseau, *Organizer, Presiding*
J. J. Mousseau, *Presiding*

- 1:00** Introductory Remarks.
- 1:05 573.** Conformationally-restricted motifs as bioisosteres for aromatics: Playground for new methods development. **T. Fessard**
- 1:35 574.** Cubanes in medicinal chemistry. **M. Kassiou**
- 2:20 575.** Synthesis of new chemical motifs for drug discovery: 4-Membered heterocycles as fragments and bioisosteres. **J.A. Bull**
- 3:05** Intermission.
- 3:20 576.** Use of aliphatic bioisosteres in medicinal chemistry. **A. Stepan**
- 3:50 577.** Strained rings in nature, medicines, and energetics. **P.S. Baran**
- 4:50** Concluding Remarks.

SECTION E

San Diego Convention Center
Room 7A

From Lab to Commercial Scale: The Challenges to Scaling Up Flow Chemistry in the Pharmaceutical Industry

J. R. Naber, *Organizer*
K. M. Maloney, *Presiding*

- 1:00 578.** Enabling photochemistry: Moving from lab to pilot scale. **F. Lévesque**
- 1:40 579.** Drug substances continuous process development: From the bench to demonstration pilot. **M. Etienne**
- 2:20 580.** Development of continuous API manufacturing technologies at Pfizer. **A. Dion**

Asymmetric Reactions & Syntheses

Cosponsored by MEDI

E. C. McLaughlin, *Organizer*

7:00 - 9:00

590. Multikilogram-scale synthesis of esomeprazole using enantioselective iron catalysis. **S. Nishiguchi**, T. Izumi, T. Kouno, J. Sukegawa, L. Ilies, E. Nakamura

591. Design of helical peptide foldamers for asymmetric reactions. **T. Umeno**, A. Ueda, T. Kato, M. Doi, M. Tanaka

592. Helical peptide-catalyzed asymmetric Michael addition reactions of malonates to α,β -unsaturated ketones and their synthetic applications. **A. Ueda**, M. Higuchi, T. Umeno, A. Sugiyama, M. Tanaka

593. New practical method for direct asymmetric reductive amination of *p*-trifluoromethoxy acetophenone. **M. Yamada**, K. Murai, M. Yamano

594. Mechanism and stereoselection of catalytic asymmetric propargylboration of hydrazonoesters. **S. Jonker**, C. Diner, G. Schulz, H. Iwamoto, L. Eriksson, K.J. Szabo

595. Organocatalyzed three-component reaction of γ -arylenals and nitroalkenes. D. Majee, S. Jakkampudi, H.D. Arman, **C.C. Zhao**

596. Asymmetric carbon atom synthesis by samarium (II)-water allylic benzoate reductions. **M.A. Leitch**, **D.R. Turner**, G.W. O'Neil

597. Change the enantioselectivity of enzymes: Rational structural-modification of functional proteins catalyzing Diels-Alder reactions with the reversed enantioselectivity. **Y. Zou**, K.N. Houk

598. Organoboron bifunctional catalysis of asymmetric nitro-Michael addition. **Y. Du**

599. Gold catalyzed asymmetric intramolecular [4+3] cycloadditions. **R. Ma**

600. Stimuli-responsive asymmetric catalysis. **S. Spring**, C.G. Frost

601. Enantioselective formation of γ -lactams with multiple chiral carbon centers by Ni(0)-catalyzed asymmetric carbonylative cycloaddition. **K. Ashida**, Y. Hoshimoto, S. Ogoshi

602. Synthesis and characterization of ethylenediamine-cored optoelectronic starburst materials. **T. Lee**, Y. Kim, K. Park

603. Ir catalyzed asymmetric tandem reaction of meso-diols. **T. Suzuki**

3:00 **581.** Development of a continuous flow process from lab to production at Vertex Pharmaceuticals.

B. Lewandowski

3:40 **582.** Safe scale-up of an exothermic grignard reaction based on thermal hazard understanding and engineering control. **A. Allian**

4:20 **583.** Enabling commercial continuous manufacturing through robust control strategies. **A. O'Brien**

SECTION F

San Diego Convention Center

Ballroom 20A

Technical Achievements in Organic Chemistry

T. Braden, J. Calvin, Organizers, Presiding

1:40 Introductory Remarks.

1:45 **584.** Discovery of potent small molecule inhibitors of the PICK1 PDZ-domain that modulate amyloid beta-mediated synaptic dysfunction. **E.Y. Lin**, L.F. Silvian, D. Marcotte, C.C. Banos, F. Jow, T.R. Chan, R.M. Arduini, F. Qian, D.P. Baker, C. Bergeron, C.A. Hession, R.L. Haganir, C.F. Borenstein, I. Enyedy, J. Zou, E. Rohde, M. Wittmann, G. Kumaravel, K.J. Rhodes, R.H. Scannevin, A.W. Dunah, K.M. Guckian

2:15 **585.** Discovery of tetflupyrolimet: New mode-of-action herbicide that interferes with *de novo* pyrimidine biosynthesis. **K.A. Hughes**, T.P. Selby, A.D. Satterfield, A. Puri, D.A. Travis, M.J. Campbell, A.E. Taggi

2:45 **586.** Discovery of pyrrolidine sulfonamides as TRPV4 antagonists. **E. Brnardic**

3:15 Intermission.

3:30 **587.** Use of structure-based design in the discovery of the BCL-2 selective inhibitor Venclexta® and the bromodomain and extra-terminal domain (BET) inhibitors mivebresib and ABBV-744. **L.A. Hasvold**

4:00 **588.** Synthetic chemistry enabling hit-to-lead progression of T-type Ca²⁺ channel antagonists and ASC-1 inhibitors. **K. Schlegel**

4:30 **589.** Identification of a novel ASGPr ligand and application to receptor mediated delivery and cell-type specific gene editing with CRISPR-Cas9 ribonucleoproteins. **B. Thuma**

Covalent & Non-Covalent Dimers as Therapeutic Agents in Drug Discovery

Sponsored by BIOL, Cosponsored by MEDI and ORGN

Interface between Experiments & Modeling in Unraveling the Physical & Chemical Properties of Charged Droplets

Sponsored by ANYL, Cosponsored by COMP, ORGN and PHYS

- 604.** Atroposelective nucleophilic aromatic substitution of fluorinated pyrrolopyrimidines. **M.A. Saputra**, A. Weng, J.L. Gustafson
- 605.** Circularly polarized luminescence from chiral molecules based on planar chiral [2.2] paracyclophane. **Y. Morisaki**
- 606.** Diastereodivergent and enantioselective synthesis of α -fluoro- β -aminonitriles via copper(I) catalyzed asymmetric Mannich reaction. **R. Ding**, Z. De los Santos, C. Wolf
- 607.** Accessing pharmaceutically relevant 3-arylated *N*-heterocycles via atroposelective synthetic methodologies. **M.M. Cardenas**, M.A. Saputra, A.N. Sanchez, E. Valle, J.L. Gustafson
- 608.** Catalytic enantioselective synthesis of α -allylic alcohol- α -aryl oxindoles. **E. Judge**, P. Guiry
- 609.** Atroposelective halogenation of biaryl anilines. **S.D. Vaidya**, S. Toenjes, J.L. Gustafson
- 610.** Asymmetric ring-opening of donor-acceptor cyclopropanes with primary arylamines catalyzed by a chiral heterobimetallic catalyst. **W. Luo**, H. Wang
- 611.** Development of late-stage functionalization of chiral bisphosphorylimides. **A. Smolin**, O. Apolinar, R.G. Iafe
- 612.** Enantioselective, copper-catalyzed alkynylation of cyclic iminium ions lacking stabilizing groups. **W. Guan**, J. Liao, M.P. Watson
- 613.** Enaminone, metal Lewis acid catalyzed inverse electron demand Aza-Diels Alder reaction to synthesize dihydropyridine derivatives. **H.N. Fernando**

SECTION A

San Diego Convention Center
TBD

CH Activation

Cosponsored by MEDI
E. C. McLaughlin, *Organizer*

7:00 - 9:00

- 614.** Mono- and bis-norbornene annulated biaryl-amines through pseudo-Catellani intermediates by Pd-catalyzed C-H activation. **S. Chuang**
- 615.** Enantioselective α -amino C-H functionalization by cooperative actions of $B(C_6F_5)_3$ and chiral Mg-PyBOX complex. **J. Chan**, M. Wasa
- 616.** Pd-catalyzed C(4)-H functionalization of pyrrolidines and piperidines with C(3)-directing groups: Mechanistic insight into regio- and stereoselectivity. **D. Antermite**, J.A. Bull
- 617.** Unified approach to C-H amination via imidate radicals. **M. Shea**, D. Nagib, A. Prusinowski

- 618.** Mechanistic insights and kinetic studies of Lewis base chlorination of arenes and heterocycles. **A.N. Dinh**, L. Janke, S.M. Maddox, J. Gustafson
- 619.** Catalytic dimerization of terminal alkynes to *gem*-enynes using a binuclear Lewis acid-base complex. **A. Brar**, S. Mummadi, D. Unruh, C. Krempner
- 620.** Synthesis of α -Keto esters using platinum-catalyzed C-H acylation reaction with ethyl chlorooxoacetate. **S. Huo**, E. Javed, J.D. Guthrie, G. Chirayath
- 621.** Chelation-assisted decarboxylative amidation. **K. Das**, P. Kilaru, P. Zhao

SECTION A

San Diego Convention Center
TBD

Metal-Mediated Reactions & Syntheses

Cosponsored by MEDI
E. C. McLaughlin, *Organizer*

7:00 - 9:00

- 622.** Solid-state aldol reaction of lithium enolate of pinacolone. **H. Pang**, P.G. Williard
- 623.** Copper-catalyzed photoinduced radical domino cyclization of ynamides and cyanamides: Unified entry to rosettacin, luotonin A and deoxyvasicinone. **H. Baguia**, C. Deldaele, E. Romero, B. Michelet, G. Evans
- 624.** Stereoselective synthesis of mono and fused, carbo- and heterocyclic compounds via cobalt-assisted radical cyclizations. **N. Babayans**, E. Artashyan, S. Guarina, G.G. Melikyan
- 625.** Rhodium-catalyzed oxy-trifluoromethylthiolation of diazocarbonyl substrates. **M. Lübcke**, W. Yuan, K.J. Szabo
- 626.** Quaternary carbons via palladium-catalyzed aryl prenylation. **J. Leister**, M. Mendoza, K. Billingsley
- 627.** Intramolecular C-N bond formation: Reactivity and selectivity of hypervalent iodine oxidants in the generation of carbamate-derived nitrenes. **A. Bunnell**, M. Lasky, B. Lee, E.C. McLaughlin
- 628.** Copper-catalyzed hydro-oxycarboxylation of terminal alkynes. **Q. Tan**, S. Seo, M.C. Willis
- 629.** Tungsten dearomatization of electron deficient arenes: Synthesis of functionalized cyclohexenes via tandem additions. **S. Simpson**, W.D. Harman
- 630.** Regio- and enantioselective CuH-catalyzed ketone allylation with terminal allenes. **E. Tsai**, R.Y. Liu, Y. Yang, S.L. Buchwald

631. Intermolecular Heck coupling with hindered alkenes directed by potassium carboxylates. **T.R. Huffman**, Y. Wu, A. Emmerich, R.A. Shenvi
632. Exploring sulfonamide substrates for cyclopropane formation by cross-electrophile coupling. **A. Izad**, E. Lucas, K.A. Hewitt, E.R. Jarvo
633. Synthesis of cyclopentenones via Ni-catalyzed formal [3+2] cycloaddition of cyclopropanones and internal alkynes. **Y. Jang**, V. Lindsay
634. Expansion of scope for nickel-catalyzed cross-electrophile couplings of sulfonamides for cyclopropane synthesis. **Y. Tiemsanjai**, A. Castro, E. Lucas, K.A. Hewitt, E.R. Jarvo
635. Non-precious metal catalyzed direct synthesis of Guerbet alcohol. **E. Sehovic**, P. Kaur
636. Green preparation of Au(I) complexes via mechanochemistry. **F. Ingner**
637. Stereocontrolled synthesis of (*E*)-stilbene derivatives by palladium-catalyzed Suzuki-Miyaura cross-coupling reaction. H.H. Rau, **N.S. Werner**
638. Nickel-catalyzed Kumada cross-coupling reactions of sulfonamides. **A.C. Matus**, K.A. Hewitt, E.R. Jarvo
639. Nickel catalyzed synthesis of alkynylphosphonates. **P. Kaur**
640. Synthesis of fluorescent compounds to detect ethylene gas. **S. Rezgui**, S. Toussaint, B.W. Michel
641. Selective deuteration of a broad variety of halogenated compounds using Pd/C-Al-D₂O system as the deuterium source and reaction medium. **N. Zorigt**, **C. Schaefer**, **B. Torok**
642. Mechanism of a chromium-salen catalyzed oxidative cross-coupling of phenols. **T. Paniak**, M. Kozlowski
643. Mechanistic origins of site-selectivity in Pd-NHC-catalyzed cross-couplings. **E. Reeves**, S. Neufeldt
644. Studies directed toward the development of transition metal-halloysite nanocomposite materials for organic transformations. **J. Hamdi**, B. Diehl, A. Blanco, J.B. Wiley, M. Trudell*

SECTION A

San Diego Convention Center
TBD

Photoredox Chemistry

Cosponsored by MEDI
E. C. McLaughlin, Organizer

7:00 - 9:00

645. Enablement of C(sp³)-C(sp³) coupling for DNA encoded library synthesis: Decarboxylative alkylation of α amino acids via mild, aqueous photoredox catalysis. D.K. Kölmel, **R.P. Loach**, T. Knauber, M.E. Flanagan

646. Visible light-mediated radical process for the synthesis of C-glycoamino acids. **P. Ji**, Y. Zhang, Y. Wei, H. Huang, W. Hu, W. Wang
647. Synthesis of chemical libraries and building blocks for drug discovery using photoredox catalysis. **K. Tai**, Y. Mori, C. Kikuchi, M. Kurimura, K. Kondo
648. Organocatalytic thioesterification of aldehydes with visible light. **Y. Zhang**, P. Ji, W. Hu, Y. Wei, H. Huang, W. Wang
649. Lead halide perovskites for photocatalytic organic synthesis. **X. Zhu**, Y. Lin, Y. Sun, D. Zhu, Y. Yan
650. Withdrawn
651. Silicon for pharmaceutical molecule synthesis: Alkenyl-passivated Si quantum dots for C-H activation of tertiary amine. **Y. Sun**, J. San Martin, Y. Yan
652. Radical cation vinylcyclopropane rearrangements by TiO₂ photocatalysis. **N. Maeta**, H. Kamiya, Y. Okada
653. Nitrene generation via visible-light photocatalysis: Aziridination from electrophilic amine sources. **V. Wu**, C.P. Anyanwu, W. Mohamed, E.C. McLaughlin
654. Continuous flow photocatalytic Minisci reaction using *N*-(aceloxy)phthalimide esters. **G. Ignacz**, T. Noel, G. Sipos
655. Silicon quantum dots for synthesis of pyrroles and pyrazoles. **J. San Martin**, Y. Sun, Y. Yan
656. Carboamination strategy for sultam synthesis enabled by photoredox catalysis. R. McAtee, **E.A. Noten**, C. Stephenson
657. Perovskite CsPbBr₃ nanocrystal with a rich possibility of photocatalysis reactions. **D. Zhu**
658. Chiral lead-halide perovskite as efficient photocatalysts for atroposelective pyrroles and indoles synthesis. **Y. Lin**, Y. Sun, C. Manabat, J. San Martin, D. Zhu, X. Zhu, Y. Yan
659. Oxidative photo-catalyzed sulfenylation of substituted indoles and benzothiamides. A.N. Dinh, **A.D. Nguyen**, **E. Millan**, S. Albright, M.R. Cedano, D.K. Smith, J.L. Gustafson

SECTION A

San Diego Convention Center
TBD

Total Synthesis of Complex Molecules

Cosponsored by MEDI
E. C. McLaughlin, Organizer

7:00 - 9:00

660. Total synthesis and absolute configuration of simpotentin, a potentiator of amphotericin B activ-

ity. **M. Ohtawa**, R. Uchida, H. Tomoda, T. Nagamitsu

661. Enantioselective total synthesis of (+)-ieodomycin B and its optical isomers: Synthesis and biological evaluation. D. Choi, J. Lee, Y. Lee, H. Lee, **J. Lee**

662. Withdrawn

663. Asymmetric total syntheses of bridged indole alkaloids with medium sized ring via regioselective indolization. C. Cho, **J. Kim**, H. Kang

664. Kinetically controlled Fischer indolization for the total syntheses of (+)-uleine, (-)-tubifolidine, (-)-tabersonine, and polyveoline. C. Cho, **D. Kim**, T. Jeon, Y. Kim, J. Lim

665. Progress toward total synthesis of (-)-platensimycin and (-)-cyanthiwigin F by internal H-bonding mediated intramolecular Diels-Alder reaction. C. Cho, **H. Kim**, J. Lee, J. Oh

666. Synthetic approach to ergotryptamine, norpsilocin, and aurantioclavine. **S. Rahman**

667. Synthetic studies on strophasterols A-D. **S. Sato**, S. Kuwahara

668. Synthesis of the N-Acyl amycolose moiety of amycolamicin and its methyl glycosides. **y. meguro**, S. Kuwahara

669. Aleutianamine: Architecturally-complex pyrroloiminoquinone alkaloid with selective cytotoxicity toward pancreatic cancer cell lines. **Y. Zou**, X. Wang, J. Sims, B. Wang, P. Pandey, C. Welsh, R. Stone, M. Avery, R.J. Doerksen, D. Ferreira, C. Anklin, F.A. Valeriote, M. Kelly, M.T. Hamann

670. Scalable and convenient syntheses of molecular baskets. **T.A. Neal**, **M. Gunther**, J. Badjic

671. Total synthesis of unique monoterpene-polyketides, cryptolaevilactones, from *Cryptocarya laevigata*. **Y. Miura**, Y. Saito, K. Nakagawa-goto

672. Structure-activity relationship study of antiproliferative abietane diterpenes: Syntheses of 4-*epi*-parviflorons and its derivatives. Y. Miyajima, **Y. Saito**, M. Takeya, M. Goto, K. Nakagawa-goto

673. 11-step catalytic asymmetric synthesis of (-)-bilobalide. **M. Baker**, R. Demoret, M. Ohtawa, R.A. Shenvi

674. Total synthesis of furanosteroids natural products: Viridin and nodulisporiviridin E. **Y. Ji**, S. Gao

675. Studies towards the total synthesis of anguidine. **D. Zhao**, R. Manetsch

676. Progress toward an enantioselective total synthesis of paecilomycine A. **J.M. Nguyen**, S.D. Townsend

677. Synthesis and biological evaluation of illudalic acid derivatives: Inhibition of protein tyrosine phosphatase activity. **B.S. McCullough**, P. Batsomboon, G.B. Dudley, A.M. Barrios

THURSDAY MORNING – ORGN

SECTION A

San Diego Convention Center
Room 7B

New Reactions & Methodology

S. M. Silverman, *Organizer*

D. Weingarten, *Presiding*

- 8:00** **678.** Aerobic C(sp²)-H hydroxylations of 2-aryloxazolines: Fast access to novel ES IPT-based luminophores. **D. Göbel**, B.J. Nachtsheim
- 8:20** **679.** Synthesis of NIR dyes by C-H functionalization for applications in cellular imaging. **C. Rathnamalala**
- 8:40** **680.** C-H activation: Viable route to materials. **C.N. Scott**, I. Rajapaksha, D. Feng, C. Rathnamalala
- 9:00** **681.** Confirmation and quantification of fatty amides and nonamides in direct vegetable oil stripping. **O. Abel-Anyebe**, D. Keita, K.I. Ekpenyong, A. Sodipe, M. Yakubu
- 9:20** **682.** Reverse pharmacology and systems approaches for chemical biology, drug discovery and development: Inspiration from the wisdom of mother nature. **M. Chorghade**
- 9:40** **683.** Surveying iron-organic framework TAL-1 derived and related materials in ligandless heterogenous oxidative catalytic transformations. **K. Ping**, M. Alam, R. Bhadoria, P. Starkov
- 10:00** **684.** Catalytic enantioselective C(sp²)-H and C(sp³)-H alkylation: From organocatalysis to transition metal catalysis. **S. Mukherjee**
- 10:20** **685.** High throughput quantitative and qualitative analysis of high-density kinetic data leads to improved understanding of complex catalytic reactions. **A. Nazarova**, V.V. Fokin
- 10:40** **686.** Cross-coupling of amides by N-C activation. **M. Szostak**
- 11:00** **687.** Multicomponent reactions for the introduction of SCF₃ groups into diazocarbonyl compounds. **M. Lübcke**, W. Yuan, D. Bezhan, K.J. Szabo
- 11:20** **688.** Chemoenzymatic approaches to the total synthesis of epoxyquinoid natural products. **J.A. Collins**, M.S. Duncan, W.B. Kline, Z.T. Clark

SECTION B

San Diego Convention Center
Room 10

Asymmetric Reactions & Syntheses

S. M. Silverman, *Organizer*

A. Lo, *Presiding*

- 8:00 689.** Synthesis of axially chiral biaryl-carboxylic acids (BINA-Cox) and their evaluation as ligands in asymmetric titanium-catalyzed hydroalkoxylation. **S.L. Helmbrecht**, L. Hintermann
- 8:20 690.** Applications of boronic acids in asymmetric synthesis. **S. Jonker**, C. Diner, G. Schulz, H. Iwamoto, L. Eriksson, K.J. Szabo
- 8:40 691.** Diastereodivergent synthesis of tricyclic chromanone derivatives using modularly designed organocatalysts. **C.C. Zhao**, S. Jakkampudi, R. Parella, H.D. Arman
- 9:00 692.** Asymmetric synthesis of azepine-fused cyclobutanes via a gold(I)-catalyzed cyclopropanation/C-C cleavage/chirality-memorized Wagner-Meerwein rearrangement of yne-methylenecyclopropanes. **C. Li**, Z. Yu
- 9:20 693.** Asymmetric synthesis of fused bicyclic N,O- and O,O-acetals via cascade reaction by gold(I)/N,N'-dioxide-nickel(II) bimetallic relay catalysis. **B. Hu**, X. Feng
- 9:40 694.** Acyclic stereocontrol in the additions of nucleophilic alkenes to α -chiral *N*-sulfonyl imines. **A. Lo**, L.C. Moore, J.T. Shaw, J.S. Fell
- 10:00 695.** Enantioselective [3 + 2] cycloaddition and rearrangement of thiazolium salts to synthesize thiazole and 1,4-thiazine derivatives. **X. Zhang**, X. Liu, X. Feng
- 10:20 696.** Bimetallic rhodium(II)/indium(III) relay catalysis for tandem insertion/asymmetric claisen rearrangement. **Y. Chen**, X. Liu, X. Feng
- 10:40 697.** Bimetallic catalytic asymmetric tandem reaction of β -alkynyl ketones to synthesize 6,6-spiroketal. **S. Ge**, X. Feng
- 11:00 698.** Enantioselective synthesis of 2,2,3-trisubstituted indolines via bimetallic relay catalysis of α -diazoketones with enones. **J. Yang**, X. Liu, X. Feng
- 11:20 699.** Catalytic enantioselective ene-type reactions of vinylogous hydrazone: Construction of α -methylene- γ -butyrolactone derivatives. **H. Zhang**, X. Liu, X. Feng
- 8:40 702.** Withdrawn
- 9:00 703.** [4+2] Cycloaddition methodology for the synthesis of functionalised aromatic scaffolds. **B. Emery**, S.D. Bull
- 9:20 704.** Rapid assembly of saturated nitrogen heterocycles in one-pot for biological screening collections. **A.J. Boddy**, D. Affron, C. Cordier, E. Rivers, A.C. Spivey, J.A. Bull
- 9:40 705.** Synthesis of novel 3,3-disubstituted azetidines for medicinal chemistry: Divergent catalytic functionalization of 3-aryl-3-azetidins. **M. Dubois**, C. Denis, A. Lazaridou, V. Anne Sophie, R. Bureau, J.J. Mousseau, C. Choi, J.A. Bull
- 10:00 706.** Synthesis of small sensory models for development as pH probes. **I. Rajapaksha**
- 10:20 707.** *In vivo* monitoring of carbonic anhydrases expression with fluorescence turn-on enrichment. **C. Chou**
- 10:40 708.** Synthesis of β -lactams via metal-catalyzed formal [3+1] cycloaddition of cyclopropanones. **C.M. Poteat**, Y. Jang, J.D. Johnson, V. Lindsay
- 11:00 709.** Regio- and stereoselective synthesis of isoindolinones through superbases-mediated iodoaminocyclization of 2-(1-alkynyl)benzamides. **S. Mehta**, D. Brahmchari
- 11:20 710.** Unprecedented and efficient synthesis of DMDPP and its conversion to the arylalkenyl π -system through C-H transition-metal-free approach. **D. Feng**
- 11:40 711.** One-pot, multicomponent synthesis of azolo[1,3,5]triazines via selective 1,3,5-triazine ring annulation onto aminoazoles. **F.P. Lim**, A.V. Dolzhenko

SECTION D

San Diego Convention Center
Room 8

Metal-Mediated Reactions & Syntheses

S. M. Silverman, *Organizer*
H. Shenouda, *Presiding*

- 8:00 712.** Nickel-catalyzed, ring-forming aromatic C-H alkylations with unactivated alkyl halides. **Q.D. Tercentio**, E.J. Alexanian
- 8:20 713.** Formation of new C-C bonds via H₂-mediated coupling of ketenimines with carbonyl electrophiles. **M.M. Sikes**, L.V. Hale, N.K. Szymczak
- 8:40 714.** Transition metal-catalyzed highly regioselective azide-internal alkynes cycloaddition under mild conditions. **W. Song**
- 9:00 715.** Iron-catalyzed site-selective oxidation of phenols and anisoles. L. Göttemann, **M. Chojnacka**, A. Pan, K. Kou

SECTION C

San Diego Convention Center
Room 9

Heterocycles & Aromatics

S. M. Silverman, *Organizer*
F. P. Lim, *Presiding*

- 8:00 700.** Magnesium ethoxide promoted conversion of nitriles to amidines and its application in 5,6-dihydro-imidazobenzoxazepine synthesis. **M.E. Dalziel**, J. Deichert, D. Carrera, D. Beaudry, C. Han, H. Zhang, R. Angelaud
- 8:20 701.** Withdrawn

- 9:20 716.** Synthesis of benzoxocine heliannuols via the intramolecular Nicholas reaction. **B. St Onge**, J.R. Green
- 9:40 717.** Stereospecific, manganese-catalyzed hydroxymethylation of unactivated alkyl tosylates. **H. Shenouda**, E.J. Alexanian
- 10:00 718.** Iridium catalyzed hydrogen-borrowing reactions of β -amino alcohols. **C.J. Hall**, W.R. Goundry, T.J. Donohoe
- 10:20 719.** Vinylation of benzylic amines via C-N bond functionalization of benzylic pyridinium salts. **W. Guan**, J. Liao, M.P. Watson
- 10:40 720.** Cyclic(alkyl)amino carbenes synthesis and applications. **R.F. Jazzar**, G. Bertrand
- 11:00 721.** Expansion of the Chan–Evans–Lam reaction with functionalized potassium vinyl trifluoroborates. **G.I. Elliott**, T.E. Cole
- 11:20 722.** Activation of trifluorotoluene towards hydroamination type reactions by a tungsten dearomatization agent. **K.B. Wilson**, H.S. Nedzbala, W.D. Harman
- 11:40 723.** Synthesis of long expanded helicenes via a diyne-selective [2+2+2] cycloaddition strategy. **G.R. Kiel**, T. Tilley
- 8:40 726.** Biocatalytic C–H oxidation as an enabling tool for complex molecule total synthesis. **H. Renata**
- 9:00 727.** Biocatalyst-initiated *ortho*-quinone methide generation and diversification. **J. Perkins**, T. Doyon, E. Romero, S.A. Dockrey, K. Skinner, P.M. Zimmerman, A.R. Narayan
- 9:20 728.** Enantioselective syntheses of concave-substituted dioxabicyclo[3.3.0]octanone spongian diterpenoids. **T.K. Allred**, P. Zhao, G. Lackner, L.E. Overman
- 9:40 729.** Eleven-step synthesis of (–)-bilobalide. **R. Demoret**, M. Baker, M. Ohtawa, R.A. Shenvi
- 10:00 730.** Total synthesis of streptothricin F and streptolidine lactam. **M. Dowgiallo**, M. Kassu, J. Kirby, R. Manetsch
- 10:20 731.** Biocatalytic synthesis of anthelmintics using a cascade assembly approach. **S. Kelly**, A.E. Fraley, S. Newmister, Y. Ye, D.H. Sherman
- 10:40 732.** Stereodivergent, chemoenzymatic synthesis of azaphilones natural products. **J. Pyser**, S.A. Dockrey, L. Joyce, A. Rodriguez Benitez, R. Wiscons, A.R. Narayan
- 11:00 733.** Progress toward the synthesis of arimetamycin A. **E.D. Huseman**, S.D. Townsend
- 11:20 734.** Thioenamide synthesis inspired by peptide macrocycles. **J. Lutz**, C.M. Taylor

SECTION E

San Diego Convention Center
Room 7A

Total Synthesis of Complex Molecules

S. M. Silverman, *Organizer*
R. Demoret, *Presiding*

- 8:00 724.** New strategies for the concise synthesis of complex terpenes. **P. Hu**
- 8:20 725.** Total synthesis of (–)- γ -lycorane. **C.J. Hall**, I. Marriott, W.R. Goundry, T.J. Donohoe

Interface between Experiments & Modeling in Unraveling the Physical & Chemical Properties of Charged Droplets

Sponsored by ANYL, Cosponsored by COMP, ORGN and PHYS

PHYS

DIVISION OF PHYSICAL CHEMISTRY

A. McCoy, *Program Chair*

SUNDAY MORNING – PHYS

SECTION A

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 13

Chemistry in Real Space & Time

Plasmon-Assisted Spectroscopy/Phenomena

V. A. Apkarian, V. Bommisetty, *Organizers*
E. Potma, *Organizer, Presiding*

- 8:00 Introductory Remarks.
- 8:05 1. Excited-state dynamics in quantum-engineered systems. **P. Narang**
- 8:40 2. Plasmons and hot electrons: Open-circuit photovoltages and bias-driven light emission. **D. Natelson**, C.I. Evans, L. Cui, Y. Zhu
- 9:15 3. Gold nanoparticle-based plasmon enhanced fluorescence of polyallylamine hydrochloride: An efficient and selective sensor for picric acid in aqueous media. S. Kaja, D.P. Damera, **A. Nag**
- 9:35 4. Ultrafast proton transport along solvent bridges governed by a hydroxide/methoxide transfer mechanism. M. Ekimova, F. Hoffmann, G. Bekçioğlu-Neff, A. Rafferty, O.A. Kornilov, D. Sebastiani, **E. Nibbering**
- 9:55 Intermission.
- 10:15 5. Plasmon-enhanced stimulated Raman scattering microscopy with single-molecule detection sensitivity. **J. Cheng**
- 10:50 6. Insights from single particle spectroscopy of plasmonic nanostructures. **S. Link**
- 11:25 7. Optical forging of graphene into 3D shapes as a potential way to control plasmonic properties. **M. Pettersson**

SECTION B

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 12

Computational Quantum Chemistry: From Promise to Prominence: A Symposium in Honor of Henry F. Schaefer

Cosponsored by COMP

T. Crawford, P. R. Schreiner, D. D. Sherrill, *Organizers*
E. F. Valeev, *Organizer, Presiding*

- 8:30 8. Some recent developments in quantum chemical methods for treating electron correlations. **M.P. Head-Gordon**
- 9:00 9. Accuracy versus complexity in computational quantum chemistry. **W. Thiel**
- 9:30 10. New tight-binding quantum chemistry methods for the exploration of chemical space. **S. Grimme**
- 10:00 11. Towards non-adiabatic dynamics simulations using semiempirical extended tight-binding (xTB) methods. **C. Bannwarth**, T.J. Martinez
- 10:15 Intermission.
- 10:40 12. Kicking it up a NOTCH. **F. Neese**
- 11:10 13. Quantum-chemical methods for biochemical systems. **C. Ochsenfeld**
- 11:40 14. Numerical evidence invalidating textbook finite-temperature perturbation theory. **S. Hirata**, P.K. Jha

SECTION C

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 11

Nanoscale & Molecular Assemblies: Designing Matter to Control Energy Transport

Cosponsored by INOR
Financially supported by Coherent
J. R. Caram, J. J. Foley, D. Hayes, *Organizers*
J. Foley, *Presiding*

- 8:30 15. Coupling between molecules and plasmons using highly confined fields. **L. Jensen**
- 9:10 16. Mesoscale quantum dynamics in molecular aggregates. **D. Bennett**
- 9:30 17. Energy transport in a strongly coupled photosynthetic system revealed by novel time resolved circular dichroism spectroscopy. **S. Savikhin**, V. Stadnytskyi, Z. Mitchell, G.S. Orf, R.E. Blankenship, Y. Kim, L.V. Slipchenko
- 9:50 Intermission.
- 10:05 18. Excited-state properties of imperfect 2D materials: Impact of defects and temperature from first principles. **S. Sharifzadeh**

- 10:45** 19. Eumelanin in a new light: Natural nanostructures with the excitonic properties of graphene oxide. **C. Grieco**, F. Kohl, B. Kohler
- 11:05** 20. Controlling energy transport with DNA-chromophore assemblies. J. Banal, W. Chen, S. Hart, W. Bricker, M. Bathe, **G. Schlau-Cohen**

SECTION E

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 1

Getting to the Bottom: Optical & Electron Imaging of Reactive Chemical Systems

High-Resolution Optical Imaging of Chemical Processes

Cosponsored by ANYL

J. S. Biteen, E. Ringe, J. Sambur, *Organizers*
R. Sharma, *Presiding*

- 8:30** 21. Single-turnover at molecular catalysts. **S. Blum**
- 9:05** 22. Influence of single nanoparticle electrochromic dynamics on the speed and durability of smart windows. **J. Sambur**
- 9:40** 23. Probing and understanding single molecule redox reactions. **N. Tao**
- 10:15** Intermission.
- 10:30** 24. Watching single nanoparticle chemistry using a whispering gallery mode optical microresonator. **R.H. Goldsmith**
- 11:05** 25. Spatiotemporal studies of the mechanism of corrosion by single molecule fluorescence spectroscopy. **L. Kiskey**
- 11:25** 26. Unusual catalog of hydrocarbons captured in plasmon-catalyzed chemistry. **P.K. Jain**

SECTION F

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 2

Hydration from the Gas to the Condensed Phase Hydration of Protons, Hydroxides, & Electrons

Financially supported by Phasetech

E. Backus, M. Bonn, *Organizers*
F. Paesani, *Organizer, Presiding*

- 8:30** Introductory Remarks.
- 8:35** 27. Proton continuum at the liquid/vapour interface. **E. Tyrode**
- 9:05** 28. Hydrated excess protons in acetonitrile/water mixtures: Solvation species and ultrafast proton motions. **B.P. Fingerhut**, A. Kundu, F. Dahms, E. Nibbering, E. Pines, T. Elsaesser

- 9:35** 29. Structure of protonated water solvates in acetonitrile reveals the importance of the protonated water trimer $H_7^+O_3$. E. Kozari, M. Sigalov, D. Pines, **E. Pines**
- 9:55** 30. Promiscuous nature of liquid water: Profiling its density and charge fluctuations. **A. Hassanali**, N. Ansari, E. Poli, A. Laio, G. Sosso
- 10:25** Intermission.
- 10:40** 31. Investigation of ion-pairing and covalent states in hydrated HCl: From clusters to the air-water interface. **R. Kumar**, C. Bresnahan, R. David
- 11:10** 32. Influence of electron scattering on the properties of the hydrated electron. **R. Signorell**
- 11:40** 33. Hydration of excess protons in aqueous systems: Addressing complexity and misconception. **G.A. Voth**

SECTION G

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 3

At the Interfaces of Experimental & Theoretical Nonlinear Optical Molecular Spectro-Imaging Hyperspectral Imaging

L. Wang, *Organizer*

W. Xiong, *Organizer, Presiding*

- 8:30** 34. Probing microscale disorder with time-resolved emission and reflection microscopies. J.J. Thiebes, A. Hathaway, C.L. Kennedy, **E. Grumstrup**
- 9:00** 35. Sensitively probing spatiotemporal photogenerated quasiparticle dynamics with on- and off-resonant light scattering. M. Delor, H. Weaver, E. Zsoldos, J. Utterback, Q. Yu, **N.S. Ginsberg**
- 9:30** 36. Ultrafast dynamic microscopy of carrier and exciton transport. **L. Huang**
- 9:50** Intermission.
- 10:10** 37. Tip-enhanced spectroscopic imaging of nanoscale chemical and electronic structure. **J. Atkin**
- 10:40** 38. Super-multiplex vibrational imaging for biomedicine. **W. Min**
- 11:00** 39. Water perspective on neuronal activity using wide field second harmonic imaging. **S. Roke**

SECTION H

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 4

Molecular, Electronic, & Ionic Transport in Materials for Energy

Moving Ions: New Mechanisms & New Measurements

X. Roy, *Organizer*

L. A. Madsen, *Organizer, Presiding*

- 8:30** Introductory Remarks.
- 8:35** **40.** Identifying the underlying causes of ionic current rectification behavior and optical phenomena in purely protonic solar cells composed of photoacid-sensitized ion-exchange membranes. **L. Schulte**, W. White, S. Ardo
- 8:55** **41.** Role of fabrication parameters on the properties of purely protonic solar cells composed of photoacid-modified ion-exchange membranes. **J. Neal, III**, L. Schulte, S. Ardo
- 9:15** **42.** Energy transduction via metal nanofilms. **F. Geiger**, T.F. Miller
- 9:45** **43.** Predicting the performance of lithium metal electrodes stabilized by polymer electrolytes. **N.P. Balsara**
- 10:15** Intermission.
- 10:35** **44.** Neutron reflectivity studies of ionic copolymer films under applied electric fields. **B.S. Lokitz**, J. Dugger, J. Browning
- 10:55** **45.** *Operando* and three-dimensional visualization of ion depletion and lithium growth by stimulated raman scattering microscopy. **Y. Yang**, W. Min
- 11:25** **46.** Li-ion dynamics in next generation cathode materials. **L.E. Marbella**
- 11:55** **47.** Design of polymer architecture to enhance Li⁺ transport in solid polymer electrolytes: Insight from molecular dynamics simulations. **D. Dong**, **D. Bedrov**, A. Choudhary

Nanotechnology & Single Cell Analysis in Biology & Medicine

Nanoscience, Biology & Medicine

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

Future Insights into Syngas Conversion Catalysis: Symposium in honor of Burtron H. Davis

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

Zarefest: Symposium in honor of Richard Zare's Love for Science

Sponsored by ANYL, Cosponsored by PHYS

Solvent Effects in Metal-Catalyzed Reactions

Sponsored by CATL, Cosponsored by ENFL and PHYS

Water in the Solid State: Reactions & Interactions with Impurities

Nucleation & Growth

Sponsored by ENVR, Cosponsored by PHYS

Advances in Catalysis with Ceria & Other Reducible Oxides

Model Ceria Catalyst

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

SUNDAY AFTERNOON – PHYS

SECTION A

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 13

Chemistry in Real Space & Time

Molecular Videography

V. A. Apkarian, V. Bommisetty, E. Potma, *Organizers*
R. Wu, *Presiding*

- 1:30** **48.** Advances in ultrafast terahertz scanning tunneling microscopy. **F. Hegmann**
- 2:05** **49.** Single switching events of one molecule observed by femtosecond STM. **D. Peller**, T. Buchner, L. Kastner, C. Roelcke, R. Huber, J. Repp
- 2:40** **50.** Ultrafast terahertz nanoscopy: From near fields to single atoms. **T. Cocker**
- 3:00** **51.** Direct imaging of nanoscale anisotropic structural dynamics with ultrafast electron microscopy. **Y. Zhang**, D.J. Flannigan
- 3:20** Intermission.
- 3:35** **52.** Phase-controlled optical pump-probe STM and its applications. **H. Shigekawa**
- 4:10** **53.** Towards understanding molecule-plasmon interactions on ultrafast timescales. **T. Ueltschi**, R.P. Van Duyne
- 4:30** **54.** Multimodal characterization of localized and propagating plasmons in real space, time, and frequency. **K. Crampton**, A. Joly, P.Z. El-Khoury
- 4:50** **55.** Direct imaging of incoherent-to-coherent structural dynamics in plasmonic nanorods with ultrafast electron microscopy. **R. Gnasik**, D.T. Valley, M.K. Quan, V.E. Ferry, D.J. Flannigan
- 5:10** Concluding Remarks.

SECTION B

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 12

Computational Quantum Chemistry: From Promise to Prominence: A Symposium in Honor of Henry F. Schaefer

Cosponsored by COMP

P. R. Schreiner, D. D. Sherrill, E. F. Valeev, *Organizers*

T. Crawford, *Organizer, Presiding*

- 1:30 56. Adventures in DFT by a wavefunction theorist. **R.J. Bartlett**
- 2:00 57. Fractional perspectives and quasiparticle and excitation energies from ground state DFT calculations. **W. Yang**
- 2:30 58. Recent progress in density functional and pair-density functional theory. **D.G. Truhlar**, P. Verma, X. He, Y. Wang, L. Gagliardi, P. Sharma, V. Bernales, S. Knecht, C. Zhou, J. Bao
- 3:00 59. Solving the density functional conundrum: Elimination of systematic errors to derive accurate energies for complex chemical reactions. S. Deb Nath, A. Sengupta, B. Thapa, **K. Raghavachari**
- 3:15 Intermission.
- 3:40 60. Robust all-electron optimization of orbital-free density-functional theory. **T. Helgaker**, M.S. Ryley, A.M. Teale
- 4:10 61. Other axis of error: DFT integration grids and relative free energies of organic molecules. **S.E. Wheeler**, A.N. Bootsma
- 4:40 62. Development of a machine-learning finite-range nonlocal density functional. **Z. Chen**, W. Yang
- 4:55 63. Density functional theory correction to CASSCF. **A.R. Mclsaac**, J.J. Shepherd, T.A. Van Voorhis

SECTION C

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 11

Nanoscale & Molecular Assemblies: Designing Matter to Control Energy Transport

Cosponsored by INOR

Financially supported by Coherent

J. R. Caram, J. J. Foley, D. Hayes, *Organizers*

D. Bennett, *Presiding*

- 1:30 64. Nonradiative energy transfer and hot-electron generation in plasmonic bio-assemblies and metastructures with hot spots. **A. Govorov**, L. Khosravi Khorashad, L.V. Besteiro
- 2:10 65. Solvent effect of energy relaxation of amyloid beta peptide 1-40 at nano-scale gold surface. **K. Yokoyama**

- 2:30 66. Expanded theory for molecular aggregate photophysics. **F.C. Spano**
- 3:10 Intermission.
- 3:25 67. Design principles for near-infrared and shortwave infrared molecular aggregates of cyanine dyes. **A. Deshmukh**, D. Koppel, C. Chuang, D.M. Cadena, J. Cao, J.R. Caram
- 3:45 68. Tubular J-aggregates of amphiphilic cyanine dyes as functional scaffolds for self-assembly of complex hybrid inorganic/organic systems. E. Steeg, K.A. Herman, H. Kirmse, Y. Qiao, J.P. Rabe, **S. Kirstein**
- 4:25 69. Design of multilayer nanostructures for thermal radiation control. **J.F. Varner**, J.J. Foley
- 4:45 70. Vibrational cooling in linear and branched oligomeric viologens. **M. Liu**, T. Kawauchi, T. Iyoda, P.G. Piotrowiak
- 5:05 71. Tuning electronic properties of well-defined nanoscale objects by locking in pi-conjugated superstructures. **J. Olivier**, A. Ashcraft, V. Paulino, K. Liu

SECTION D

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 10

Water in the Universe

S. Ioppolo, *Organizer*

G. A. Blake, *Organizer, Presiding*

- 1:30 Introductory Remarks.
- 1:35 72. Water megamaser emission in galaxies. **V. Impellizzeri**
- 2:10 73. Water vapor in galaxies at high redshift. **C. Yang**
- 2:45 74. Chemistry of water in our galaxy and beyond. **S. Viti**
- 3:20 Intermission.
- 3:40 75. Influence of water on reactivity in and on icy grain surfaces. **A. Lamberts**
- 4:15 76. Three things you probably didn't know about amorphous solid water. **M.R. McCoustra**
- 4:50 77. Rotational spectroscopy as a probe for gas-phase products of thermal- and photo-processed ices. **S.L. Widicus Weaver**, K. Yocum, A. Jones, E. Todd, P.A. Gerakines, S.N. Milam

SECTION E

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 1

Getting to the Bottom: Optical & Electron Imaging of Reactive Chemical Systems

Visualizing Biology in Living Cells and In Vitro

Cosponsored by ANYL

E. Ringe, J. Sambur, *Organizers*
J. S. Biteen, *Organizer, Presiding*

- 1:30 78.** Optical microscopy of dynamic systems: From graphene reactions to intracellular diffusion. **K. Xu**
- 2:00 79.** Label-free optical detection of neural electric potentials. **B. Cui**, F. Alfonso
- 2:30 80.** Imaging the cellular response to TiO₂ nanoparticles. **C.K. Payne**
- 3:00** Intermission.
- 3:15 81.** Fluorescence studies of protein disorder, single molecules to droplets. **A.A. Deniz**
- 3:45 82.** Getting to the bottom of bacterial type 3 secretion by tracking biomolecular complexes in living cells. J. Rocha, A.M. Achimovich, A. Rivera, **A. Gahlmann**
- 4:15 83.** Optical charge transfer transitions in charged amino acids: New label free spectroscopic markers to probe protein structure and dynamics. **R. Venkatramani**, I. Mandal
- 4:35 84.** Close look at the mechanisms of protein folding and unfolding via single molecule fluorescence and force spectroscopy methods. **V. Muñoz**

SECTION F

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 2

Hydration from the Gas to the Condensed Phase Water in Biology

Financially supported by Phasetech
E. Backus, M. Bonn, F. Paesani, *Organizers*
S. Sarupria, *Presiding*

- 1:30 85.** Weird hydration: Water in living cells and the strange case of PEG vs. POM. **S. Woutersen**
- 2:00 86.** Protein hydration and cold unfolding. **J.C. Palmer**
- 2:30 87.** Protection against hydration: How do cells withstand freezing temperatures?. **N.E. Levinger**, F.D. Samuels
- 2:50 88.** Interfacial H-bond dynamics in reverse micelles: Role of surfactant heterogeneity. **C.P. Baryames**, M. Teel, C.R. Baiz
- 3:10** Intermission.
- 3:40 89.** Heterogeneous dynamics in self-assembled materials revealed by transient VSFG microscopy. **H. Wang**, W. Chen, J. Wagner, W. Xiong
- 4:00 90.** 2D IR study of NMA-water mixtures. **M. Pshenichnikov**, E. Salamatova, A. Cunha, R. Bloem, S. Roeters, S. Woutersen, T.C. Jansen
- 4:20 91.** Molecular dynamics study of structure and vibrational spectra at aqueous lipid and polymer interfaces. **T. Ishiyama**
- 4:50 92.** Hydrophobic vs. hydrophilic interactions of TMAO and urea. **Y. Nagata**

SECTION G

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 3

At the Interfaces of Experimental & Theoretical Nonlinear Optical Molecular Spectro-Imaging Hyperspectral Imaging

L. Wang, W. Xiong, *Organizers*
E. Grumstrup, *Presiding*

- 1:30 93.** Compressive-sensing sum frequency generation imaging of surfaces. **S. Baldelli**, K. Kelly, D. Zheng, Z. Sun, H. Li
- 2:00 94.** Chemical imaging with sum-frequency generation microscopy and scattering scanning near-field optical microscopy. **N. Ge**
- 2:30 95.** Phase transformations in pharmaceutical materials through nonlinear optical imaging and spectroscopy. **G.J. Simpson**
- 3:00** Intermission.
- 3:20 96.** Exploring the spatial dependence of chemical dynamics under a voltage bias using 2D IR imaging. C. Tibbetts, N.J. Gimble, B.M. Luther, A.L. Prieto, **A.T. Krummel**
- 3:50 97.** 4D super-resolution imaging of interfacial protein dynamics. **C.F. Landes**
- 4:10 98.** Non-equilibrium crystal geometries involved in singlet fission visualized with ultrafast 2D white-light microscopy. **M.T. Zanni**
- 4:40 99.** Decay associated Fourier spectra: Visible to shortwave infrared time-resolved emission spectra. **T.L. Atallah**, A.J. Shin, A.V. Sica, J.R. Caram

SECTION H

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 4

Molecular, Electronic, & Ionic Transport in Materials for Energy

Transport Mechanisms for Ions & Small Molecules

X. Roy, *Organizer*
L. A. Madsen, *Organizer, Presiding*

- 1:30 100.** Ion conduction and phase behaviors of imidazolium-based ionic plastic crystals and semicrystalline copolymers. **M. Lee**, H. Chae, U. Choi
- 1:50 101.** Ion transport in polymerized ionic liquid-ionic liquid blends. S. Mogurampelly, **V. Ganesan**
- 2:20 102.** Transport of ions and small molecules in self-assembled materials based on polymers and ionic liquids for application in energy and sustainability. **M. Watanabe**

- 2:50** **103.** Structure and transport properties of lithium-doped aprotic and protic ionic liquid electrolytes. **A. Taghavi Nasrabadi**, V. Ganesan
- 3:10** Intermission.
- 3:30** **104.** Influence of morphology on ion transport in polymerized ionic liquid. **Z. Zhang**, J. Krajniak, V. Ganesan
- 3:50** **105.** Tuning self-assembly and macromolecular properties in ion-conducting block copolymer systems by controlling monomer segment distribution. **T.H. Epps**
- 4:20** **106.** Ion transport in battery electrolytes from molecular dynamics simulations. **O. Borodin**
- 4:50** **107.** Membrane science and technology for water and energy applications. **B.D. Freeman**

Nanotechnology & Single Cell Analysis in Biology & Medicine

Nanoscience

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Zarefest: Symposium in honor of Richard Zare's Love for Science

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Future Insights into Syngas Conversion Catalysis: Symposium in honor of Burtron H. Davis

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Water in the Solid State: Reactions & Interactions with Impurities

Microstructural & Mechanical Aspects of Ice

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Solvent Effects in Metal-Catalyzed Reactions

Sponsored by CATL, Cosponsored by ENFL and PHYS

Advances in Catalysis with Ceria & Other Reducible Oxides

Theory of Ceria Catalysts

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Advances in Fluorescence & Bioluminescence Imaging Probes

Sponsored by ANYL, Cosponsored by PHYS

SUNDAY EVENING – PHYS

Zarefest: Symposium in honor of Richard Zare's Love for Science

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MONDAY MORNING – PHYS

SECTION A

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 13

Chemistry in Real Space & Time

TERS & SERS Theory

V. A. Apkarian, V. BommiSETTY, E. Potma, *Organizers*
L. Jensen, *Presiding*

- 8:00** **108.** Theories of SERS, TERS, and plasmon-enhanced energy transfer. **G.C. Schatz**
- 8:35** **109.** Electron transfer in confined electromagnetic fields. A. Semenov, **A. Nitzan**
- 9:10** **110.** Real-time simulation of spin-polarized molecular plasmon dynamics. **C.T. Chapman**
- 9:30** Intermission.
- 9:50** **111.** Quantum plasmonics and hot carrier generation. **P.J. Nordlander**
- 10:25** **112.** Theoretical insights into tip-enhance Raman scattering images. **P. Liu**, X. Chen, L. Jensen
- 10:45** **113.** Semiempirical modeling of SERS and TERS enhancement mechanisms. **R. Gieseeking**
- 11:20** **114.** Theoretical study on high-resolution tip-enhanced Raman scattering: From plasmonic near field to sub-molecular density change. **X. Chen**, P. Liu, L. Jensen
- 11:40** **115.** Recent advances in modeling SERS and TERS. **L. Jensen**

SECTION B

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 12

Computational Quantum Chemistry: From Promise to Prominence: A Symposium in Honor of Henry F. Schaefer

Cosponsored by COMP
T. Crawford, P. R. Schreiner, D. D. Sherrill, E. F. Valeev, *Organizers*
A. Sokolov, *Presiding*

- 8:30** **116.** Classical molecular dynamics simulations of electronically non-adiabatic processes. **W.H. Miller**

- 9:00 **117.** Computational treatment of the Jahn-Teller and pseudo Jahn-Teller effects. **J.F. Stanton**
- 9:30 **118.** Accurate nonadiabatic dynamics. **D.R. Yarkony**
- 10:00 **119.** Excited-state specific multireference wavefunction methods. **L. Tran**, E. Neuscammann
- 10:15 Intermission.
- 10:40 **120.** Dramatic enhancement of quantum tunneling rates in water clusters via librational excitation. **R.J. Saykally**
- 11:10 **121.** Multicomponent quantum chemistry: Integrating electronic and nuclear quantum effects. **S. Hammes-Schiffer**
- 11:40 **122.** Electroweak quantum chemistry and quantum dynamics of chiral molecules: High resolution spectroscopy and the parity violating energy difference between enantiomers. **M. Quack**

SECTION C

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 11

Nanoscale & Molecular Assemblies: Designing Matter to Control Energy Transport

Cosponsored by INOR

Financially supported by Coherent

J. R. Caram, J. J. Foley, D. Hayes, *Organizers*

C. Grieco, *Presiding*

- 8:00 **123.** Silicon based stabilizers for self-assembled nanoparticles. **B.P. Chauhan**, G. Longia, E. Cook, Z. Perez, Q.R. Johnson
- 8:40 **124.** The dynamics and spectroscopy of molecular excitons in large aggregates of chromophores. **S.J. Jang**
- 9:20 **125.** What should be considered to control the electronic structure of excited states: Impact upon topological arrangement. **J. Yu**, P. Deria
- 9:40 Intermission.
- 9:55 **126.** Gas-phase synthesis of hierarchically structured and responsive metal-organic frameworks. **T.J. Kempa**
- 10:35 **127.** Geometric and material effects of thermal evanescent near-field of metal-based nanoparticles and forster resonant energy transfer. **X. Chen**
- 10:55 **128.** Optics and energy transport of excitons in self-assembled molecular nanotubes. **J. Knoester**
- 11:35 **129.** Molecular thermal transport at room temperature: Stochastic nonequilibrium molecular dynamics simulations of heat conduction through extended molecule junctions. **R. Chen**, I. Sharony, A. Nitzan

SECTION D

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 10

Water in the Universe

G. A. Blake, S. Ioppolo, *Organizers*

M. R. McCoustra, *Presiding*

- 8:30 **130.** Water at the dawn of star formation. **P. Caselli**
- 9:05 **131.** Water in protostellar systems: Past, present, and future. **L. Kristensen**
- 9:40 **132.** Water ice observations, from dense clouds to protoplanetary disks. **A. Boogert**
- 10:15 Intermission.
- 10:35 **133.** Behavior of OH radical on ice. **N. Watanabe**, A. Miyazaki, W. Sameera, T. Hama, A. Kouchi
- 11:10 **134.** Activation energy of OH-radical diffusion on water ice surface. **A. Miyazaki**, N. Watanabe, W. Sameera, T. Hama, H. Hidaka, A. Kouchi
- 11:30 **135.** Inversion of surface voltage on H₂O films affecting sublimation of CO underlayer. **A. Ishibashi**, Y. Oba, T. Hama, A. Kouchi, N. Watanabe
- 11:50 **136.** Water forming reaction H₂ + OH → H₂O + H: Atom tunneling, kinetic isotope effects and influence of an ice surface. **J. Meisner**, A. Lamberts, J. Kästner

SECTION E

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 1

Getting to the Bottom: Optical & Electron Imaging of Reactive Chemical Systems

Imaging Plasmon-Coupled Processes

Cosponsored by ANYL

J. S. Biteen, E. Ringe, J. Sambur, *Organizers*

R. R. Frontiera, *Presiding*

- 8:30 **137.** Active binary control of the thermal near field via plasmon hybridization. **D.J. Masiello**
- 9:05 **138.** Photoelectrodissolution of single plasmonic nanoparticles. **A. Al-Zubeidi**, B. Hoener, S. Collins, W. Wang, S. Kirchner, S. Hosseini Jebeli, A. Joplin, W. Chang, S. Link, C.F. Landes
- 9:25 **139.** Fractal plasmonics: Optical properties from the visible to the mid-IR spectral range. **F.A. Lagugne-Labarthet**, G.Q. Wallace, D. McRae, D. Therien
- 9:45 Intermission.
- 10:00 **140.** Monitoring electrochemical reactions at plasmonic nanoparticle surfaces. **K.A. Willets**
- 10:35 **141.** Resolving mislocalization in plasmon-enhanced single-molecule microscopy. **H.J. Goldwyn**, D.J. Masiello

- 10:55 142.** Single-molecule emission polarization modification by plasmonic nanorods. **T. Zuo**, H.J. Goldwyn, B. Isaacoff
- 11:15 143.** Imaging hot carrier chemistry at plasmonic interfaces. **C.F. Landes**, S. Link

SECTION F

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 2

Hydration from the Gas to the Condensed Phase

Water at Charged Interfaces

Financially supported by TOPAG
E. Backus, F. Paesani, *Organizers*
M. Bonn, *Organizer, Presiding*

- 8:30 144.** Exploring the interfacial structure of water at buried silica/aqueous interfaces with nonlinear optical spectroscopy. **J. Gibbs**
- 9:00 145.** Water at fluorite/water interface: Structure and vibrational spectroscopy from *ab initio* simulations. **M. Sulpizi**
- 9:30 146.** Second-order vibrational lineshapes from the air/water interface. **F. Geiger**
- 10:10** Intermission.
- 10:30 147.** Ion solvation at mineral-aqueous interfaces. **E. Borguet**
- 11:00 148.** Hydration revealed by DFT-MD simulations: From gas phase ionic clusters to mineral-water interfaces. **M.P. Gaigeot**
- 11:30 149.** Beyond linear dielectric hydration models. **R. Netz**

SECTION G

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 3

Physical Chemistry of the Atmosphere

Gas-Phase Chemistry

A. Asa-Awuku, M. Freedman, J. H. Kroll, *Organizers*,
Presiding

- 8:00 150.** Mapping urban emissions and chemistry. **R.C. Cohen**
- 8:25 151.** How to make sense of “missing” OH reactivity. **S. Kim**, A. Guenther, D. Sanchez, D. Jeong
- 8:50 152.** Acetonylperoxy and hydroperoxy kinetics from the perspective of the product hydroxyl radical. **K. Zuraski**, A.O. Hui, F.J. Grieman, M. Okumura, S.P. Sander
- 9:05 153.** Atmospheric autoxidation via fast peroxy radical hydrogen shift reactions. **H.G. Kjaergaard**, K. Moller, R.V. Otkjaer, P. Wennberg, J.D. Crouse, L. Xu, E.J. Praske, K. Bates

- 9:30 154.** Unimolecular chemistry of organic peroxy radicals in the atmosphere. **P. Wennberg**, L. Xu, J.D. Crouse, K. Moller, H. Kjaergaard
- 9:55** Intermission.
- 10:10 155.** Direct measurements of vinoxy radicals and formaldehyde from ozonolysis of *trans*- and *cis*-2-butenes: New insights into OH radical formation and secondary chemistry. **M. Campos-Pineda**, **J. Zhang**
- 10:25 156.** Probing isoprene photochemistry at atmospheric relevant nitric oxide levels. **X. Zhang**
- 10:50 157.** Reaction of limonene with HOCl and Cl₂ in the dark followed by particle formation under indoor irradiation conditions. **C. Wang**, D.B. Collins, J.P. Abbatt
- 11:05 158.** Chemistry of organic reduced nitrogen in a rural environment. **E.C. Browne**, H. Stark, A. Abdelhamid, J. Nowak, J. Smith, J.T. Jayne, D.R. Worsnop
- 11:30 159.** Power of combined experiments and theory for understanding atmospheric processes. **B.J. Finlayson Pitts**, R.B. Gerber

SECTION H

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 4

Molecular, Electronic, & Ionic Transport in Materials for Energy

Understanding Electrolytes: From Liquids to Solids

X. Roy, *Organizer*

L. A. Madsen, *Organizer, Presiding*

- 8:00 160.** Comparative capacitive study of room temperature imidazolium-based ionic liquids with differing cation chain lengths near a charged polycrystalline gold electrode. **N.R. Pitawela**, S.K. Shaw
- 8:20 161.** Polymeric ionic liquids for multivalent ion transport. **R.A. Segalman**, N. Michenfelder-Schauser, S. Jones
- 8:50 162.** Solid-state divalent ion conduction in ZnPS₃. **K.A. See**
- 9:20 163.** Intercalated cation disorder in Prussian blue analogues: First principles and grand canonical analyses. **S. Liu**, **K.C. Smith**
- 9:40** Intermission.
- 10:00 164.** When dynamics matters: Structure-matching alone is insufficient in the development of realistic force fields for nonaqueous electrolyte solutions. **Z. Li**, L. Robertson, J.S. Moore, Y. Zhang

- 10:20 165.** Designing polymer-based Li⁺ electrolytes with high conductivity and Li⁺ transference number. **B.D. McCloskey**
- 10:50 166.** Understanding the relationship between permittivity and ion conduction in polymer electrolyte materials. **R. Hickey, R. Colby, W. Mei, J. Rinehart, J. Bostwick**

Frontiers in Interdisciplinary Research: New Paradigms for Integration of Theory & Experiment

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Ice in Earth & Environmental Systems

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Advances in Fluorescence & Bioluminescence Imaging Probes

Sponsored by ANYL, Cosponsored by PHYS

Advances in Catalysis with Ceria & Other Reducible Oxides

Reactions of Ceria Catalysts

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

Future of Biomacromolecules at a Crossroads of Polymer Science & Biology

Synthetic Cells

Sponsored by POLY, Cosponsored by BIOL, CARB, CELL, COLL, ENVR, MEDI, PHYS and PMSE

MONDAY AFTERNOON – PHYS

SECTION A

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 13

Chemistry in Real Space & Time

TERS & SERS Experimental

V. A. Apkarian, V. Bommisetty, E. Potma, *Organizers*
J. Lee, *Presiding*

- 1:30 167.** STM-based single-molecule optical spectroscopy. **Z. Dong**
- 2:05 168.** Probing intermolecular and molecule-substrate interactions at angstrom scale by ultrahigh vacuum tip-enhanced Raman spectroscopy. **N. Jiang**
- 2:40 169.** Chemical and chemical reaction imaging at the solid-liquid interface via TERS. **A. Bhattarai, P.Z. El-Khoury**
- 3:00** Intermission.
- 3:20 170.** Aspects of high resolution TERS under ambient conditions. **V. Deckert, M. Richard-Lacroix**
- 3:55 171.** Back and forth ambient TERS nanoscopy and chemical reaction imaging. **P.Z. El-Khoury**
- 4:30 172.** Withdrawn
- 5:05 173.** Progress in surface- and tip-enhanced Raman spectroscopy experiments. **J. Lee**

SECTION B

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 12

Computational Quantum Chemistry: From Promise to Prominence: A Symposium in Honor of Henry F. Schaefer

Cosponsored by COMP

T. Crawford, P. R. Schreiner, D. D. Sherrill, E. F. Valeev, *Organizers*

K. B. Bravaya, *Presiding*

- 1:30 174.** Optimization of carbon dioxide reduction at functionalized semiconductor electrodes. **E.A. Carter**
- 2:00 175.** Theoretical design of energy materials: Electrocatalysts and perovskite solar cells. **K. Kim**
- 2:30 176.** Dynamical bonding driving new type of mixed valency, phase transitions, Raman anomalies, and more, in samarium hexaboride. **A. Alexandrova**
- 3:00 177.** Neutral excitation energies of crystalline solids from periodic equation-of-motion coupled-cluster theory. **X. Wang, T.C. Berkelbach**
- 3:15** Intermission.
- 3:40 178.** Coupled cluster methods in condensed phase chemistry. **G.K. Chan**
- 4:10 179.** Density matrix embedding theory with multi-reference solvers for extended systems. **L. Gagliardi**
- 4:40 180.** Minding the gap: Quantum studies of aromatic diradicals. **C.A. Parish**
- 4:55 181.** Density matrix renormalization group pair-density functional theory (DMRG-PDFT). **P. Sharma, V. Bernales, S. Knecht, D.G. Truhlar, L. Gagliardi**

SECTION C

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 11

Nanoscale & Molecular Assemblies: Designing Matter to Control Energy Transport

Cosponsored by INOR

Financially supported by Coherent

J. R. Caram, J. J. Foley, D. Hayes, *Organizers*

N. Korovina, *Presiding*

- 1:30** **182.** Plasmonic antenna-reactors and other nanoscale complexes for sensing and photocatalysis. **N.J. Halas**
- 2:10** **183.** Assessing possible mechanisms of micrometer scale electron transfer in heme free geobacter sulfurreducens pili. **X. Ru**, P. Zhang, D.N. Beratan
- 2:30** **184.** Multiple electron transfer from quantum dots to molecular electron acceptors. Y. Sun, H. Zhu, T. Mani, O. Chen, **J. Zhao**
- 3:10** Intermission.
- 3:25** **185.** Chromophore vibrations and energy transfers in photosynthetic complexes: Case studies with FMO and LH2. **Y.M. Rhee**
- 3:45** **186.** Applications of controlled energy transfer in quantum dot-molecule complexes: From sensing to catalysis. Y. Jiang, C. Rogers, **E.A. Weiss**
- 4:25** **187.** Elastic interfacial transistor enabled by superhydrophobic self-assembled nanowires on graphene. **T. Tian**, C. Sharma, N. Ahuja, M. Varga, R. Selvakumar, Y. Lee, Y. Chiu, C. Shih
- 4:45** **188.** Time-dependent electronic structure methods for plasmon-molecule interactions. **A.E. DePrince**

SECTION D

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 10

Water in the Universe

G. A. Blake, S. Ioppolo, *Organizers*

E. Bergin, *Presiding*

- 1:30** **189.** Chemistry on mantles of water ice surrounding interstellar dust particles. **E. Herbst**
- 2:10** **190.** Interactions and dynamics in interstellar ices. **H. Cuppen**
- 2:50** **191.** Structure and composition of interstellar ice: Linking observations to laboratory studies via IR spectroscopy. **J.A. Noble**
- 3:30** Intermission.
- 3:50** **192.** Combined laboratory and theoretical studies on the formation of alcohols in the H₂O-rich ice phase of prestellar cores. **D. Qasim**, G. Fedoseev, A. Lamberts, K. Chuang, J. He, J. Kästner, S. Ioppolo, H. Linnartz

- 4:30** **193.** Catalytic role of water ice in the formation of prebiotic molecules. **E. Congiu**, T. Nguyen, F. Dulieu

SECTION E

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 1

Getting to the Bottom: Optical & Electron Imaging of Reactive Chemical Systems

Observing Chemical Processes and Nanostructures In Situ at the Atomic Level

Cosponsored by ANYL

J. S. Biteen, J. Sambur, *Organizers*

E. Ringe, *Organizer, Presiding*

- 1:30** **194.** Imaging dynamic processes in liquids by scanning transmission electron microscopy (STEM). **N.D. Browning**, H. Amari, N. Johnson, D. Nicholls, J. Lee, A. Stevens, B.L. Mehdi
- 2:05** **195.** Growth mechanisms of metallic helical nanowires: Combined electron tomography and *in-situ* microscopy study. X. Song, A. Bruefach, P. Pelz, **M. Scott**
- 2:40** **196.** Nanoparticle mechanochemistry. **M.R. Jones**
- 3:15** Intermission.
- 3:35** **197.** Plasmonic metalattices probed by high energy resolution using STEM/EELS. **N. Alem**
- 4:10** **198.** Electron energy-loss spectroscopy for designing plasmonic catalysts. **R. Sharma**, W. Yang, C. Wang, A. Bruma

SECTION F

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 2

At the Interfaces of Experimental & Theoretical Nonlinear Optical Molecular Spectro-Imaging

Interface & Surface Sensitive Vibrational Spectroscopy and Theoretical Vibrational Spectroscopy

L. Wang, W. Xiong, *Organizers*

Y. Rao, *Presiding*

- 1:30** **199.** Beyond the Gouy-Chapman model with heterodyne-detected second harmonic generation. **F. Geiger**
- 2:00** **200.** Nonlinear interferometric detection of complex surfaces. **M.J. Shultz**, P.J. Bisson, J. Marmolejos, A.N. Carey, N.J. Anderson
- 2:30** **201.** Asymmetry of the interfacial water response to positive vs. negative electric field. **A.V. Benderskii**
- 3:00** Intermission.

- 3:10** **202.** Mott transition of interlayer excitons at 2D van der Waals heterojunctions. **X. Zhu**
- 3:40** **203.** Counterion effects on aqueous hydroxide mobility. T. Miller, **S. Corcelli**
- 4:10** **204.** Stories that are encoded in vibrational spectra: Obtaining insights into the spectroscopy of water from studies of ion-water complexes. **A.B. McCoy**, M.A. Boyer, R. Dirisio
- 4:40** **205.** Development of vibrational frequency maps for znucleobases. Y. Jiang, **L. Wang**
- 5:10** **206.** Chemical Structure, Dynamics, and Mechanisms-A: Updates and opportunities in the division of chemistry and the National Science Foundation. **C.A. Foss**

SECTION G

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 3

Physical Chemistry of the Atmosphere

Surface Chemistry & Ice

A. Asa-Awuku, M. Freedman, J. H. Kroll, *Organizers, Presiding*

- 1:30** **207.** Residential reservoir and reactor: Chemistry on indoor surfaces. **D.B. Collins**
- 1:55** **208.** Heterogeneous reaction kinetics of authentic biomass burning aerosol with nitrogen oxides under nocturnal conditions. **R.C. Sullivan**, L. Jahl, L. Goldberger, J.A. Thornton, B. Bowers, L. Jahn
- 2:20** **209.** Is the dielectric constant a macroscopic predictor of N_2O_5 reactivity at complex atmospheric interfaces?. **J.R. Gord**, S. Staudt, E. Rossich Molina, R. Gerber, G.M. Nathanson, T.H. Bertram
- 2:35** **210.** Impact of adsorption energies on gas-surface interactions and multiphase chemical kinetics. **D.A. Knopf**, M. Ammann, U. Pöschl, M. Shiraiwa
- 3:00** **211.** Reaction networks of peroxy radicals and Criegee intermediates and their role in governing the heterogeneous oxidation of organic aerosols. **K.R. Wilson**
- 3:25** Intermission.
- 3:40** **212.** Production of reactive oxygen species at the air: Water interface. **C. George**, N. Hayeck, S. Perrier
- 4:05** **213.** Elucidating how trace gases interact with ice surfaces. **J.D. Cyran**, E. Backus, M. van Zadel, M. Bonn
- 4:20** **214.** Using model metal oxide systems to study ice nucleation activity. **E. Chong**, M. King, Y. Li, M. Freedman
- 4:35** **215.** Heterogeneous ice nucleation by proteins. **V. Molinero**
- 5:00** **216.** Molecular insight on organic matter's atmospheric ice nucleating ability. **N. Borduas**, S. Bogler, K. Brennan, A. Miller

SECTION H

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 4

Molecular, Electronic, & Ionic Transport in Materials for Energy

Effects of Confinement on Ion & Molecular Transport

L. A. Madsen, *Organizer*
X. Roy, *Organizer, Presiding*

- 1:30** **217.** Macroscopic salt rejection through electrostatically gated nanoporous graphene. **T. Tian**, R. Wyss, K. Yazda, H. Park, C. Shih
- 1:50** **218.** Transport of nanoconfined ionic liquids: Molecular physics and applications. **R. Qiao**
- 2:20** **219.** Modeling ion conduction through block copolymers: Morphology, ion solvation, and correlated ion motion. **L.M. Hall**
- 2:50** **220.** Confinement effects on diffusion in nanostructured polymers. **L.A. Madsen**, R. Zhang, Y. Chen, A.G. Korovich, Y. Wang, D. Troya
- 3:20** Intermission.
- 3:40** **221.** Conical nanopores for efficient ion pumping and desalination. **Y. Zhang**, G.C. Schatz
- 4:00** **222.** Influence of framework flexibility of zeolitic imidazolate framework crystals on intracrystalline diffusion of guest molecules by high field NMR. **S. Vasenkov**
- 4:30** **223.** Confinement-entitled morphology and transport in charge-containing polymers. **M. Park**
- 5:00** **224.** Understanding and controlling proton transport for efficient fuel catalysis. A. Wuttig, B. Yan, J. Ryu, R. Bisbey, **Y. Surendranath**

Frontiers in Interdisciplinary Research: New Paradigms for Integration of Theory & Experiment

Sponsored by BIOL, Cosponsored by COMP, ORGN and PHYS

Nanotechnology & Single Cell Analysis in Biology & Medicine

Nanoscience

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

Water, Ice, & Clathrate Hydrate Geochemistry: Molecular Structures, Microscopic Properties, & Energetics

Sponsored by GEOC, Cosponsored by COLL and PHYS

Computational Methods for Lanthanides & Actinides: Theory & Applications

Sponsored by NUCL, Cosponsored by PHYS

Engaging Students in Physical Chemistry

Sponsored by CHED, Cosponsored by PHYS

Advances in Catalysis with Ceria & Other Reducible Oxides

Reactions and Other Metal Oxides

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

Advances in Fluorescence & Bioluminescence Imaging Probes

Sponsored by ANYL, Cosponsored by PHYS

Future of Biomacromolecules at a Crossroads of Polymer Science & Biology

Tissue Engineering

Sponsored by POLY, Cosponsored by BIOL, CARB, CELL, COLL, ENVR, MEDI, PHYS and PMSE

MONDAY EVENING – PHYS

SECTION A

San Diego Convention Center
TBD

Sci-Mix

A. B. McCoy, *Organizer*

8:05 - 10:05

410, 412, 413, 414, 415, 416, 417, 418, 419, 421, 423, 428, 429, 431, 432, 437, 438, 440, 441, 447, 448, 452, 455, 577. See Subsequent Listings.

TUESDAY MORNING – PHYS

SECTION A

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 13

Chemistry in Real Space & Time

Nanoscopy & Beyond

V. A. Apkarian, V. BommiSETTY, E. Potma, *Organizers*
H. Wickramasinghe, *Presiding*

- 8:00 225. Metasurface flat optics. **F. Capasso**
8:35 226. Force-detected nanoscale absorption spectroscopy in water at room temperature using an optical trap. A. Parobek, J. Black, M. Kamenetska, **Z. Ganim**

- 9:10 227. Nanoscale spectroscopic studies by using tip-enhanced force: Dipole and thermal. **J. Jahng**, E. Lee
9:30 228. Charge carrier dynamics in PbSe quantum-dot films studied by femtosecond pump-probe scattering scanning near-field optical microscopy. H. Maekawa, A. Abelson, M. Law, **N. Ge**
9:50 Intermission.
10:10 229. Quantum dissipation driven by electron transfer within a single molecule investigated by means of atomic force microscopy. **P. Jelinek**
10:45 230. Direct measurement of the photo-induced force for nanoscale imaging and spectroscopy at 10 nm spatial resolution. **X. Xu**, L. Wang
11:05 231. Frontiers in the atomistic modeling of single-molecule force-conductance spectroscopies. **I. Franco**
11:40 232. Microscopy based on measuring the optical trapping force between a scanning probe tip and sample. **H. Wickramasinghe**

SECTION B

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 12

Computational Quantum Chemistry: From Promise to Prominence: A Symposium in Honor of Henry F. Schaefer

Cosponsored by COMP
T. Crawford, P. R. Schreiner, D. D. Sherrill, E. F. Valeev, *Organizers*
N. Mayhall, *Presiding*

- 8:30 233. Physical concepts for chemical bonding. **K. Ruedenberg**
9:00 234. Fascinating world of silicon chemistry: Tribute to H.F. Schaefer's pioneering contributions. **Y. Apeloig**
9:30 235. Travelling in valence space. **G. Frenking**
10:00 236. Construction of reaction networks using the *ab initio* nanoreaction coupled to a kinetic model. **J. Meisner**, X. Zhu, K. Thompson, H. Hirai, T.J. Martinez
10:15 Intermission.
10:40 237. Modeling the behavior of strongly correlated electrons. **P. Gill**
11:10 238. Learning (from/about) the ground-state electron density. **C. Corminboeuf**, M. Ceriotti, A. Fabrizio, A. Grisafi, B. Meyer, D. Wilkins
11:40 239. SCGVB-based multiconfiguration description of molecules. **T.H. Dunning**, L.T. Xu

SECTION C

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 11

Nanoscale & Molecular Assemblies: Designing Matter to Control Energy Transport

Cosponsored by INOR

Financially supported by Coherent

J. R. Caram, J. J. Foley, *Organizers*

D. Hayes, *Organizer, Presiding*

- 8:10** **240.** Using STEM/EELS to image energy transfer processes in plasmonic nanostructures: Nanodimers spanning the gap between weak and strong coupling. **J.P. Camden**, D.J. Masiello, J. Idrobo, P. Rack
- 8:30** **241.** Stark control of electrons at interfaces. **I. Franco**
- 9:10** **242.** Functional ligands for improved nanocrystal energy transport. M.S. Azzaro, A.K. Le, **S.T. Roberts**
- 9:30** **243.** Towards all-optical chiral resolution and few-molecule circular dichroism spectroscopy with dielectric metasurfaces. **J. Dionne**, M. Solomon, J. Hu, J.M. Abendroth, M. Lawrence, L. Poulikakos
- 10:10** **244.** Nonadiabatic molecular dynamics in extended systems: Toward nanoscale materials. **A.V. Akimov**
- 10:30** Intermission.
- 10:45** **245.** 3D periodic subphthalocyanine-based covalent organic framework for high-efficiency crystalline organic photovoltaics. J. Cox, **S.A. Lopez**
- 11:25** **246.** Exploring size dependency of hot carrier generation through interband and intraband transitions in gold nanorods. **B. Ostovar**, Y. Cai, A. Ahmadvand, R. Zhang, L.J. Tauzin, P.J. Nordlander, S. Link
- 11:45** **247.** Computationally aided design of copper-based two-dimensional composites as alternative, active carbon dioxide reduction catalysts. **Z. Lin**, K. Jiang, A.J. Garza, A.T. Bell, M.P. Head-Gordon

SECTION D

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 10

Hydration from the Gas to the Condensed Phase Ion Hydration

E. Backus, M. Bonn, F. Paesani, *Organizers*

B. P. Fingerhut, *Presiding*

- 8:00** **248.** Echoes in 2D-Raman-THz spectroscopy of water. A. Shalit, D. Sidler, R. Ciardi, A. Berger, **P. Hamm**
- 8:30** **249.** Inhomogeneity of the intermolecular terahertz modes in aqueous salt solutions. L. Vietze, M. Bonn, **M. Grechko**

- 9:00** **250.** Towards single shot multidimensional terahertz spectroscopy of hydrogen-bonded liquids. **G. Mead**, H. Lin, G.A. Blake
- 9:20** **251.** Probing liquid water and aqueous solution with two-color high-harmonic and X-ray spectroscopy. **Z. Yin**, T. Luu, S. Thürmer, S. Malerz, M. Pohl, E. Chatzigeorgiou, Y. Cui, K. Yamazoe, J. Miyawaki, T. Tokushima, C. Sathe, J. Grasjö, Y. Harada, B. Winter, J. Rubensson, H. Wörner
- 9:40** Intermission.
- 10:10** **252.** Hydration and ion pairing at surfaces. **H.C. Allen**
- 10:40** **253.** Ions at hydrophobic interfaces. **Y. Levin**
- 11:10** **254.** Closer look at salt dissolution: Microhydration of LiX_2^- ($X = \text{Cl}^-, \text{I}^-$) studied by cryogenic ion trap vibrational spectroscopy. **A. Chakraborty**, S. Schmahl, T. Brumme, J. Dahme, C. Baldauf, **K.R. Asmis**
- 11:30** **255.** Using quantum simulation of ion hydration to predict electrolyte solution properties. **T.T. Duignan**, M.D. Baer, C. Mundy, G.K. Schenter, X. Zhao

SECTION E

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 1

Getting to the Bottom: Optical & Electron Imaging of Reactive Chemical Systems

Spectroscopy of Reactive Chemical Systems

Cosponsored by ANYL

J. S. Biteen, E. Ringe, *Organizers*

J. Sambur, *Organizer, Presiding*

- 8:30** **256.** *In situ* transient reflectance probe of water reduction/oxidation kinetics at semiconductor photoelectrode/liquid interface. **T. Lian**
- 9:00** **257.** Ultrafast and nanoscale Raman probes of plasmonic photocatalysis and organic photovoltaics. **R.R. Frontiera**
- 9:30** **258.** Stimulated Raman excited fluorescence spectroscopy and imaging. **W. Min**
- 10:00** Intermission.
- 10:15** **259.** Resolving chemical bond dynamics at an electrode surface by time-resolved optical and vibrational spectroscopy. **T. Cuk**
- 10:45** **260.** Electron dynamics at metal oxide surfaces and interfaces. **T. Hamann**
- 11:15** **261.** Visualizing electrolyte-free electrochemical intercalation. **M.S. Stark**, H. Kim, J. Cheng, K.L. Kuntz, S.C. Warren
- 11:35** **262.** Building functional organic/inorganic interfaces for triplet energy transfer. E. Raulerson, J.A. Bender, D.E. Cotton, A.P. Moon, A.K. Le, **S.T. Roberts**

SECTION F

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 2

At the Interfaces of Experimental & Theoretical Nonlinear Optical Molecular Spectro-Imaging

Interface & Surface Sensitive Vibrational Spectroscopy

L. Wang, W. Xiong, *Organizers*
J. Atkin, *Presiding*

- 8:30** 263. Charge dynamics at surfaces and interfaces with the development of time-resolved electronic sum frequency generation. G. Deng, Y. Qian, **Y. Rao**
- 9:00** 264. Theoretical description of the polarization dependence of vibrational sum frequency generation spectroscopy at the water/vapor interface. **P.B. Moore**, B. Space
- 9:20** 265. Monitoring charge localization at organic thin film interfaces by interferometric vibrational sum frequency generation. **A.M. Massari**
- 9:50** Intermission.
- 10:10** 266. Protein characterizations by chiral vibrational sum frequency generation spectroscopy. **E.C. Yan**
- 10:40** 267. Molecular structures of polymer and biological molecules at buried interfaces studied by sum frequency generation vibrational spectroscopy. **Z. Chen**
- 11:10** 268. *In situ* vibration sum frequency generation spectroscopic probe of molecular structures and dynamics at electrochemical interfaces. **T. Lian**

SECTION G

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 3

Physical Chemistry of the Atmosphere

Multiphase Chemistry

A. Asa-Awuku, M. Freedman, J. H. Kroll, *Organizers*,
Presiding

- 8:00** 269. Reactive uptake of amines and ammonia by secondary organic aerosols. **S.A. Nizkorodov**, J. Montoya-Aguilera, N. Smith, L.M. Wingen, J. Horne, S. Zhu, D. Dabdub, J. Laskin, A. Laskin, P. Lin
- 8:25** 270. Effects of gas-phase methylamine and cloud processing on aerosol chemistry, water uptake, viscosity, and optical properties. **D.O. Dehaan**, A. Pajunoja, L.N. Hawkins, M. Riva, J. Surratt, J. Doussin
- 8:50** 271. Quantifying pyrazine-based products in cloud water mimics containing ammonium sulfate and methylglyoxal: Effects of evaporation and pH on product formation. **L. Hawkins**, S.J. Jones, L.R. Mazzoleni, S.K. Schum, M. Khaksari

- 9:15** 272. Simulated atmospheric processing and iron mobilization of combustion particles: Effects of acid media and solar flux. **J.G. Navea**, K. Deborah, Y. Xiao, R. Karchere-Sun, E. Richmond
- 9:30** 273. Relationships between aerosol acidity, organic acids, and water-soluble metals in fine particulate matter. **J. Murphy**, Y. Tao
- 9:55** Intermission.
- 10:10** 274. Turning over a new leaf on IEPOX SOA formation. **V.F. McNeill**, A. Fankhauser
- 10:35** 275. New insights into physical chemistry on cloud/aerosol water surfaces. **C. Zhu**, L. Li, X.C. Zeng, J.S. Francisco
- 10:50** 276. *In-situ* surface tension measurements of hanging droplet methylglyoxal/ammonium-sulfate aerosol mimics under photooxidative conditions. **J. Woo**, T. Beier
- 11:05** 277. Photolysis of secondary organic aerosol: Chromophore photobleaching and chemical transformations over extended timescales. **R. O'Brien**, E. Walhout, H. Yu, C. Thrasher, J. Shusterman, J.H. Kroll
- 11:30** 278. Multiphase photochemistry relevant to marine environments and sea spray aerosol. **V.H. Grassian**

SECTION H

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 4

Molecular, Electronic, & Ionic Transport in Materials for Energy

Transport in Optoelectronic Materials

L. A. Madsen, *Organizer*
X. Roy, *Organizer, Presiding*

- 8:30** 279. Synthesis of nitrile-functionalized ladder-type oligo(*p*-phenylene)s for probing electron delocalization. **J. Yan**, T. Mani, J.R. Miller
- 8:50** 280. Twistacenes, helicenes, and macrocycles as optoelectronic materials. **C.P. Nuckolls**
- 9:20** 281. Halide perovskites and the halogens. A. Slavney, N.R. Wolf, A. Saldivar Valdes, H. **Karunadasa**
- 9:50** 282. Towards artificial light-harvesting organelle mimics: Exciton dynamics in conjugated polyelectrolyte complex coacervates. **A. Johnston**, A. Ayzner
- 10:10** Intermission.
- 10:30** 283. Electronic coupling and dissipative transport in non-covalent inorganic nanoscale assemblies. X. Lan, E.M. Janke, M. Chen, M.H. Hudson, P. Guyot-Sionnest, **D.V. Talapin**

- 11:00** **284.** Synthetic versatility of colloidal magnetic nanoparticles as a tool for understanding and control of nanocomposite magnetotransport. **J.D. Rinehart**, B. Zhou
- 11:30** **285.** Intriguing case of excited state intramolecular charge transfer: T- and V-shaped molecules with pyridoquinoxaline acceptor. **B. Sk**, S. Khodia, S. Sharma, A. Patra
- 11:50** **286.** Engineering a redox-active proton wire with proton-coupled electron transfer. **J.J. Goings**, E. Odella, B.L. Wadsworth, S. Mora, M.T. Huynh, J.D. Gust, T. Moore, G.F. Moore, S. Hammes-Schiffer, A.L. Moore

Computational Methods for Lanthanides & Actinides: Theory & Applications

Sponsored by NUCL, Cosponsored by PHYS

ACS Award in Pure Chemistry: Symposium in Honor of Danna Freedman

Sponsored by INOR, Cosponsored by PHYS

Water, Ice, & Clathrate Hydrate Geochemistry: Molecular Structures, Microscopic Properties, & Energetics

Sponsored by GEOC, Cosponsored by COLL and PHYS

Future Insights into Syngas Conversion Catalysis: Symposium in honor of Burtron H. Davis

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

Advances in Catalysis with Ceria & Other Reducible Oxides

Reactions and Other Metal Oxides

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

TUESDAY AFTERNOON – PHYS

SECTION A

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 13

PHYS Division Awards

A. B. McCoy, *Organizer, Presiding*

- 1:30** **287.** Role of topological phases in quantum molecular dynamics. **A.F. Izmaylov**

- 2:00** **288.** Predicting properties, learning design rules, and accelerating discovery in inorganic chemistry with computational chemistry. **H.J. Kulik**
- 2:30** **289.** Ultrafast IR spectroscopy for molecular vibrational polaritons and self-assembled materials. **W. Xiong**
- 3:00** Intermission.
- 3:15** **290.** ‘Clean’ carbon: Old material, new surface. **H. Liu**
- 3:45** **291.** Ultrafast functional motions in proteins: Single-molecule FRET perspective. **G. Haran**
- 4:15** **292.** Markov state modeling: State of the art and future prospects. **F. Noe**
- 4:45** **293.** Accurate quantum chemical methods for excited electronic states and transition-metal compounds. **L. Gagliardi**

Future Insights into Syngas Conversion Catalysis: Symposium in honor of Burtron H. Davis

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

TUESDAY EVENING – PHYS

Future of Biomacromolecules at a Crossroads of Polymer Science & Biology

Sponsored by POLY, Cosponsored by BIOL, CARB, CELL, COLL, ENVR, MEDI, PHYS and PMSE

Water in the Solid State: Reactions & Interactions with Impurities

Sponsored by ENVR, Cosponsored by PHYS

WEDNESDAY MORNING – PHYS

SECTION A

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 13

Chemistry in Real Space & Time Cavity Optomechanics & Conductive Junctions

V. BommiSETTY, E. Potma, *Organizers*
V. A. Apkarian, *Organizer, Presiding*

- 8:00** **294.** Addressing atomically resolved molecular spectroscopy in plasmonic cavities. **J. Aizpurua**

- 8:35 295. Effect of Stokes shift on strongly coupled hybrid states between organic molecules and confined light. S. Baieva, S. Pikker, E. Hulkko, T. Heikkilä, G. Groenhof, **J. Toppari**
- 9:10 296. Vibrational polariton chemistry. **J. Yuen Zhou**
- 9:45 297. Single-molecule interfacial electron transfer dynamics. **H. Lu**
- 10:20 Intermission.
- 10:35 298. Plasmon controlled quantum transport in nano-scale junctions. **Y. Selzer**
- 11:10 299. Green function methods for optoelectronics and molecular dynamics. **M. Galperin**
- 11:45 300. Spectromicroscopy in the atomistic near-field. **V.A. Apkarian**

SECTION B

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 12

Computational Quantum Chemistry: From Promise to Prominence: A Symposium in Honor of Henry F. Schaefer

Cosponsored by COMP

T. Crawford, P. R. Schreiner, D. D. Sherrill, E. F. Valeev,
Organizers

L. Slipchenko, Presiding

- 8:30 301. Quantum chemistry for strong correlation. **G.E. Scuseria**
- 9:00 302. Multireference perturbation theory for metastable electronic states. **K.B. Bravaya**
- 9:30 303. Multireference configuration interaction beyond singles and doubles. **M.R. Hoffmann**
- 10:00 304. Turning multiconfigurational methods into “black-box” routines for an accurate description of strongly correlated enzymatic systems. **E. Sayfutyarova**
- 10:15 Intermission.
- 10:40 305. Uniform theoretical framework for bound and metastable excited states. **A. Krylov**
- 11:10 306. Multi-reference algebraic diagrammatic construction theory for excited states and spectroscopy. **A. Sokolov**
- 11:40 307. Quantum chemistry with excited state variational principles. **E. Neuscamman**

SECTION C

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 11

Nanoscale & Molecular Assemblies: Designing Matter to Control Energy Transport

Cosponsored by INOR

Financially supported by Coherent

J. R. Caram, J. J. Foley, D. Hayes, *Organizers*

Z. Lin, *Presiding*

- 8:00 308. Photophysical detective story: Forbidden emission and photobrightening in self-assembled organic nanoparticles. **R.H. Goldsmith**
- 8:40 309. Active binary control of the thermal near field via plasmon hybridization. **S. Hosseini Jebeli**, U. Bhattacharjee, S. Link, K.A. Willets, D.J. Masiello, C. West, H.J. Goldwyn, E. Beutler
- 9:00 310. NIR-to-visible upconversion sensitized by lead halide perovskite thin films. S. Wieghold, A. Bieber, Z. VanOrman, J. Correa-Baena, **L. Nienhaus**
- 9:40 311. Computational study of surface and bulk excited states on quantum dots. **A.R. Mclsaac**, T.G. Goldzak, T.A. Van Voorhis
- 10:00 Intermission.
- 10:15 312. Spatial and spectral mapping of a random nanoscale lasing media with sub-micron resolution. **K. Appavoo**
- 10:55 313. Effects of transition dipole moment coupling on endothermic singlet fission in perylene oligomers. **N. Korovina**, J. Johnson
- 11:15 314. Self-organization of electrostatically and sterically stabilized colloidal nanocrystals: Roles of topology, image charges, and non-classical nucleation. E.M. Janke, I. Coropceanu, M.A. Boles, **D.V. Talapin**

SECTION D

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 10

Hydration from the Gas to the Condensed Phase

Electronic Structure & Hydration

Financially supported by Elsevier

E. Backus, M. Bonn, F. Paesani, *Organizers*

H. C. Allen, *Presiding*

- 8:30 315. Structure, dynamics, and vibrational SFG spectroscopy of water at electrified graphene interfaces. Y. Zhang, G. Stirnemann, H. B. de Aguiar, J.T. Hynes, **D. Laage**
- 9:00 316. Bonding structure of electrically gated oxide/water interfaces. **W. Liu**
- 9:30 317. Water on semiconducting and insulating surfaces: Structural and electronic properties from first principles. **G.A. Galli**
- 10:00 Intermission.
- 10:30 318. Aqueous-phase energetics and electronic properties of redox reactants in solution: Study of the permanganate/manganate redox pair using liquid jet photoelectron spectroscopy. **K. Mudryk**, R. Seidel, B. Winter, I. Wilkinson
- 10:50 319. Experimental measurements of the impact of solvation on the electronic structure of organic molecules in solution. **J.C. Hemminger**, J.P. Bruce, R.P. Galhenage

11:10 320. Withdrawn

SECTION E

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 1

Water in the Universe

G. A. Blake, S. Ioppolo, *Organizers*

S. L. Widicus Weaver, *Presiding*

- 8:30 321. GOTHAM and ARKHAM: First results from programs to explore aromatic chemistry at the earliest stages of star formation. **B. McGuire**
- 9:05 322. Constraining the formation of interstellar methanol using isotopologues. **O. Wilkins**, B. Carroll, G.A. Blake
- 9:25 323. Quantum chemical perspective of biomolecule synthesis via UV-irradiation of their precursors in astrophysical ices. **P. Bera**
- 9:45 324. Producing accurate theoretical anharmonic infrared cascade spectra of PAHs. **C.J. Mackie**, A. Candian, X. Huang, E. Maltseva, A. Petrigiani, T. Chen, J. Oomens, W. Buma, T.J. Lee, A.G. Tielens
- 10:20 Intermission.
- 10:40 325. Theoretical study of the formation of glycolonitrile on icy grain mantles from the reaction of C⁺ and HCN. **D.E. Woon**
- 11:15 326. Vacuum ultraviolet photodissociation of CS. Z. Xu, Y.C. Chang, C. Ng, W.M. Jackson, S.R. Federman, L. Wang, **K.N. Crabtree**
- 11:50 327. Synthesis of alkylphosphonic acids in interstellar analogue ices of phosphine and water. **A.M. Turner**, M. Abplanalp, C. Meinert, R. Kaiser

SECTION F

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 2

At the Interfaces of Experimental & Theoretical Nonlinear Optical Molecular Spectro-Imaging

Theoretical Electronic Spectroscopy

W. Xiong, *Organizer*

L. Wang, *Organizer, Presiding*

- 8:30 328. Atomistic modeling of electronic spectroscopy for organic chromophores in aqueous solutions. T.J. Zuehlsdorff, H. Hong, J. Wilmer, **L. Shi**, C. Isborn
- 9:00 329. Ultrafast nonlinear X-ray spectroscopy and quantum imaging of molecules. **S. Mukamel**, D. Cho, K. Dorfman, S. Rahav
- 9:30 330. Characterising spectral lineshapes in water-solvated adenine from first-principles. **J. Segarra-Martí**, F. Segatta, T.A. Mackenzie, A. Nenov, I. Rivalta, M. Garavelli, M. Bearpark
- 9:50 Intermission.

- 10:10 331. Computing nonlinear vibrational, vibronic, and vibrational-vibronic spectra from classical trajectories. **R.F. Loring**, K. Polley
- 10:40 332. Fluorescence-detected two-dimensional electronic spectroscopy of multichromophoric systems. **T.C. Jansen**
- 11:10 333. On the structure and dynamics of the hydrated excess proton in acetonitrile. A.P. Seitsonen, R. Vuilleumier, W.H. Thompson, **D. Laage**

SECTION G

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 3

Physical Chemistry of the Atmosphere

Organic Aerosol

A. Asa-Awuku, M. Freedman, J. H. Kroll, *Organizers*,
Presiding

- 8:00 334. Consideration of a carbon number-polarity grid based approach for defining lumped surrogates in secondary organic aerosol modeling. **K. Barsanti**, A. Carlton, I. Afreh, J. Jiang, C. Wiedinmyer
- 8:25 335. Sources of secondary aerosol species in a highly polluted urban environment: Insights from online composition measurements for PM₁ and PM_{2.5}. **Q. Chen**, Y. Zheng, Y. Li, X. Cheng, Y. Liu, T. Zhu, J.T. Jayne, D.R. Worsnop
- 8:50 336. Chemical composition and viscosity of SOA formed by VOCs emitted from healthy and stressed pine trees. **N. Smith**, Y. Huang, A. Hettiyadura, C.L. Faiola, A. Laskin, A.K. Bertram, M. Shiraiwa, S.A. Nizkorodov
- 9:05 337. Mechanism of the nitrate oxidation of -pinene under simulated ambient conditions. **T.B. Nguyen**, G. Burke, Y. Li
- 9:30 338. Aerosol formation from NO₃ + isoprene: Field and laboratory studies on mechanism and yields. **J.L. Fry**
- 9:55 Intermission.
- 10:10 339. Chemical composition of sub-20 nm particles formed from the reaction of methanesulfonic acid with methylamine. **V. Perraud**, X. Li, J. Smith, B.J. Finlayson Pitts
- 10:25 340. Advancing our understanding of ocean biology impacts on atmospheric chemistry, clouds, and climate. **K.A. Prather**
- 10:50 341. Gel formation from low molecular-mass organic gelators in model marine aerosols: Synergistic role of water, organic, and inorganic components. **R.D. Davis**, D. Richards, K. Trobaugh
- 11:05 342. Role of water in nanoparticle growth by monoterpene ozonolysis. **M.V. Johnston**

- 11:30 343.** It's the water: Exploring the impacts of water vapor on new particle formation mechanisms. **J. Smith**, S. Chee, N. Myllys, X. Li, J. Jiang

SECTION H

Marriott Marquis San Diego Marina

Marriott Grand Ballroom Section 4

Molecular, Electronic, & Ionic Transport in Materials for Energy

Transport in Battery & Solar Materials

L. A. Madsen, *Organizer*

X. Roy, *Organizer, Presiding*

- 8:00 344.** Reevaluation of thermal stability of Ni-rich oxide cathode $\text{LiNi}_{0.8}\text{Co}_{0.1}\text{Mn}_{0.1}\text{O}_2$. **C. Yan**, X. Yang, J. Shan, H. Zhao, G. Ma, Y. Ju
- 8:20 345.** Electronic transport in Fe and Co chalcogenides prepared from intercalation chemistry. B. Wilfong, H. Zheng, **E.E. Rodriguez**
- 8:50 346.** Battery diagnostics with inside-out MRI. **A. Jerschow**
- 9:20 347.** Using nanoporous and nanostructured materials to improve ion diffusion for fast charging battery and pseudocapacitor applications. **S.H. Tolbert**
- 9:50** Intermission.
- 10:20 348.** Proton intercalation/deintercalation chemistry on H_xWO_3 photoelectrodes for oxygen evolution. **B.M. Bartlett**
- 10:50 349.** Element-specific measurement of hole transport and kinetics in a Ni-TiO₂-Si photoelectrode using transient extreme ultraviolet spectroscopy. **S.K. Cushing**
- 11:20 350.** Structure and dopant engineering in PEDOT thin films for the development of all-polymeric transparent heaters and thermoelectric applications. **A. Carella**, M.N. Gueye, A. Schultheiss, R. Demadrille, J.P. Simonato
- 11:40 351.** Understanding the structure-conductivity relationship of P3HT doped with redox-tuneable dodecaborane clusters. **K. Winchell**, T. Aubry, V. Basile, B.J. Schwartz, S.H. Tolbert

Future Insights into Syngas Conversion Catalysis: Symposium in honor of Burtron H. Davis

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

Future of Biomacromolecules at a Crossroads of Polymer Science & Biology

Delivery Systems

Sponsored by POLY, Cosponsored by BIOL, CARB, CELL, COLL, ENVR, MEDI, PHYS and PMSE

Understanding the Role of Water in Solid Acid-Base Catalysis

Sponsored by CATL, Cosponsored by ENFL, INOR and PHYS

Interface between Experiments & Modeling in Unraveling the Physical & Chemical Properties of Charged Droplets

Sponsored by ANYL, Cosponsored by COMP, ORGN and PHYS

WEDNESDAY AFTERNOON – PHYS

SECTION A

Marriott Marquis San Diego Marina

Marriott Grand Ballroom Section 13

Chemistry in Real Space & Time

Plasmon Driven Chemistry

V. A. Apkarian, V. Bommisetty, E. Potma, *Organizers*

M. Law, *Presiding*

- 1:30 352.** Plasmon-mediated surface chemistry. **W. Wei**
- 2:05 353.** Directly observing plasmon-driven oxidation of ferrocyanide using SERS: Towards a model system for plasmonic reactions. **Y. Qi**, V. Brasiliense, T. Ueltschi, J. Park, R.P. Van Duyne
- 2:25 354.** SERS tags for intracellular monitoring of viral evolution in individual intact cells. K. Dardir, H. Wang, **L. Fabris**
- 3:00 355.** Reversible aggregation of covalently cross-linked gold nanocrystals by linker oxidation. **M. Law**, Z. Luan, A. Abelson
- 3:20** Intermission.
- 3:40 356.** Energy and charge flow in the multi-component plasmonic materials: Opportunities, challenges, and unresolved questions. **S. Linic**
- 4:15 357.** Withdrawn
- 4:50 358.** Light-induced self-assembly of plasmonic nanoparticles. **Z. Yan**

SECTION B

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 12

Computational Quantum Chemistry: From Promise to Prominence: A Symposium in Honor of Henry F. Schaefer

Cosponsored by COMP

T. Crawford, P. R. Schreiner, D. D. Sherrill, E. F. Valeev,

Organizers

C. Corminboeuf, *Presiding*

- 1:30 359. Electronic structure theory in the exascale era. **M.S. Gordon**
- 2:00 360. Free-complement theory and chemical-formula theory leading to the solutions of Schrödinger equation. **H. Nakatsuji**
- 2:30 361. Many-body expanded full configuration interaction. **J. Gauss**, J.J. Eriksen
- 3:00 362. Quantum chemistry at the edge of exact correlation energies. **P.M. Zimmerman**
- 3:15 Intermission.
- 3:40 363. Challenges of using quantum computers for quantum chemistry. **J.E. Rice**
- 4:10 364. Classical and quantum approaches to strong electron correlation. **F.A. Evangelista**
- 4:40 365. ADAPT-VQE: Quasi-optimally compact wavefunctions for simulating molecules on a quantum computer. H. Grimsley, S. Economou, E. Barnes, **N. Mayhall**

SECTION C

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 11

Nanoscale & Molecular Assemblies: Designing Matter to Control Energy Transport

Cosponsored by INOR

Financially supported by Coherent

J. R. Caram, J. J. Foley, D. Hayes, *Organizers*

L. Nienhaus, *Presiding*

- 1:30 366. Direct imaging of exciton transport in molecular aggregates by ultrafast microscopy. **L. Huang**
- 2:10 367. From inverse design to implementation of practical photonics. **J. Vuckovic**
- 2:50 368. Nanoparticle patterning via chemical lift-off lithography. **N. Chiang**, L. Scarabelli, G.A. Vinnacombe, T.D. Young, P.S. Weiss, S.J. Jonas
- 3:10 Intermission.
- 3:25 369. Understanding and controlling white-light emission from halide perovskites. M.D. Smith, B. Connor, E. Crace, K. Lindquist, **H. Karunadasa**
- 4:05 370. Visualizing chemical dynamics to control energy transfer. **M.A. Allodi**

- 4:25 371. Terahertz quantum beats and nano-imaging of metal halide perovskites. **J. Wang**

SECTION D

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 10

Hydration from the Gas to the Condensed Phase

Financially supported by Newport Spectra-Physics

E. Backus, M. Bonn, F. Paesani, *Organizers*

D. Laage, *Presiding*

- 1:30 372. Quantum tunnelling and the geometric-phase effect in molecules and the condensed phase. **J.O. Richardson**
- 2:00 373. Modeling hydration, one water molecule at a time: Towards realistic computer simulations through many-body representations and data-driven algorithm. **M. Riera Riembau**, P. Bajaj, C. Egan, B. Bizzarro, F. Paesani
- 2:20 374. Ultrafast 2DIR spectroscopy from gas to liquid phase: *J*-scrambling, rovibrational relaxation, and the onset of liquid character. **M.C. Rotondaro**, G. Ng Pack, P.P. Shah, A. Mandal, S. Erramilli, L.D. Ziegler
- 2:40 375. Fully polarizable embedding model for molecular spectroscopy of aqueous solutions. **C. Cappelli**
- 3:00 Intermission.
- 3:30 376. Soft X-ray spectroscopy of hydrogen-bonded molecular systems in protic and aprotic solvents. **M. Ekimova**, C. Kleine, J. Ludwig, M. Ochmann, M. Kubin, N. Huse, P. Wernet, M. Odelius, **E. Nibbering**
- 3:50 377. H-bond details and dynamics via artificial and intrinsic IR and Raman probes. **C.H. Londergan**, N.R. John, C. Fu
- 4:10 378. Aggregation of methane molecules in water. **O. Akin-Ojo**, K. Szalewicz
- 4:30 379. Effect of crowding on hydrophobic crossover. **A. Bredt**, P. Wise, D. Ben-Amotz

SECTION E

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 1

Water in the Universe

G. A. Blake, S. Ioppolo, *Organizers*

R. C. Fortenberry, *Presiding*

- 1:30 380. Interstellar water and organic molecules in protoplanetary disks. **C. Favre**
- 2:10 381. Does the early planetesimal get the water?. **M. McClure**, C. Dominik
- 2:50 382. Water in planet formation: What do we know and what do we want to know?. **E. Bergin**
- 3:30 Intermission.

- 3:50 **383.** Molecular snow lines in protoplanetary disks. **G.A. Blake**, D. Anderson, E. Bergin
- 4:10 **384.** Importance of zero-point energy for crystalline ice phases: Comparison of force fields and density functional theory. **J. Meyer**
- 4:45 **385.** Water-ice: Quest to understand its physical forms and chemical processes. **M.S. Gudipati**

SECTION F

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 2

At the Interfaces of Experimental & Theoretical Nonlinear Optical Molecular Spectro-Imaging Coherent 2D Spectroscopy

L. Wang, W. Xiong, *Organizers*
L. Shi, *Presiding*

- 1:30 **386.** Water dynamics at the molecular interfaces. **W. Zhuang**
- 2:00 **387.** Direct observation of proton hopping in water/HCl solutions by 2D IR spectroscopy and *ab initio* simulations. **M.D. Fayer**, R. Yuan, J. Napoli, T. Markland
- 2:30 **388.** Site-specific interrogation of protein structure and dynamics via 1D and 2D IR spectroscopies. **F. Gai**
- 3:00 Intermission.
- 3:20 **389.** Residue-specific characterization of protein dynamics in molecular recognition via 2D IR spectroscopy. **M.C. Thielges**
- 3:50 **390.** Ultrafast IR spectroscopic investigation on molecular vibrational polaritons. **B. Xiang**, R. Florentino Ribeiro, A. D. Dunkelberger, J. Wang, Y. Li, B. Simpkins, J. Owrutsky, J. Yuen-Zhou, W. Xiong
- 4:10 **391.** Mapping structure and dynamics with site-specific vibrational probe pairs via 2D IR. **M.J. Tucker**

SECTION G

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 3

Physical Chemistry of the Atmosphere

Water & Phase State

A. Asa-Awuku, M. Freedman, J. H. Kroll, *Organizers*,
Presiding

- 1:30 **392.** Impact of particle phase state on multiphase processes of secondary organic aerosols. **M. Shiraiwa**
- 1:55 **393.** Modification of aerosol phase, acidity, and structure by heterogeneous and multiphase chemistry. **A.P. Ault**, N.E. Olson, Z. Lei, Y. Chen, Y. Zhang, J. Surratt

- 2:20 **394.** Diffusion of organics in sucrose-water solutions as a function of temperature: Measurements and atmospheric relevance. **K.J. Kiland**, A. Maclean, S. Kamal, A.K. Bertram
- 2:35 **395.** Surface tension measurements of aqueous organic and inorganic aerosol particles. **T. Preston**
- 3:00 **396.** Aerosol phase, age, and liquid water: Recent analyses from field and laboratory studies of terrestrial and marine aerosol systems. **J.H. Slade**, A.P. Ault, V.H. Grassian, K.A. Prather, P.B. Shepson, P. Tumminello
- 3:25 Intermission.
- 3:40 **397.** Impact of shape on optical properties: Study of mineral dust. **M.E. Greenslade**, J. Morang, T. Galpin
- 3:55 **398.** Cloud activation potentials for atmospheric α -pinene and β -caryophyllene ozonolysis products. **F. Geiger**, A. Be, D. Liu, A. Bellcross
- 4:10 **399.** Frenkel Halsey and Hill activation theory: Toward closure between cloud condensation nuclei activity and water adsorption. **C.D. Hatch**, P.R. Tumminello, M. Cassingham, A.L. Greenaway, R. Parham, K. Morris, C. Botner, O. Eddings
- 4:35 **400.** Modeling water uptake and cloud droplet formation potential of multiphase aerosols. **A. Zuend**, K. Gorkowski
- 5:00 **401.** Going through a phase: Particulate water in atmospheric aerosol. **M. Tolbert**, R.D. Davis, S. Ushijima

SECTION H

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 4

Recent Developments in Biomaterials

A. Alexander-Katz, L. Yang, *Organizers*
T. Xu, *Organizer, Presiding*

- 1:30 **402.** Design of functional protein membranes. **M. Olvera De La Cruz**
- 2:05 **403.** Design of redox-active antibacterial peptide hydrogels to prevent implant-related infections. **J.P. Schneider**
- 2:40 **404.** Multiscale modeling framework with the 3D-RISM-KH molecular solvation theory for supramolecular structures, nanomaterials, and biomolecules: Where are we going?. **A. Kovalenko**
- 3:00 Intermission.
- 3:20 **405.** Supramolecular dynamics and bioactivity of biomaterials. **S.I. Stupp**
- 3:55 **406.** Ionic liquids as potential drug delivery and drug formulation biomaterials: Studies of membrane permeability and cytotoxicity. G.A. Caputo, B. Carone, **T.D. Vaden**

- 4:15 407.** Elucidation of the molecular structure and dynamics of egg sac spider silks using solid-state NMR. **S.K. Davidowski**, J.B. Addison, G.P. Holland, J.L. Yarger
- 4:35 408.** Networking of amyloidogenic peptides over nano-gold colloidal particles' surfaces. **K. Yokoyama**
- 4:55 409.** Computational insights into multivalent binding of patterned polymers. **E. Zumbro**, A. Alexander-Katz

In Situ & Operando Spectroscopy

Sponsored by CATL, Cosponsored by ENFL and PHYS

Future of Biomacromolecules at a Crossroads of Polymer Science & Biology

Biomaterials

Sponsored by POLY, Cosponsored by BIOL, CARB, CELL, COLL, ENVR, MEDI, PHYS and PMSE

Understanding the Role of Water in Solid Acid-Base Catalysis

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Interface between Experiments & Modeling in Unraveling the Physical & Chemical Properties of Charged Droplets

Sponsored by ANYL, Cosponsored by COMP, ORGN and PHYS

WEDNESDAY EVENING – PHYS

SECTION A

San Diego Convention Center

TBD

PHYS Poster Session

A. B. McCoy, *Organizer*

6:00 - 8:00

- 410.** Influence of methanol on transport of OH⁻ in anion-exchange membranes. **D. Dong**, D. Bedrov, A.C. Van Duin, W. Zhang
- 411.** Quantum numerical control of nuclei. **Q. Wang**
- 412.** Incoherent upconversion in oligoacenes. **H.C. Friedman**, L.S. Forte, S. Tenney, J.R. Caram
- 413.** NEXAFS spectra and specific dissociation of oligo-peptide model molecules. **C. Liu**
- 414.** AdNDP 2.0: Flexible and efficient way of chemical bonding deciphering in novel clusters and solids. **N.V. Tkachenko**, A.I. Boldyrev

- 415.** Thermodynamic studies of orthorhombic cesium lead halide (CsPbX₃) materials. **B. Wang**, A. Navrotsky
- 416.** Laboratory submillimeter spectroscopic analysis of desorbed H₂O and D₂O ices. **K. Yocum**, A. Jones, E. Todd, S.L. Widicus Weaver, P.A. Gerakines, S.N. Milam
- 417.** Immersion freezing of substrate deposited atmospherically relevant aerosol particles using micro-Raman spectroscopy. **L. Mael**, **H. Busse**, V.H. Grassian
- 418.** Titration of aerosol pH through droplet coalescence. **E. Coddens**, **K. Angle**, V.H. Grassian
- 419.** Spectroscopic signatures of water confined inside metal-organic frameworks with open metal sites. **K.M. Hunter**, F. Paesani
- 420.** Combined experimental and computational studies of the absorption spectra and photochemistry of nitenpyram and analogs. **M.J. Ezell**, W. Wang, D. Shemesh, A.Z. Ni, R.B. Gerber, B.J. Finlayson Pitts
- 421.** Toward electrocatalysis on metal clusters coupled to an electron reservoir. **C.J. Stein**, M.P. Head-Gordon
- 422.** Elusive electrides: From solids to molecules. **M. Kulichenko**, N. Fedik, K.V. Bozhenko, A.I. Boldyrev
- 423.** Partitioning space for electronic correlation: Number-counting Jastrow factors. **B. Van Der Goetz**, E. Neuscamman
- 424.** High-throughput analysis of protein phase separation via temperature gradient microfluidics. **E.A. Graff**, B.A. Rogers, K.B. Rembert, J. Zhang, P.S. Cremer
- 425.** Experimental determination of root mean square (RMS) and molecular velocity of an atom. **S.N. Olatunji**
- 426.** Ultrafast energy-transfer in a hybrid system composed of a wide-bandgap conjugated polymer and quantum dots. **D. Lee**, K. Cho
- 427.** TDDFT study of the valence excited states of Br₂ in clathrate cages. C. Morera Boado, M. Bernal-Uruchurtu, **R. Hernandez**
- 428.** Second-order multi-reference algebraic diagrammatic construction theory for excited electronic states. **I. Mazin**, A. Sokolov
- 429.** Multi-reference algebraic diagrammatic construction theory for ionization energies. **K. Chatterjee**, A. Sokolov
- 430.** Searching for peptides that fold into interesting conformations: Combined experimental and computational study. **C. Patcher**, E.R. Civitello, G.E. Lindberg
- 431.** Regulating the femtosecond excited-state lifetime of a single molecule. **K. Rusimova**, P.A. Sloan, R.M. Purkiss

- 432.** Polarized MUPPETS (multiple population-period transient spectroscopy) distinguishes between heterogeneous local viscosities and local anisotropy in SDS micelles. **J. Darvin**, M.A. Berg
- 433.** Study of processes reduction-oxidation of ions of chromium in the aqueous solution under the action of the DC discharge of atmospheric pressure in oxygen. **A. Izvekova**
- 434.** Quantitative analysis of krypton and xenon isotopes in ambient air with a cost-efficient benchtop mass spectrometer. **I. Beta**, **G. Thier**, J. Wei, **B. Regel**, L. Kephart
- 435.** Synthesis of magnetic iron oxide nanoparticles by precipitation technique and their use in the bituminous composite materials. **N. Barashkov**, A. Mantel, S. Mendigaliyeva, A. Aldongarov, I. Irgibayeva
- 436.** Cavity ringdown spectroscopy of intermediates in the reactions of aromatics + OH. **J. Messinger**, J. Vinson, Q. Meng, M. Okumura
- 437.** Translationally transformed coupled-cluster (TT-CC) theory in a local basis for periodic systems. **B. Gutierrez Cortes**, A.D. Dutoi
- 438.** Solvation thermodynamics of intrinsically disordered proteins (IDP). **S. Maiti**, M. Heyden
- 439.** Comparing wave function optimization algorithms in real space variational Monte Carlo. **L. Otis**, E. Neuscamman
- 440.** Scattering approach to quantum thermodynamics. **A. Semenov**, A. Nitzan
- 441.** Towards the dissociation dynamics of multiply-charged ions. **E. Castracane**, J. Gibbard, R.E. Continetti
- 442.** Treating multi-electron excitations with a QMC-based approach. **R. Hanscam**, E. Neuscamman
- 443.** State specific quantum Monte Carlo targeting of core excited states. **S. Garner**, E. Neuscamman
- 444.** Searching for a self consistent field approach to excited state mean field theory. **T. Hardikar**, J. Shea, E. Neuscamman
- 445.** Robust optical band gap predictions using state-specific orbital optimization within quantum Monte Carlo. **S. Pineda Flores**, E. Neuscamman
- 446.** Solid versus solution phase ultraviolet-visible absorption of secondary organic aerosols. **M. Olsen**, S.A. Nizkorodov, N. Smith
- 447.** Proton hydration in gas phase clusters: Born–Oppenheimer molecular dynamics hybrid DFT study of HCl in a water nanodroplet. C. León-Pimentel, J. Hernández-Cobos, A. Ramírez-Solís, **H. Saint-Martin**
- 448.** 1,000-fold enhancement of light-induced magnetism in plasmonic Au nanoparticles. **H. Cheng**, M.T. Sheldon, D.H. Son
- 449.** QMC-initialized GW for excited states in solids. **C. Robinson**, E. Neuscamman
- 450.** Fluorescence quenching mechanism by the interaction of amyloid beta peptide and nano-gold particle. **A. Ichiki**, **S. Hamazaki**, **K. Yokoyama**
- 451.** Determination of the nano-scale adsorption orientation of amyloidogenic peptides. **A. Ichiki**, **S. Hamazaki**, **K. Yokoyama**
- 452.** Dualism of electronically enriched boron clusters: From transmutation to nitrogen to formation of inverse Lewis pair. **N. Fedik**, G. Liu, X. Zhang, K.H. Bowen, A.I. Boldyrev
- 453.** Excited state Møller–Plesset perturbation theory. **R. Clune**, J. Shea, E. Neuscamman
- 454.** Ultrathin PdPt bimetallic nanowires with enhanced electrocatalytic performance for hydrogen evolution reaction. **H. Lv**, Y. Hu, D. Xu, B. Liu
- 455.** Ice-nucleating bacteria and fungi: Increased order of water molecules at low temperatures. **M. Lukas**, A.T. Kunert, J. Fröhlich-Nowoisky, A. Abdelmonem, U. Pöschl, M. Bonn, E. Backus
- 456.** Simulating nonlinear surface-enhanced vibrational spectroscopy in aqueous solution. **J. Becca**, L. Jensen
- 457.** Water in hydrophobic and other environmental multi-component interfaces. **J.M. Marmolejos**, P.J. Bisson, M.J. Shultz
- 458.** Synthesis of ZnSe: Mn doped nanoparticles for tuning charge carrier lifetimes. **K. Schlegel**
- 459.** Sulfurous and sulfonic acids: Predicting a spectrum and setting the surface straight. **J. Misiewicz**, K.B. Moore, W. Morgan, H.F. Schaefer
- 460.** Ultrafast solvation dynamics of cresyl violet probed by two-dimensional electronic spectroscopy. **J. Lu**, Y. Lee, J.M. Anna
- 461.** Thermodynamic characterization of micelle formation of gemini surfactants. T. Sutorius, B. Britt, S.J. Bachofer, **R.D. Sheardy**
- 462.** Investigation of thermal management in perovskite optoelectronic materials using time-resolved infrared spectroscopy. **J.R. Swartzfager**, J.B. Asbury
- 463.** Recent advances of tunable femtosecond stimulated Raman spectroscopy to design and develop superphotoacids and redder fluorophores. **C. Chen**, L. Zhu, M.S. Baranov, N.S. Baleeva, I.V. Yampolsky, K. Solntsev, C. Fang
- 464.** Comparison between hydrogen and halogen bonding: Hypohalous acid-water dimers, HOX—H₂O (X=F, Cl, Br). **M. Wolf**, B. Zhang, J. Turney, H.F. Schaefer
- 465.** Synthesis and characterization of single-

- atom Pt and Pd dopants on Fe-doped ultra-nano titanium dioxide nanoparticles. T. Xu, **N.J. Anderson**, M. Ouyang, M.J. Shultz
- 466.** Vibrational overtone induced unimolecular dissociation of peroxyformic acid. **J.E. Perez**, M. Roy, A. Sinha
- 467.** Understanding the influence of structure and solution conditions on the self-assembly of cyanine dye aggregates. **L.S. Forte**, J.R. Caram
- 468.** Reactions of water with radical cations of guanine nucleobases and nucleosides. **J. Liu**, Y. Sun, W. Zhou, M. Myat Moe
- 469.** Impact of vibrational excitation on the dynamics of the HOCO radical. **A. Parsons**
- 470.** Conformational analysis of DEET analogs with asymmetric nitrogen arms. **M.C. Coppedge**, D. Morrelli, K.V. Krishnan, S. Maitra
- 471.** Effects of sunlight on the optical properties of methylamine–aldehyde brown carbon aerosol particles. D.Z. Uglund, **D.O. Dehaan**
- 472.** Effects of long-wave UV irradiation on the optical properties of methylamine-aldehyde-ammonium sulfate aerosol particles. C. Carmona, **D.O. Dehaan**
- 473.** Infinite-order connected moments for the many-body calculation of ground and excited state systems. **B. Ganoe**, M.P. Head-Gordon
- 474.** Binding of steroid-based ligands to the HMG-CoA reductase: Molecular docking study. **M. Hackbarth**, V.F. Waingeh
- 475.** Capillary condensation of single- and multi-component fluids in nanopores. **X. Li**, G. Yang
- 476.** Gas transport modeling with multilayer adsorption in nanopores. X. Li, **D. Chai**
- 477.** Effect of water models on the simulated redox potentials of molecules in aqueous solutions. **M. Burrows**, K.B. Bravaya
- 478.** Measuring water uptake and loss in viscous aerosol particles. **B. Wallace**, J. Davies, T. Preston
- 479.** Reactions of N_2O_5 with ions in water: Computational studies of mechanisms and dynamics for Cl^- , SO_4^{2-} , and ClO_4^- . **N. Karimova**, J.R. Gord, S. Staudt, T.H. Bertram, G.M. Nathanson, R. Gerber
- 480.** Many-body effects determine the hydration structure of alkali ions in solution. **D. Zhuang**, M. Riera, F. Paesani
- 481.** Computational study of the photodegradation and thermal decomposition channels of gas-phase and aqueous pyruvic acid. **M.L. Mayes**, M.P. Barquilla
- 482.** Janus: Extensible open-source software package for adaptive QM/MM methods. **B. Zhang**, D. Altarawy, T. Barnes, J. Turney, H.F. Schaefer
- 483.** Temperature-dependent hygroscopic behaviors of atmospherically relevant water-soluble carboxylic acid salts studied by ATR-FTIR spectroscopy. **Y. Liu**, X. Gao
- 484.** PES-Learn: Open-source software package for the automated generation of machine learning models of molecular potential energy surfaces. **A. Abbott**, J. Turney, B. Zhang, D. Smith, D. Altarawy, H.F. Schaefer
- 485.** Computational analysis of a hindered bond rotation in atropisomers. **H. Pearce**, S. Toenjes, V. Garcia, J.L. Gustafson, A. Cooksy
- 486.** Theoretical investigation of the addition of methanol to criegee intermediates. **G.J. Aroeira**, A. Abbott, S. Elliott, J. Turney, H.F. Schaefer
- 487.** Many-body effects in protonated and deprotonated water clusters. **C. Egan**, F. Paesani
- 488.** Silica coating of tubular J-aggregates from amphiphilic cyanine dyes for stabilization and functionalization. **K.A. Herman**, H. Kirmse, J.P. Rabe, S. Kirstein
- 489.** Critical organic hydrophobic modifier aliphatic tail-length for formation of poly(methyl methacrylate) (PMMA)-montmorillonite nanocomposites. R. Tiwari, **U. Natarajan**
- 490.** Bismuth tetramer Bi_4 : The v_3 key to experimental observation. **M. Lahm**, P. Hoobler, J. Turney, K.A. Peterson, H.F. Schaefer
- 491.** Toward ultrafast vibrational dynamics of cobalt-coordinated alkynyl fatty acids. **J.H. Meadows**, K.J. Kubarych
- 492.** Understanding electrocatalytic mechanisms using spectroelectrochemical techniques. **L.B. Michocki**, K.J. Kubarych
- 493.** Interaction-induced dipole of a hydrogen molecule colliding with a hydrogen atom. **H. Lee**, X. Li, E. Miliordos, K.C. Hunt
- 494.** Withdrawn
- 495.** High-level theoretical characterization of the vinoxy radical ($^-\text{CH}_2\text{CHO}$) + O_2 reaction. **J. Weidman**, R. Allen, K.B. Moore, H.F. Schaefer
- 496.** Using geometric phases to separate overall rotation and internal motions in classical and quantum three-body molecular dynamics. **F.J. Lin**
- 497.** Stimulated emission pumping spectroscopy of SiC_2 : Key molecular progenitor of dust in carbon stars. **S. Ross**, N. Reilly
- 498.** Water diffusion measurements of single charged aerosol using $\text{H}_2\text{O}/\text{D}_2\text{O}$ isotope exchange and Raman spectroscopy in an electrodynamic balance. **P. Kim**
- 499.** Thermochemistry for core combustion species: Automating with PACChem. **S. Elliott**, M. Keceli, A.V. Copan, C. Cavallotti, Y. Georgievski, S.J.

- Klippenstein, H.F. Schaefer
- 500.** Spectroscopic studies of membrane protein folding into nanodiscs. **D.K. Asamoto**, G. Kang, J.E. Kim
- 501.** Using commercial 3D-printers to study chemical reactor and flow-cuvette designs for pseudo-first order degradation of methyl-green. **M.M. Allard**, R. Rakijian
- 502.** Highly excited states of cumulenone chlorides in the vacuum-ultraviolet region. **Q.L. Nguyen**, W.K. Peters, R.C. Fortenberry
- 503.** Hydration from no man's land to proteins and metal oxides: Molecular-dynamics insights from nanoclusters to the condensed state. P. Nandi, J. Martínez González, Z. Futera, C. Burnham, **M. Ghaani**, N. English
- 504.** Cavity hydration and competitive binding in methylated β -cyclodextrin. **D. Mendes de Oliveira**, D. Ben-Amotz
- 505.** Subsaturated kappa factor determination and comparison for model systems. **J.N. Dawson**, M. Freedman
- 506.** Aqueous solutions of TMAO and urea under pressure: Molecular dynamics simulation study. **X. Teng**, T. Ichiye
- 507.** On the origins of the surface charge at water-hydrophobic interfaces. **E. Poli**, A. Hassanali
- 508.** Entangled trajectories Hamiltonian dynamics for treating quantum nuclear effects. **B.A. Smith**, A.V. Akimov
- 509.** Analytic energy gradient derivation of the fragment molecular orbital method in the adaptive frozen orbital treatment (FMO/AFO). **Y. Kim**, M.S. Gordon
- 510.** New methods for revealing the effects of solvent in optical spectroscopy. **T.J. Zuehlsdorff**, A. Montoya Castillo, S.V. Shedje, J. Napoli, M. Servis, A.E. Clark, L. Shi, T. Markland, C. Isborn
- 511.** Atmospheric evolution of the ice nucleation properties of biomass burning aerosol. **L. Jahn**, L. Jahl, M.J. Polen, T. Brubaker, S. Graves, R.C. Sullivan
- 512.** Exchange-repulsion for QM/EFP excitations: Aye or nay?. **C.I. Viquez Rojas**, L.V. Slipchenko
- 513.** Electronic energy transfer dynamics in anharmonic environments. **P.L. Walters**
- 514.** *Ab initio* magnetic properties via non-perturbative fields. **B. Ganoe**, M.P. Head-Gordon, T. Stauch, J. Lee
- 515.** Active marine enzymes in the ocean and the air control heterogeneous reactivity of atmospheric aerosols. **C. Lee**, O.S. Ryder, F. Malfatti, J. Schiffer, J. Michaud, J.S. Sauer, M.A. Pendergraft, R.E. Amaro, M.D. Burkart, F. Azam, V.H. Grassian, K.A. Prather
- 516.** Using pyrene excimer dynamics to probe the geometry of triplet-triplet annihilation. **A.J. Berges**, K.M. Hanson, C.J. Bardeen
- 517.** On the interactions and phase separation for the mixture of 1-butyl-3-methylimidazolium bis(trifluorosulfonyl)imide and water from molecular dynamics simulations. G. Jordy, T. Costa, **L.T. Costa**
- 518.** Stochastic dynamics of molecular systems and upconversion materials from experiments and simulations. **G.H. Oliveira**, B. Barja, F. Sigoli, R. Nome
- 519.** Towards the complete basis set and full configuration interaction limits for excited states. **M. Davis**, J. Turney, H.F. Schaefer
- 520.** Effect of water complexation on the chemical kinetics of the β -hydroxyethylperoxy radical. **F. Winiberg**, A.O. Hui, K. Zuraski, M.D. Smarte, R. Caravan, G.H. Jones, J. Messinger, M. Okumura, D.L. Osborn, C. Percival, C.A. Taatjes, S.P. Sander
- 521.** Withdrawn
- 522.** Understanding the reactive uptake of N_2O_5 in the atmospheric aerosol using machine learning and *ab initio* molecular dynamics. **M. Galib**, D. Limmer
- 523.** TERS-relayed molecular force microscopy using CO-terminated tips. **K. Roy**, J. Lee, B. Taber, V.A. Apkarian
- 524.** How ice and water conduct electricity from direct current to terahertz. **V. Artemov**, H. Ouerdane
- 525.** Towards reduced-scaling higher-order coupled-cluster methods via tensor decompositions. **K. Pierce**, E.F. Valeev
- 526.** Observation of trochoidal dichroism. **L.A. McCarthy**, K.W. Smith, S. Hosseini Jebeli, X. Lan, L. Bursi, W. Chang, P.J. Nordlander, S. Link
- 527.** Development of accurate potential energy functions for molecular-ion–water interactions through the many-body expansion. **S.E. Brown**, F. Paesani
- 528.** Semiclassical energy transfer: What is the right Hamiltonian?. **T. Li**, H. Chen, M. Sukharev, A. Nitzan, J.E. Subotnik
- 529.** Theoretical modeling of the vibrational spectra of nucleic bases. **Y. Jiang**, L. Wang
- 530.** Triplet tuning: Novel family of non-empirical exchange–correlation functionals. **Z. Lin**, T.A. Van Voorhis
- 531.** Calculation of reaction rates in the atmosphere using instanton theory: Rigorous inclusion of tunneling and zero-point energy. **P. Winter**, J. Richardson
- 532.** Study of the elusive hydration of Pb(II) from

- the gas phase to the infinitely diluted aqueous solution. **C. León-Pimentel**, J. Amaro-Estrada, H. Saint-Martin, A. Ramírez-Solís
- 533.** Orientational distribution of the free O-H group at the water-air interface. **S. Sun**, F. Tang, S. Imoto, D. Moberg, T. Ohto, F. Paesani, M. Bonn, E. Backus, Y. Nagata
- 534.** General purpose nonadiabatic dynamics with Libra: Implementation, comparative analysis of methodologies, and application to excited state dynamics in lead halide perovskites. **B.A. Smith**, A.V. Akimov
- 535.** Impact of temperature on the reactive uptake kinetics of OH by amorphous organic aerosol surrogates. **J. Li**, D.A. Knopf
- 536.** Investigating particle growth and organic nitrate uptake into secondary organic aerosol particles from the ozonolysis of α -pinene. **A. Vander Wall**, V. Perraud, L.M. Wingen, B.J. Finlayson Pitts
- 537.** Emergent structures in cold water. **A.S. Urbina**, T. Morawietz, P. Wise, X. Wu, W. Lu, D. Ben-Amotz, T. Markland
- 538.** Multicomponent coupled cluster singles and doubles method for molecules in the ground and excited states. **F. Pavosevic**, S. Hammes-Schiffer
- 539.** Mueller tensor framework for nonlinear-optical polarization analysis in turbid media. **J.R. Ulcickas**, c. ding, F. Deng, G.J. Simpson
- 540.** Hydrogen bond dynamics of TADDOL asymmetric organo-catalyst correlate with catalytic activity. **S. Cha**, B. Marekha, M. Wagner, J. Hunger
- 541.** Ultrafast vibrational dynamics of alkyne-coordinated dicobalt hexacarbonyl complexes. **J.H. Meadows**, K.J. Kubarych
- 542.** Halogen bonding and cooperative effects in chlorine clathrate hydrate: *Ab initio* periodic study. C. Cuautli, **R. Hernandez**
- 543.** New excited state density functional theory for single excitations. **L. Zhao**, E. Neuscamman
- 544.** Optical properties of molecules with cycling centers for quantum information science: Insights from equation-of-motion coupled-cluster theory. **M. Ivanov**, F. Bangerter, A. Krylov
- 545.** Polarization effects on protein-ligand interaction energies. S. Yoo Willow, B. Xie, B. Eisenberg, **D.D. Minh**
- 546.** Studying dynamics of engineered peptide systems using transition metal carbonyls. **L.B. Michocki**, K.J. Kubarych
- 547.** Ion-specific effects on the hydrophobic collapse of thermoresponsive polymers: Role of interfacial water structure. **B.A. Rogers**, H. Okur, C. Yan, C.I. Drexler, T. Yang, J. Heyda, P.S. Cremer
- 548.** Active thermochemical tables: Partition function of hydroxymethyl (CH_2OH) revisited. **D. Bross**, H. Yu, L.B. Harding, B. Ruscic
- 549.** Investigating nonadditive ion effects in salt mixtures. **P.T. Bui**, E. Bruce, B.A. Rogers, N. van der Vegt, P.S. Cremer
- 550.** Exploring the diversity of local hydration water environments. **M. Heyden**
- 551.** Advances in stimulated Raman nanoscopy and spectroscopy measured using photon-induced forces. **A. Tamma**, **H. Wickramasinghe**
- 552.** Kinetics and products of multiphase ozonolysis of unsaturated lipids. **Z. Zhou**, S. Zhou, J.P. Abbatt
- 553.** Surface and bulk contribution to sum-frequency vibrational spectroscopy of surface of single crystal ice. **X. Xu**, C. Tian, Y. Shen
- 554.** Glycerol and water: Cluster formation, and photoionization destruction pathways. **C.J. Mackie**, M. Ahmed, M.P. Head-Gordon
- 555.** Reversible point-to-point excited state proton transfer in bifunctional photoacids. D. Pines, H. Rozler, D. Eliovich, D. Aminov, D.I. Huppert, **E. Pines**
- 556.** Electric field-induced orientation and vibrational Stark effect of water molecules in an argon matrix. **Y. Park**, H. Kang
- 557.** Withdrawn
- 558.** Effective modeling of photobiology with the effective fragment potential method. **Y. Kim**, D. Kaliakin, L.V. Slipchenko
- 559.** Time-resolved strong-field photoemission dynamics of isolated, ligand-free nanoparticles using UV, visible, and mid-infrared laser fields. **Q.L. Nguyen**, K.M. Dorney, J.L. Ellis, N.J. Brooks, D. Hickstein, A.G. Grennell, G. Dukovic, E. Campbell, H. Kapteyn, M.M. Murnane
- 560.** Aqueous inorganic textbook ions revisited: Photoelectron spectroscopy study. **R. Seidel**, B. Winter, S.E. Bradforth
- 561.** Approximating quasiparticle and excitation energies from ground state generalized Kohn-Sham calculations. **Y. Mei**, C. Li, N. Su, W. Yang
- 562.** Probing radical-neutral interactions and “improper” hydrogen bonds with analysis tools based on absolutely localized molecular orbitals. **Y. Mao**, M.P. Head-Gordon
- 563.** Understanding random heteropolymer morphology through simulation. **S. Hilburg**, A. Alexander-Katz
- 564.** New, scalable Hartree-Fock algorithm for the exascale computing era. **D. Poole**, G. Barca, A. Rendell, M. Gordon
- 565.** Morphology of ice formation controlled by

supercooling. **T. Zhou**, F. Bridges, D. Lin
566. Development of a polarizable water model for molecular dynamics simulations. **S. Naseem Khan**, L. Lagardère, G.A. Cisneros, N. Gresh, J.A. Piquemal
567. Simulation of Hofmeister effects in intrinsically disordered proteins via explicit ion coarse-grained simulations utilizing hydrophobicity scale interactions. **T. Dannenhoffer-Lafage**, R. Best
568. Development of a generalized linear scaling reference term for accurate prediction of ¹³C solid-state NMR isotropic chemical shifts. **N. Gonnella**, D. Xin, K. Sarpal
569. Activation of actinide dioxide cations by water: Weaker bonds are less reactive. **T. Jian**, P. Dau, J.K. Gibson

THURSDAY MORNING – PHYS

SECTION A

Marriott Marquis San Diego Marina
 Marriott Grand Ballroom Section 13

Chemistry in Real Space & Time

Chiroptical Plasmons & Chemistry

V. A. Apkarian, V. Bommisetty, E. Potma, *Organizers*
 J. S. Shumaker-Parry, *Presiding*

- 8:00** **570.** Plasmonic hot electrons from metastructures for photochemistry: Hot spots and chiral reactions. **A. Govorov**
- 8:35** **571.** Giant circular dichroism at visible frequencies with broken-symmetry plasmonic nano-apertures. **M. Rajaei**, J. Zeng, M. Albooyeh, M. Kamandi, M. Hanifeh, F. Capolino, H. Wickramasinghe
- 8:55** **572.** Chiroptical activity of symmetric and asymmetric aluminum nanocrescents. P.R. Stevenson, K. Rodriguez, M. Du, J. Yuen-Zhou, V.A. Apkarian, **J.S. Shumaker-Parry**
- 9:15** **573.** Tunable chiral optical properties in semiconductor nanocrystals and metamaterials. **V. Ferry**
- 9:50** Intermission.
- 10:10** **574.** Light years: Combined optical and environmental electron microscopy to visualize dynamic photochemical processes with atomic-scale resolution. **J. Dionne**
- 10:45** **575.** Bimetallic nanoparticle optimization for surface enhanced Raman. **C. Mueller**, M. Bourgeois, G.C. Schatz
- 11:05** **576.** Nanoscale plasmon-driven electron transfer for solar energy applications. **E. Sprague**, M. Cardinal, Z. Mansley, Y. Shin, Y. Guo, R.P. Van Duyne
- 11:25** **577.** Second harmonic imaging of real-time spatially resolved chemical reaction constants. **S. Roke**

SECTION B

Marriott Marquis San Diego Marina
 Marriott Grand Ballroom Section 12

Computational Quantum Chemistry: From Promise to Prominence: A Symposium in Honor of Henry F. Schaefer

Cosponsored by COMP
 T. Crawford, P. R. Schreiner, E. F. Valeev, *Organizers*
 D. D. Sherrill, *Organizer, Presiding*

- 8:30** **578.** Recent efforts in calculating free energy based properties using QM and QM/MM methods, and progress towards better MM methods to support more accurate QM/MM free energies. **B. Brooks**
- 9:00** **579.** Making the inaccessible accessible: Novel techniques for obtaining accurate QM/MM free energies at affordable costs. **H.L. Woodcock**, S. Boesch
- 9:30** **580.** Influence of electrostatic and hydrogen bonding effects on radical abstraction reactions in amino acids and peptides. **L. Radom**, B. Chan, C.J. Easton
- 10:00** **581.** Reproducible, rational, and rigorous QM-cluster enzyme models. **N.J. Deyonker**, t.J. summers, Q. Cheng, M. Palma
- 10:15** Intermission.
- 10:40** **582.** *Ab initio* many-body potentials from “machine learning” before we knew that terminology. **J.M. Bowman**
- 11:10** **583.** Effective fragment potential method: New models, new tools. **L.V. Slipchenko**
- 11:40** **584.** Applications of a layered, ONIOM-like approach to the many body expansion for weakly bound clusters to hydrogen bonding, water clusters, and explicit hydration. **G.S. Tschumper**
- 12:10** **585.** Symmetry of the hydrogen bonds of two enols in solution. **C. Perrin**, Y. Wu

SECTION C

Marriott Marquis San Diego Marina
 Marriott Grand Ballroom Section 11

Nanoscale & Molecular Assemblies: Designing Matter to Control Energy Transport

Cosponsored by INOR
 Financially supported by Coherent
 J. R. Caram, J. J. Foley, D. Hayes, *Organizers*
 H. Lu, *Presiding*

- 8:00** **586.** Photophysics and photochemistry of organic polaritons. **J. Yuen Zhou**
- 8:40** **587.** Designing amphiphilic assemblies with controlled structure to facilitate excited state electron transfer. **Y. Wu**, Y.L. Li, S.H. Tolbert, Y.F. Rubin

- 9:00 **588.** Extraordinary optics from structured nanoparticles. **D. Wang**, G.C. Schatz, T.W. Odom
- 9:40 **589.** Withdrawn
- 10:00 Intermission.
- 10:15 **590.** Time-dependent DFT and DFTB studies of electron dynamics in silver nanoparticle arrays. **C.M. Aikens**
- 10:55 **591.** Uncovering design rules for environmentally friendly nanoparticle enabled energy storage via machine learning. **C.A. Daly**, R.J. Hamers, C.L. Haynes, V. Feng, R. Hernandez
- 11:15 **592.** Photogenerated spin-entangled (qubit) radical pairs in DNA hairpins. **J.H. Olshansky**, M.D. Krzyaniak, R. Young, M.R. Wasielewski

SECTION D

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 10

Hydration from the Gas to the Condensed Phase

Water at Low Temperatures

Financially supported by Newport Spectra-Physics
E. Backus, M. Bonn, F. Paesani, *Organizers*
S. Woutersen, *Presiding*

- 8:00 **593.** Vapor-liquid-ice environmental interactions with mineral surfaces on the molecular level using nonlinear optical spectroscopy. **A. Abdelmonem**, M. Bonn, J. Luetzenkirchen, E. Backus, J.D. Cyran, M. Lukas, S. Ratnayake
- 8:30 **594.** Understanding heterogeneous ice nucleation through water structure and dynamics. **S. Sarupria**
- 9:00 **595.** Structure outweighs chemistry: Icy water at the interface with self-assembled cholesterol monolayers. **G.C. Sosso**, P. Sudera, E. Backus, M. Bonn, A. Michaelides
- 9:30 **596.** Inducing changes in interstellar ice by IR irradiation. **H. Cuppen**, S. Ioppolo, J. Noble, S. Coussan, B. Redlich
- 9:50 Intermission.
- 10:20 **597.** Dynamics of cooled water in bulk, mixtures, and confinements: Combined experimental and computational studies. **M. Vogel**, M. Weigler, R. Horstmann
- 10:40 **598.** Proposal for the structure of high- and low-density fluctuations in liquid water. **L.G. Pettersson**
- 11:00 **599.** Amorphous ices and liquid states of water. **K. Amann-Winkel**
- 11:30 **600.** Structure of ice surface revealed by heterodyne-detected sum frequency generation spectroscopy and theoretical modeling. **Y. Nojima**, H. Torii, S. Yamaguchi

SECTION E

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 1

Water in the Universe

G. A. Blake, S. Ioppolo, *Organizers*
M. Brogi, *Presiding*

- 8:00 **601.** The delivery and evolution of water within the solar system. **G.L. Villanueva**, S.N. Milam
- 8:35 **602.** Water on solid bodies in our solar system. **R. Klima**, A. Rivkin, T.M. Orlando
- 9:10 **603.** Chemical kinetic modeling of cometary ice processing. **R.T. Garrod**
- 9:45 Intermission.
- 10:05 **604.** Making abiotic O₂ from water in comets. **R.C. Fortenberry**
- 10:25 **605.** TeraHertz time domain spectroscopy (THz TDS) of molecular ices. **G.A. Blake**, S. Ioppolo, M.A. Allodi, B. McGuire, G. Mead
- 11:00 **606.** Regenerative water sources on surfaces of airless bodies. **C. Zhu**, S. Góbi, M. Abplanalp, R. Frigge, J.J. Gillis-Davis, G. Dominguez, K. Miljković, R. Kaiser
- 11:20 **607.** On the formation and destruction cycle of solid carbonic acid in the solar system. **S. Ioppolo**, Z. Kanuchová, R.L. James, A. Dawes, N.C. Jones, S.V. Hoffmann, N.J. Mason, G. Strazzulla

SECTION F

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 2

At the Interfaces of Experimental & Theoretical Nonlinear Optical Molecular Spectro-Imaging Coherent 2D Spectroscopy

L. Wang, W. Xiong, *Organizers*
M. J. Tucker, *Presiding*

- 8:30 **608.** High resolution coherent 2D and 3D spectroscopy. **P. Chen**, T. Wells
- 9:00 **609.** Robust, rapidly dephased, excited state coherences in a photosynthetic bacteria isolated through fluorescence-detected two-dimensional electronic spectroscopy. **V. Tiwari**, Y. Acosta, A.T. Gardiner, R.J. Cogdell, J.P. Ogilvie
- 9:20 **610.** Single-molecule, multidimensional measurements of rate-domain lifetimes near the glass transition. H. Kaur, S. Verma, K. Paeng, L. Kaufman, **M.A. Berg**
- 9:40 Intermission.
- 10:00 **611.** Coherent multidimensional vibronic spectroscopies. **M.H. Khalil**

- 10:30 612.** Resonance hyper-Rayleigh and hyper-Raman scattering from II-VI semiconductor nanocrystals. **A.M. Kelley**, R. Tan, D.F. Kelley
- 10:50 613.** Simultaneous observation of donor and acceptor vibrational modes during excited state proton transfer in water. **L. Zhu**, C. Chen, L. Tang, C. Fang
- 11:10 614.** Exploring vibrational polaritonic systems using multidimensional spectroscopy. **R. Duan**, K.J. Kubarych

SECTION G

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 3

Molecular, Electronic, & Ionic Transport in Materials for Energy

Transport in Materials Assembled from Molecular Building Blocks

X. Roy, *Organizer*

L. A. Madsen, *Organizer, Presiding*

- 8:00 615.** Molecular interactions in diffusion-controlled aldol condensation with mesoporous silica nanoparticle (MSN) by the effective fragment potential (EFP) method. **Y. Kim**, M.S. Gordon
- 8:20 616.** Electronic structure of photosystem II active site models: Combined density functional theory and electron paramagnetic resonance study. **K. Mardis**, J. Niklas, O. Poluektov
- 8:50 617.** Mechanism of charge carrier propagation through organic semiconductors from non-adiabatic molecular dynamics. **S. Giannini**, A. Carof, M. Ellis, O. Zigos, S. Ghosh, **J. Blumberger**
- 9:20 618.** Structural origins of slow recombination in halide perovskites from ultrafast infrared spectroscopy. **J.B. Asbury**
- 9:50** Intermission.
- 10:10 619.** Tunable metal–oxide frameworks based on assembled metal oxide clusters. **A.M. Schimpf**, L. Chen, M. Turo
- 10:40 620.** Extended molecular materials constructed from redox-active building blocks. **M.S. Inkpen**
- 11:10 621.** Switchable transport behaviors in a phase change superatomic crystal. **X. Roy**

SECTION H

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 4

Recent Developments in Biomaterials

A. Alexander-Katz, L. Yang, *Organizers*

T. Xu, *Organizer, Presiding*

- 8:30 622.** Selective *in vivo* cell labeling mediated cancer targeting and drug delivery. **J. Cheng**
- 9:05 623.** Investigating sub-20 nm nanocarrier transport and accumulation in tumors. **M. Lim**, B. Jung, V. Dharmaraj, N. Vlahakis, T. Xu
- 9:25 624.** Advancing the development of highly-functionalizable glucose-based polycarbonates by tuning of the glass transition temperature. **Y. Song**, X. Ji, M. Dong, K.L. Wooley
- 9:45 625.** Three-component model for potato suberin biopolymer supports a self-assembly process. **A. Kligman**, K. Dastmalchi, G. John, R.E. Stark
- 10:05** Intermission.
- 10:20 626.** Supramolecular polymer prodrugs for drug-induced tissue regeneration. **P.B. Messersmith**, E. Heber-Katz
- 10:55 627.** pH-Sensitive peptide hydrogels based on semenogelin I: Characterization via global and site-specific vibrational reporters. **C.H. Londergan**, K.S. Akerfeldt, W. Fox, G. Braun, N.R. John
- 11:15 628.** Multiheme cytochromes: From biology to bioelectronic junctions. **J. Blumberger**, Z. Futera, X. Jiang
- 11:35 629.** Using combined solid-state NMR dynamics and ice growth measurements to unravel different molecular level effects of synthetic and biological anti-freeze (macro)molecules. **A.E. Fayter**, M.I. Gibson, R. Stevens, J.R. Lewandowski

Water Behavior in Concentrated Electrolytes

Sponsored by NUCL, Cosponsored by PHYS

In Situ & Operando Spectroscopy

Sponsored by CATL, Cosponsored by ENFL and PHYS

Interface between Experiments & Modeling in Unraveling the Physical & Chemical Properties of Charged Droplets

Sponsored by ANYL, Cosponsored by COMP, ORGN and PHYS

THURSDAY AFTERNOON – PHYS

SECTION A

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 13

Chemistry in Real Space & Time

Seeing Electrons in Action

V. A. Apkarian, V. BommiSETTY, E. Potma, *Organizers*

N. Ge, H. Petek, *Presiding*

- 1:30 630.** Ultrafast excited state dynamics and photoinduced phase transitions of solids probed by time resolved photoemission. **M. Wolf**
- 2:05 631.** Revealing an optical spin skyrmion at the core of a plasmonic vortex. **Y. Dai**, Z. Zhou, A. Kubo, C. Huang, H. Petek
- 2:25 632.** Fast carrier extraction from transient interlayer exciton states in twisted and stacked 2D materials. **M.W. Graham**
- 3:00 633.** Dynamics and separation of triplet pair intermediates in singlet fission measured with ultrafast infrared spectroscopy. **J.B. Asbury**
- 3:35** Intermission.
- 3:55 634.** Probing plasmon-driven electron transfer between gold nanoparticles and PCBM with pump probe SERS. **Y. Wu**, G.C. Schatz, R.P. Van Duyne
- 4:15 635.** Ferroelectric polarons in lead halide perovskites. **X. Zhu**
- 4:50 636.** Tracing from femtoseconds to seconds the dynamics of electronic states at a model electrode-electrolyte interface. **S.B. King**, A. Demling, K. Broch, J. Stähler

SECTION B

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 12

Computational Quantum Chemistry: From Promise to Prominence: A Symposium in Honor of Henry F. Schaefer

Cosponsored by COMP

T. Crawford, D. D. Sherrill, E. F. Valeev, *Organizers*

P. R. Schreiner, *Organizer, Presiding*

- 1:30 637.** Computational explorations of organic reaction mechanisms. **K.N. Houk**
- 2:00 638.** Ultrafast processes: Quantum theory and coordination chemistry. **C. Daniel**
- 2:30 639.** Riddles of the structure and vibrational dynamics of HO₃ resolved near the *ab initio* limit. M.A. Bartlett, **W.D. Allen**, H.F. Schaefer
- 3:00 640.** Near-linear scaling explicitly correlated coupled cluster singles and doubles method based on an open-shell domain-based local pair natural orbitals. **A. Kumar**, F. Neese, E.F. Valeev
- 3:15** Intermission.
- 3:30 641.** Quasistructural molecules. **A.G. Csaszar**
- 4:00 642.** Coupled-cluster theory investigations of vibrational Raman optical activity. **R.A. King**, A.G. Heide, T. Crawford
- 4:30 643.** Searching for nitrogen-containing cyclic molecules in the ISM: Formation pathways and spectroscopic characterization. **T.J. Lee**
- 5:00 644.** Can unrestricted Kohn-Sham DFT qualitatively describe dissociation of H₂? **D. Hait**, A. Rettig, M.P. Head-Gordon

SECTION C

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 11

Nanoscale & Molecular Assemblies: Designing Matter to Control Energy Transport

Cosponsored by INOR

Financially supported by Coherent

J. R. Caram, J. J. Foley, D. Hayes, *Organizers*

J. Caram, *Presiding*

- 1:30 645.** Molecular materials to manipulate and control triplet exciton dynamics. **C.J. Bardeen**
- 2:10 646.** Emerging opportunities of low-dimensional perovskite materials beyond photovoltaics: Spin, charge, and light/matter interaction. **H. Lu**, M.C. Beard
- 2:30 647.** Progress using hybrid nanomaterials for excitonic photon upconversion. **M.W. Wilson**
- 3:10** Intermission.
- 3:25 648.** Robust light-harvesting in biomimetic nanotubes through scaffold-assisted self-healing. **D. Eisele**
- 4:05 649.** Photon upconversion utilizing energy beyond the band gap of crystalline silicon with a hybrid TES-ADT/ PbS quantum dots system. **N. Nishimura**, J.R. Allardice, J. Xiao, Q. Gu, V. Gray, A. Rao
- 4:25 650.** Chiral, low-resistance organic and nanoscale frameworks that uniquely propagate spin polarized currents. **G. Bullard**, F. Tassinari, C. Ko, s. mishra, A. Mondal, R. Wang, R. Naaman, M.J. Therien

SECTION D

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 10

Hydration from the Gas to the Condensed Phase Clusters & Droplets

Financially supported by Newport Spectra-Physics

M. Bonn, F. Paesani, *Organizers*

E. Backus, *Organizer, Presiding*

- 1:30 651.** Microsolvation structure of protonated amino acids and peptides. **E. Garand**
- 2:00 652.** Many-body expansion for water clusters revisited. **S.S. Xantheas**, J.P. Heindel
- 2:20 653.** Explicit hydration of halide and alkali metal ions with density functional theory and wave function theory methods. **G.S. Tschumper**
- 2:40 654.** Thermal expansion and thermal transitions in small water clusters. N.R. Samala, **N. Agmon**
- 3:00** Intermission.

**Molecular, Electronic, & Ionic Transport in
Materials for Energy****Spectroscopic Measurement of Transport in
Materials**L. A. Madsen, *Organizer*X. Roy, *Organizer, Presiding*

- 1:30** **666.** First-principles study of the electron-phonon interaction in SrTiO₃: Temperature dependence of energy gaps and optical properties. **Y. Wu**, J. Wuenschell, W. Al-Saidi, T. Tadano, P. Ohodnicki, B. Chorpene, Y. Duan
- 1:50** **667.** Coarse-grained electronic structure in organic semiconductors via supervised machine learning. **N. Jackson**, J.J. De Pablo
- 2:10** **668.** Probing non-equilibrium electron transfer in plasmonic assemblies using two-dimensional electronic spectroscopy. **K.L. Knappenberger**
- 2:40** **669.** Understanding energy-relevant soft materials with overhauser relaxometry. **J. Franck**
- 3:10** Intermission.
- 3:30** **670.** Electron hopping and vibrational cooling in dendritic arrays of acceptors. Z. Gong, M. Liu, T. Kawauchi, **P.G. Piotrowiak**
- 4:00** **671.** Ultrafast transient absorption spectroscopy of doped P3HT films: Distinguishing free polarons, trapped polarons and bipolarons. **B.J. Schwartz**, M. Voss
- 4:30** **672.** Using time-resolved infrared spectroscopy to investigate the structural origins of slow recombination in halide perovskites. **K.T. Munson**, G. Doucette, E. Kennehan, J.R. Swartzfager, J.B. Asbury
- 4:50** **673.** Photoexcited electron dynamics in Ag nanoplatelets adsorbed on TiO₂ nanorods. **H. Fang**, Y. Rao, J. Ma, D.L. Kuhn, Z. Zachary, B.G. DeLacy, H. Dai
- 5:10** **674.** Interrogating charge-transfer mechanisms during photoacid dye-sensitization of ion-exchange membranes for light-to-ionic energy conversion. **S. Luo**, W. White, J.M. Cardon, S. Ardo

- 3:25** **655.** On the deep supercooling of nano-sized water droplets dispersed in a polymer matrix. **B.H. Milosavljevic**
- 3:45** **656.** Long-range interactions of ions with water determine the Jones-Ray effect. **S. Roke**
- 4:05** **657.** Molecular properties of low charge aqueous-hydrophobic nanoemulsion interfaces. **A. Carpenter**, E. Tran, R. Altman, G.L. Richmond
- 4:25** **658.** Water network formation and acid dissociation at “stardust conditions”. **M. Havenith**, D. Mani, R. Pérez de Tudela, R. Schwan, N. Pal, S. Koerning, H. Forbert, B. Redlich, A. van der Meer, G. Schwaab, D. Marx, C. Qu, C.J. Leforestier, J.M. Bowman
- 4:55** Concluding Remarks.

SECTION E

Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 1**Water in the Universe**G. A. Blake, *Organizer*S. Ioppolo, *Organizer, Presiding*

- 1:30** **659.** Hunting for water in the atmospheres of exoplanets. **M. Brogi**
- 2:10** **660.** Direct detection of water in the thermal emission spectra of hot jupiters. **C. Buzard**, D. Piskorz, G.A. Blake, C. Bender, B. Benneke, M. Line, A. Lockwood
- 2:30** **661.** Sources of water and other volatiles to the terrestrial planets. **C. Alexander**
- 3:10** Intermission.
- 3:30** **662.** Water on rocky planets: Atmospheres, oceans, and deep interiors. **L. Schaefer**
- 4:10** **663.** Water mediated ³SO₂ chemistry in planetary atmospheres. **V. Vaida**, J.A. Kroll, B.N. Frandsen, H. Kjaergaard
- 4:30** **664.** Confinement effects on water’s nuclear spin isomer conversion. **C. Wespiser**, P. Turgeon, J. Vermette, Y. Kalugina, P. Roy, P. Ayotte
- 4:50** **665.** Preparation, characterization, and storage of water vapours highly enriched in its ORTHO-H₂O nuclear spin isomer. **P. Ayotte**, J. Vermette, I. Braud, P. Turgeon, X. Michaut, T. Putaud, G. Alexandrowicz
- 5:10** Concluding Remarks.

SECTION H
Marriott Marquis San Diego Marina
Marriott Grand Ballroom Section 4

Recent Developments in Biomaterials

A. Alexander-Katz, L. Yang, Organizers

T. Xu, Organizer, Presiding

- 1:30** **675.** Controlled assembly pathways and conditions to access unique nanoscopic morphologies from topologically complex poly(glucose carbonate) biomaterials. **K.L. Wooley**
- 2:05** **676.** Hydrophobic interactions in soft matter. **F. Stellacci**
- 2:40** **677.** Cytoskeletal stiffening in synthetic hydrogels. **P.H. Kouwer**
- 3:00** Intermission.
- 3:20** **678.** Helical cooperativity and helical chain growth mechanism in polypeptide-containing macromolecules. **Y. Lin**
- 3:55** **679.** Using sequence and chemistry to engineer complex coacervate materials. **S.L. Perry**
- 4:30** **680.** Oscillatory behavior in a cellular automaton-based model of metal passivation. **J. Stepien, J. Stafiej**

PMSE

DIVISION OF POLYMERIC MATERIALS SCIENCE AND ENGINEERING

J. Schaefer, T. Bunning and C. Snyder, *Program Chairs*

SUNDAY MORNING – PMSE

SECTION A

Manchester Grand Hyatt San Diego
Harbor G

Novel Polymeric Materials & Polymer-Based Processes for Energy-Efficient Treatment of Water & Resource Recovery

Membrane Formation

Cosponsored by ENVR

Financially supported by North American Membrane Society, Center for Materials for Water & Energy Systems (M-WET); Advanced Materials for Energy Water Systems Center (AMEWS); ACS Innovative Project Grant

D. Bhattacharyya, S. B. Darling, Y. Ding, B. D. Freeman, E. Hatakeyama, W. A. Phillip, C. M. Stafford, *Organizers*
M. Barboiu, J. McCutcheon, *Presiding*

- 8:25** Introductory Remarks.
- 8:30** **1.** Exploring the scalability of water filtration membranes using roll-to-roll. **T.A. Harris**
- 9:10** **2.** Printing membranes: Enabling the use of conventional and novel polymers in high-performance membranes. **J.R. McCutcheon**, M. Chowdhury, X. Qian, T. Ravindran, A. Asatekin, B. Huey, S. Loudner
- 9:35** **3.** Dynameric asymmetric membranes for directional water transport. Y. Zhang, **M. Barboiu**
- 10:00** **4.** Atomic layer deposition-enabled conversion of porous polyethersulphone to laser-induced graphene for antifouling membranes. **D.S. Bergsman**, B.A. Getachew, J.C. Grossman
- 10:25** Intermission.
- 10:40** **5.** Capacitive protein separation: From electrode preparation to process design that also affects salt removal. **P. Fritz**, P. Zhang, M. Chan-Park, R. Boom, K. Schroen
- 11:05** **6.** Negatively and positively charged low-pressure NF membranes for selective water desalting. **F. Leniz**, A. Colburn, I.C. Escobar, D. Bhattacharyya
- 11:30** **7.** 3D-printed multifunctional, hyperelastic silicone rubber foam. **Q. Chen**, P. Cao, R.C. Advincula

SECTION B

Manchester Grand Hyatt San Diego
Cortez Hill C

Eastman Chemical Student Award

Financially supported by Eastman Chemical Co.

J. C. Jenkins, *Organizer*

J. W. Gilmer, *Organizer, Presiding*

K. Burke, *Presiding*

- 8:25** Introductory Remarks.
- 8:30** **8.** Using monomer chemistry to predict dose reate effects during electron-beam polymerization. **N.L. Thiher**, S.M. Schissel, J.L. Jessop
- 9:00** **9.** Living polymerization of a 2-alkylthio-2-oxazoline as a divergent platform for post-polymerization functionalization. **Y.M. Wu**, T.M. Swager
- 9:30** **10.** Enhancing macroscopic properties of 3D-printed parts by tailoring interfacial interactions at the nanoscale. **D.P. Street**, S. Kilbey
- 10:00** Intermission.
- 10:15** **11.** Preclinical *in vitro* and *in vivo* assessment of linear and branched *l*-valine based poly(ester urea)s for soft-tissue applications. **N.Z. Dreger**
- 10:45** **12.** Underlying entropy-enthalpy compensation effect in relaxation dynamics of imprinted polymer surfaces. **S. Bhadauriya**, X. Wang, C.M. Stafford, J. Douglas, A. Karim
- 11:15** **13.** Directly measuring the uniaxial stress-strain response of freestanding ultra-thin glassy polymer films. **R. Bay**, A. Crosby

SECTION C

Manchester Grand Hyatt San Diego
Harbor I

PMSE Future Faculty

Financially supported by Tosoh Bioscience, LLC; IBM; Solvay Specialty Polymers USA, LLC; Royal Society of Chemistry; Jasco

C. A. DeForest, E. Pentzer, *Organizers*

C. Chang, M. A. Hillmyer, *Presiding*

- 8:30** **14.** Pearls of wisdom from an ex department chair. **S. Kumar**

- 9:00 15. Ultrafast motion of the slingshot spider powered by a 3-D conical web. **S.L. Alexander**, S. Bhamla
- 9:30 16. Molecularly engineering polymers for biodegradable and stretchable electronics. **H. Tran**, R.N. Zuckermann, L. Campos, Z. Bao
- 10:00 Intermission.
- 10:30 17. PolyMOFs: Hybridization of polymers and metal–organic frameworks as a route towards thermally processable MOFs. **K.C. Bentz**, S. Ayala, M. Kalaj, K.S. Barcus, Y. Katayama, S. Cohen
- 11:00 18. Journey from conjugated semiconducting polymers to porous conductive metal-organic frameworks. **S. Goswami**, K.S. Schanze, J.T. Hupp
- 11:30 19. Exploiting facile synthetic strategies for the development of aqueous electrolyte compatible electrochromic polymers processable from environmentally sustainable solvents. **G.S. Collier**, J.R. Reynolds

SECTION D

Manchester Grand Hyatt San Diego
Harbor D

Continuous Flow Chemistry in Polymer Science

T. Junkers, F. A. Leibfarth, *Organizers*
C. Boyer, *Organizer, Presiding*

- 8:00 20. Surface engineering through stop-flow solution exchange lithography. **C.W. Pester**, C. Boyer, M. Li, M. Fromel
- 8:25 21. Organocatalyzed atom transfer radical polymerization performed in flow. **G. Miyake**
- 8:50 22. Supramolecular chemistry under continuous flow conditions. **A. Slater**
- 9:15 23. Evolution of material function through continuous flow chemistry. **F.A. Leibfarth**
- 9:40 24. Microfluidic preparation of smart emulsions and functional microparticles. **J. Xu**
- 10:05 Intermission.
- 10:30 25. Automation of precision polymer synthesis towards unprecedented control. **T. Junkers**
- 10:55 26. Polymer hydrogelation and continuous microfiber formation in microfluidic devices. E. Hofmann, S. Seibt, M. Trebbin, **S. Förster**
- 11:20 27. Withdrawn

SECTION E

Manchester Grand Hyatt San Diego
Hillcrest A

Roy W. Tess Award: Symposium in Honor of Raymond H. Fernando

E. D. Sapper, *Organizer, Presiding*

- 8:50 Introductory Remarks.
- 9:00 28. Exploring the limits of additive molar functions for coating resin property prediction. **E.D. Sapper**
- 9:30 29. Waterborne nonleaching antimicrobial coating. **W. Ming**
- 10:00 Intermission.
- 10:30 30. Assessing high-gloss architectural paint performance using rheological techniques. **T.E. Ewert**
- 11:00 31. Methods to evaluate service life performance of nanocoatings under different environmental stressors. **L. Sung**, D. Goodwin, S. Shen, R. Lankone
- 11:30 32. Watching paint dry doesn't have to be boring. **G. Williams**

SECTION F

Manchester Grand Hyatt San Diego
Cortez Hill A/B

General Papers/New Concepts in Polymeric Materials

T. J. Bunning, *Organizer*
A. Anderson, A. Kulkarni, *Presiding*

- 9:00 33. Development of a hierarchical porous structure in syndiotactic polystyrene aerogels via Pickering emulsion. **A. Kulkarni**, S.C. Jana
- 9:20 34. Dual imprinted composite polymeric layers for improved recognition in complex mixtures. **A. Mujahid**, M. Irshad, A. Afzal, T. Hussain, S.Z. Bajwa
- 9:40 35. Tailored porous polymer scaffolds for enhanced 3D cell culture of primary human cells. **A.M. Eissa**
- 10:00 Intermission.
- 10:20 36. Exploiting catalytic chain transfer polymerization for the synthesis of carboxylated latexes via sulfur free RAFT. **A. Shegiwal**, A. Wemyss, M. Schellekens, J. Bont, J. Town, E. Liarou, G. Patias, C. J Atkins, D.M. Haddleton
- 10:40 37. Synthesis, self-assembly, and photomechanical gel actuator performance of a sequence-defined polyviologen crosslinker. **A. Delawder**, A. Natraj, N.D. Colley, T. Saak, A.F. Greene, J.C. Barnes
- 11:00 38. Hybrid polymeric gel networks crosslinked via “click” nucleic acid hybridization. **A. Anderson**, S. Bryant, C. Bowman

- 11:20** 39. Highly asymmetric ABC triblock block copolymers targeting the core-shell sphere phase region. **A. Klug**, T.S. Bailey

SECTION G

Manchester Grand Hyatt San Diego
Harbor H

Emulsification & Encapsulation by Soft Matter Techniques

Engineering of Emulsification & Encapsulation

Cosponsored by POLY

Financially supported by Princeton Chemical and Biological Engineering; Solvay; Givaudan; MANE

R. D. Priestley, R. K. Prudhomme, *Organizers*

F. Ganachaud, *Organizer, Presiding*

- 8:30** Introductory Remarks.
- 8:40** 40. Large-scale manufacturing of microfluidic emulsions and particles via parallelization. **D. Lee**
- 9:10** 41. Predictive design of polymeric capsules by microflow-SANS. **J. Cabral**
- 9:40** 42. Formulation of functional soft materials with microfluids. **D.A. Weitz**
- 10:20** Intermission.
- 10:50** 43. Flash nanoprecipitation of ionomers for the scalable production of functional colloids. **D.M. Scott**, R.K. Prudhomme, R.D. Priestley
- 11:15** 44. Electrohydrodynamic atomization synthesis route for polymer nanoparticles encapsulating hydrophobic cargoes. K. Lee, G. Yang, B.E. Wyslouzil, **J.O. Winter**
- 11:40** 45. Structured polymer colloids and encapsulation by flash nanoprecipitation. **R.D. Priestley**

Characterization of Plastics in Aquatic Environments

Sponsored by POLY, Cosponsored by ANYL, BIOL, CEI, ENVR, I&EC, PMSE and PRES

SUNDAY AFTERNOON – PMSE

SECTION A

Manchester Grand Hyatt San Diego
Harbor G

Novel Polymeric Materials & Polymer-Based Processes for Energy-Efficient Treatment of Water & Resource Recovery

Membrane Processes

Cosponsored by ENVR

Financially supported by North American Membrane Society, Center for Materials for Water & Energy Systems (M-WET); Advanced Materials for Energy Water Systems Center (AMEWS); ACS Innovative Project Grant D. Bhattacharyya, S. B. Darling, Y. Ding, B. D. Freeman, E. Hatakeyama, W. A. Phillip, C. M. Stafford, *Organizers* H. Ro, N. Yin YIP, *Presiding*

- 1:25** Introductory Remarks.
- 1:30** 46. Membrane distillation, pevaporation, and ion selective membranes for desalination and resource recovery. W. cha-umpong, A. Razmjou, G. Dong, **V. Chen**
- 2:10** 47. Donnan dialysis desalination with thermolytic salts. **H. Fan**, N. Yip
- 2:35** 48. Driving water down the nano-highways for effective dehumidification. **F. Akhtar**, K. Ng
- 3:00** 49. Novel isothermal membrane distillation with acid collector for selective and energy efficient removal and recovery of ammonia. S. McCartney, C. Boo, N. Williams, X. Chen, **N. Yip**
- 3:25** Intermission.
- 3:40** 50. Recovery of dissolved methane from wastewater using omniphobic membranes: Maximizing the energy benefits towards water sustainability. **X. Li**, A. Dutta, Q. Dong, S. Rollings-Scattergood, J. Lee
- 4:05** 51. Dissolved methane harvesting using omniphobic membrane contactor. **A. Dutta**, X. Li, J. Lee
- 4:30** 52. Direct capture of rare earth elements via electrochemical precipitation on an electrically conductive ultrafiltration membrane. **Z. Hendren**, E. Reid

SECTION B

Manchester Grand Hyatt San Diego
Cortez Hill C

Design, Synthesis & Engineering of Polypeptides for Biological & Biomedical Application

Self-Assembly & Engineering of Functional Polypeptides

Cosponsored by POLY

J. Cheng, T. J. Deming, M. J. Vicent, L. Yin, *Organizers*

C. A. Alabi, D. J. Pochan, *Presiding*

- 1:00** 53. Biomolecules for biomedical materials: Peptide design and solution assembly to construct nanostructures and hydrogel networks. **D.J. Pochan**
- 1:30** 54. Controlling the self-assembly of difficult to assemble proteins. **B.D. Olsen**, J.M. Paloni, T. Suguri
- 2:00** 55. Engineering pleiotropic peptides for immunomodulation. **G. Wong**

- 2:30** 56. Multiscale property control through self-assembly and photopolymerization. A. Hilderbrand, E. Ford, **A.M. Kloxin**
- 3:00** Intermission.
- 3:20** 57. Synthesis and self-assembly of biomimetic polypeptide-based copolymers towards functional nanomedicines. **S. Lecommandoux**, E. Garanger, C. Bonduelle
- 3:50** 58. Self-assembly of short synthetic peptides into hydrogels for biomedical applications. **Y. Yang**
- 4:20** 59. Engineering macromolecular oligoTEA conjugates for biological applications. **C.A. Alabi**

SECTION C

Manchester Grand Hyatt San Diego
Harbor I

PMSE Future Faculty

Financially supported by Tosoh Bioscience, LLC; IBM; Solvay Specialty Polymers USA, LLC; Royal Society of Chemistry; Jasco

C. A. DeForest, E. Pentzer, *Organizers*

R. H. Grubbs, A. Murphy, *Presiding*

- 1:30** 60. Nature-inspired strategies for reinforcement of polymer gels and composites. **L. Korley**
- 2:00** 61. Catalyst-controlled stereoselective polymerization of vinyl ethers to access new polar thermoplastics. **A. Teator**, F.A. Leibfarth
- 2:30** 62. Expanding the scope of catalyst-transfer polymerization. **T. Kubo**, K. Souther, M.S. Young, A.J. McNeil
- 3:00** Intermission.
- 3:30** 63. Advances in aqueous metathesis chemistry. **J. Foster**, S. Varlas, L.A. Arkinstall, R.K. O'Reilly
- 4:00** 64. Ring-opening metathesis of cyclopropenes for polymer sequence control. **B.R. Elling**, Y. Xia
- 4:30** 65. Development of polymeric biomaterials using high-throughput experimentation and statistical learning. **R. Kumar**, N. Le, Z. Tan, T.M. Reineke

SECTION D

Manchester Grand Hyatt San Diego
Harbor D

Continuous Flow Chemistry in Polymer Science

C. Boyer, T. Junkers, *Organizers*

F. A. Leibfarth, *Organizer, Presiding*

- 1:15** 66. Programmable synthesis of polycarbonates and polyesters via continuous-flow ring-opening polymerization. **N. Park**
- 1:40** 67. Fluid mechanics meet controlled polymerizations: Theory, experiments, and beyond. D. Walsh, **D. Guironnet**

- 2:05** 68. Continuous reactor cascades for block copolymer synthesis. **E. Baeten**, T. Junkers
- 2:30** 69. Oxygen free copper(II) mediated polymerisation in a flow reactor. **D.M. Haddleton**, M. Laurel, A. Marathianos, E. Liarou, A. Anastasaki, R. Whitfield
- 2:55** Intermission.
- 3:25** 70. Continuous primary processing: From an R&D concept to implementation at an industrial scale. **C. Wiles**
- 3:50** 71. Continuous flow polymerizations: Lessons from the factory floor. Y. Zhu, I. Martinez-Botella, T. Kohl, D. Fullston, M. Skidmore, C. Hornung, J. Tsanaktsidis, **S. Saubern**
- 4:15** 72. Intelligent continuous-flow polymer synthesis. **N. Warren**

SECTION E

Manchester Grand Hyatt San Diego
Hillcrest A

Roy W. Tess Award: Symposium in Honor of Raymond H. Fernando

E. D. Sapper, *Organizer, Presiding*

- 1:30** 73. Influence of the first normal stress differences on model HEUR-thickened waterborne paints brush drag. **J.J. Rabasco**, D. Saucy, A. Van Dyk, T. Chatterjee, M. Linsen, A.I. Nakatani, V. Ginzburg
- 2:00** 74. Latex paint open time analysis through rheological methods. **A.Z. Prosser**
- 2:30** Intermission.
- 3:00** 75. Why can't we agree on VOCs?. **D.R. Jones**
- 3:30** 76. Hydrophobically modified, ethoxylated urethane (HEUR) associative thickeners: Thickening mechanism sensitivities to coating formulation variables. **R.H. Fernando**

SECTION F

Manchester Grand Hyatt San Diego
Cortez Hill A/B

Polymer Science & Engineering in Microelectronics

C. J. Ellison, *Organizer*

Q. Lin, *Organizer, Presiding*

J. F. Cameron, *Presiding*

- 1:30** Introductory Remarks.
- 1:40** 77. Reversibly cross-linked nonwoven fibers: Sustainability meets melt blowing. **C.J. Ellison**, K. Jin, F.S. Bates
- 2:10** 78. Chemical amplification: Past, present, and future - DuPont's perspective. **J.F. Cameron**

- 2:40 79. Metal oxide nanoparticles and MOF-inspired clusters for microlithography. **C.K. Ober**, K. Sakai, H. Xu, E.P. Giannelis
- 3:10 Intermission.
- 3:40 80. Morphological evolution of poly(solketal methacrylate)-*block*-polystyrene copolymers in thin films. D. Yu, D.M. Smith, H. Kim, J.K. Mapas, J. Rzayev, **T.P. Russell**
- 4:10 81. Rapid and selective deposition of patterned thin films via spin coating. **C.M. Bates**

SECTION G

Manchester Grand Hyatt San Diego
Harbor H

Emulsification & Encapsulation by Soft Matter Techniques

Conventional & Non-conventional Multiphase Systems

Cosponsored by POLY

Financially supported by Princeton Chemical and Biological Engineering; Solvay; Givaudan; MANE F. Ganachaud, R. K. Prudhomme, *Organizers*
R. D. Priestley, *Organizer, Presiding*

- 1:30 82. Designer polypeptides and electrostatic assembly for RNA-protein enhanced delivery. **P.T. Hammond**
- 2:10 83. Reinforced and magnetically navigated polyelectrolyte-based micro(nano)capsules as promising microreactors. **S. Zapotoczny**, K. Chojnacka-Gorka, J. Odrobinska, E. Gumieniczek-Chlopek, J. Szafraniec, M. Janik
- 2:35 84. Ultrasound-sensitive fluororous nanoemulsions enable image-guided cytosolic protein delivery. **J.N. Sloand**, E. Cook, T. Zimudzi, S. Zinck, J. Simon, S.A. Showalter, S.H. Medina
- 3:00 85. Speedy and robust ICG J-aggregation in polymer micelle through hierarchical assembling for cancer theranostics. **L. Tian**
- 3:25 Intermission.
- 3:55 86. Polyion complex vesicles (PICsomes) assembled from block ionomers in nanomedicine application. **K. Kataoka**
- 4:25 87. Precise engineering of nanocapsules using nanoprecipitation. X. Yan, R. Ramos, F. Ganachaud, **J. Bernard**
- 4:55 88. Multiphase fluid mixtures without surfactant and their applications. **J. Bibette**

Characterization of Plastics in Aquatic Environments

Sponsored by POLY, Cosponsored by ANYL, BIOL, CEI, ENVR, I&EC, PMSE and PRES

MONDAY MORNING – PMSE

SECTION A

Manchester Grand Hyatt San Diego
Harbor I

Novel Polymeric Materials & Polymer-Based Processes for Energy-Efficient Treatment of Water & Resource Recovery

Fundamentals of Water & Solute Transport in Membranes

Cosponsored by ENVR

Financially supported by North American Membrane Society, Center for Materials for Water & Energy Systems (M-WET); Advanced Materials for Energy Water Systems Center (AMEWS); ACS Innovative Projects Grant D. Bhattacharyya, S. B. Darling, B. D. Freeman, E. Hatakeyama, W. A. Phillip, C. M. Stafford, *Organizers*
Y. Ding, *Organizer, Presiding*
T. Squires, *Presiding*

- 8:25 Introductory Remarks.
- 8:30 89. Comparison of water and salt transport properties in ion exchange and desalination membranes. R.S. Kingsbury, J. Wang, **O. Coronell**
- 9:10 90. Investigating the effect of carbonyl content on water and salt dynamics in interfacially polymerized polyamide membranes. **V. Witherspoon**, K. Ito, M. Tyagi, C.L. Soles, R. Nieuwendaal, C.M. Stafford, V. Oleshko
- 9:35 91. Studying surface hydration of polymers with ambient pressure XPS. **M.E. Barry**, P. Aydogan Gokturk, E.J. Crumlin, R.A. Segalman
- 10:00 92. Fouling mechanisms in constant flux crossflow ultrafiltration. A.Y. Kirschner, **Y. Cheng**, D.R. Paul, R. Field, B.D. Freeman
- 10:25 Intermission.
- 10:40 93. Interfacial polymerization kinetics for reverse osmosis membranes. **T. Squires**, A. Nowbahar, V. Mansard, M. Paul, J. Mecca, T. Arrowood
- 11:05 94. Modulation of interface solute selectivity via chemical group patterning. **J. Monroe**, M. Shell
- 11:30 95. Activity model of membrane transport for volatile solutes and water: Concentration and pressure dependent transport of trace and high concentrations. **B. Mickols**, B. Van der Bruggen, M. Zhaohuan

SECTION B

Manchester Grand Hyatt San Diego
Cortez Hill C

Design, Synthesis & Engineering of Polypeptides for Biological & Biomedical Application

Design & Synthesis of Polypeptide Materials

Cosponsored by POLY

T. J. Deming, M. J. Vicent, L. Yin, *Organizers*

J. Cheng, *Organizer, Presiding*

J. Kramer, *Presiding*

- 8:00** **96.** Diversity of polypeptide materials: From simple linear homopolymer synthesis to bottlebrush architectures, polyelectrolytes, block polymer hydrogels, drug delivery systems, conductive composite materials, and organic radical polymers. **K.L. Wooley**
- 8:30** **97.** Introduction of complex side-chain functionality into polypeptides to develop new properties. **T.J. Deming**
- 9:00** **98.** Synthesis of brush polypeptides. **J. Cheng**
- 9:30** **99.** Enzymatic noncovalent synthesis (ENS) for peptide assemblies. H. He, H. Wang, Z. Feng, B. Kim, D. Yang, J. Wang, A. Shy, **B. Xu**
- 10:00** Intermission.
- 10:20** **100.** Moisture-tolerant and operationally simple synthesis of polypeptides by ring-opening polymerization of α -amino acid derived N-thiocarboxyanhydrides. **D. Zhang**, D. Siefker, J. Cao, A. Williams
- 10:50** **101.** Glycocalyx engineering with tunable synthetic glycopolypeptides. **J. Kramer**, Z. Clauss, C. Wardzala
- 11:20** **102.** pH-sensitive histidine-based block copolypeptide nanostructures for drug delivery. **C. Noble Jesus**, J. Forth, A. Duro Castano, E. Liatsi-Douvitsa, L. Ruiz-Perez, G. Battaglia
- 11:40** **103.** Rational design of supramolecular dynamic protein assemblies using a micelle-assisted activity-based protein labeling technology. B.S. Sandanaraj, **M. Mullapudi**, P.J. Bhandari, S. Kumar, V.K. Aswal

SECTION C

Manchester Grand Hyatt San Diego
Harbor H

PMSE Future Faculty

Financially supported by Tosoh Bioscience, LLC; IBM; Solvay Specialty Polymers USA, LLC; Royal Society of Chemistry; Jasco

C. A. DeForest, E. Pentzer, *Organizers*

J. Bae, T. M. Swager, *Presiding*

- 8:00** **104.** Withdrawn
- 8:30** **105.** Exploiting self-assembly in photoresponsive materials. **B.R. Donovan**, T.J. White
- 9:00** **106.** Next-generation mechano-responsive polymers: See the force, tame the force, and wield the force. **Y. Liu**
- 9:30** Intermission.
- 10:00** **107.** Click nucleic acids as low-cost detection probes for mononucleotide repeat sequences. **H. Culver**, J. Sinha, T. Prieto, C. Bowman
- 10:30** **108.** “Breathing” atom-transfer radical polymerization and applications of enzyme degassing systems. **A.E. Enciso**, J.F. Stoddart, K. Matyjaszewski
- 11:00** **109.** Programming protein interactions to access protein diblock copolymer assemblies. **C. Figg**, O.G. Hayes, P.H. Winegar, J.R. McMillan, C.A. Mirkin

SECTION D

Manchester Grand Hyatt San Diego
Harbor G

Continuous Flow Chemistry in Polymer Science

C. Boyer, F. A. Leibfarth, *Organizers*

T. Junkers, *Organizer, Presiding*

- 8:00** **110.** Flow chemistry and scalable surface grafted polymerization. **R.C. Advincula**
- 8:25** **111.** Flow-mediated PET-RAFT polymerization for upscaled and consistent polymer production. N. Corrigan, **C. Boyer**
- 8:50** **112.** Copper mediated polymerization in flow. **A. Anastasaki**, D.M. Haddleton, E. Liarou, A. Marathianos
- 9:15** **113.** Continuous-flow photo-controlled radical polymerization with concentrated monomer/polymer solutions. **M. Chen**, Y. Zhou, F. Zhong
- 9:40** **114.** Continuous-flow chemistry for the determination of comonomer reactivity ratios. **M.H. Reis**, F.A. Leibfarth
- 10:00** Intermission.

- 10:30 115.** High conversion PET-RAFT flow synthesis of sequence-defined oligomers in aqueous solution. A. Aerts, C. Reese, Y. Zhou, C. Boyer, J. Xu, A. Postma, S. Saubern, **G. Moad**
- 10:55 116.** Flow RAFT polymerization for multiblock copolymer synthesis. **S. Perrier**
- 11:20 117.** Anionic polymerization using flow microreactor systems and its applications to syntheses of structurally well-defined polymers. **A. Nagaki**

SECTION E

Manchester Grand Hyatt San Diego
Hillcrest A

Unique & Complex Polymer Architectures

Networks

Cosponsored by POLY

K. C. Bentz, D. A. Savin, *Organizers, Presiding*

- 8:30 118.** Elucidating the effects of hydrophobicity and branching in amphiphilic linear-dendritic block copolymers (LDBC)s. **D.L. Watkins**
- 9:00 119.** Auxetic behavior in fiber networks. **M. Shofner**, P. Verma, A. Griffin
- 9:30 120.** Creating and unraveling polymer structures with Diels-Alder chemistry. E. Wilborn, C.G. Gregory, T.M. Page, W. Ramos, M. Hunter, **P.J. Costanzo**
- 10:00 121.** Designing properties by architecture in highly aromatic polymers. **B. Voit**, R. Pöttsch, Q. Wei
- 10:20** Intermission.
- 10:35 122.** Metallo-supramolecular polymers as a route to poly[n]catenanes. **S.J. Rowan**
- 11:05 123.** Sustainable polymer network designs using robust B–O and Si–O dynamic covalent bonds. **Z. Guan**
- 11:35 124.** Synthetic approaches to model reference materials: Design and characterization of architecturally ‘perfect’ branched polyolefins. **S.V. Orski**, L.A. Kassekert, W. Farrell, M.A. Hillmyer, K. Beers
- 11:55 125.** Block copolyMOFs: Morphology control and moving towards functional polymer-MOF hybrid materials. **S. Ayala**, K.C. Bentz, S. Cohen

SECTION F

Manchester Grand Hyatt San Diego
Cortez Hill A/B

Polymer Science & Engineering in Microelectronics

Q. Lin, *Organizer*

C. J. Ellison, *Organizer, Presiding*

M. A. Hillmyer, *Presiding*

- 9:00 126.** Developing the concept of chemical amplification with Grant Willson. **J. Frechet**
- 9:30 127.** Selective grafting of polymer brushes enables directed self-assembly of high- χ block copolymers. **J. Koh**, J. Kim, Q. Zhu, N. Ito, R. Mizuochi, G. Blachut, J. Doise, S.M. Sirard, C.J. Ellison, N.A. Lynd, C.G. Willson
- 10:00 128.** Area selective atomic layer deposition for advanced nanofabrication. **S.F. Bent**
- 10:30** Intermission.
- 11:00 129.** Block copolymers for production of 50 \square lines and spaces for nanoimprint templates. **J. Kim**, X. Yang, S.M. Sirard, Q. Zhu, N. Ito, A. Lane, G. Blachut, Y. Asano, M.J. Maher, C.J. Ellison, C.R. Baiz, N.A. Lynd, C.G. Willson
- 11:30 130.** Dendrimers as an ideal calibration for mass spectrometry. **S.M. Grayson**

SECTION G

Manchester Grand Hyatt San Diego
Hillcrest B/C

Emulsification & Encapsulation by Soft Matter Techniques

Polymerization-Induced Self Emulsification & Encapsulation

Cosponsored by POLY

Financially supported by Princeton Chemical and Biological Engineering; Solvay; Givaudan; MANE

F. Ganachaud, R. D. Priestley, *Organizers*

R. K. Prudhomme, *Organizer, Presiding*

- 8:30 131.** Functional encapsulation by the miniemulsion process. **K. Landfester**
- 9:00 132.** New materials from thermodynamically stable dispersions. **J. Texter**
- 9:25 133.** Synthesis and investigation of amphiphilic polypeptoid-functionalized halloysite nanotubes (HNTS) as stabilizers towards oil spill remediation. **T. Yu**, L.T. Swientoniewski, M. Omarova, I. Negulescu, A. Panchal, N. Jiang, O.A. Darvish, Y.M. Lvov, D.A. Blake, V.T. John, D. Zhang

- 9:50 134.** Encapsulation within emulsion-templated elastomers: water and fertilizer for plant growth. K. Kapilov-Buchman, I. Berezovska, A. Stern, E. Asulin, D. Canfi, R. Effenberger, **M.S. Silverstein**
- 10:15** Intermission.
- 10:45 135.** Drug monomer: Methods for maximized loading of biologics and small molecular therapeutics on triggerable polymers and nanoparticles. **N.C. Gianneschi**, Y. Liang, M.T. Proetto, C. Battistella, O. Berger, W. Choi, H. Sullivan, M.A. Touve, K. Christman
- 11:15 136.** Radical ring-opening copolymerization-induced self-assembly (rROPISA). E. Guegain, C. Zhu, E. Giovanardi, **J. Nicolas**
- 11:40 137.** Biodegradable latex: Emulsion ring opening polymerization. **D.D. Harrier**, D. Guironnet
- 12:05** Concluding Remarks.

Future of Biomacromolecules at a Crossroads of Polymer Science & Biology

Synthetic Cells

Sponsored by POLY, Cosponsored by BIOL, CARB, CELL, COLL, ENVR, MEDI, PHYS and PMSE

MONDAY AFTERNOON – PMSE

SECTION A

Manchester Grand Hyatt San Diego
Harbor I

Novel Polymeric Materials & Polymer-Based Processes for Energy-Efficient Treatment of Water & Resource Recovery

Energy-Efficient Water Purification & Resource Recovery

Cosponsored by ENVR

Financially supported by North American Membrane Society, Center for Materials for Water & Energy Systems (M-WET); Advanced Materials for Energy Water Systems Center (AMEWS); ACS Innovative Project Grant
D. Bhattacharyya, S. B. Darling, Y. Ding, B. D. Freeman, E. Hatakeyama, C. M. Stafford, *Organizers*
W. A. Phillip, *Organizer, Presiding*
R. Sujanani, *Presiding*

- 1:25** Introductory Remarks.
- 1:30 138.** Nanoporous membranes from block polymer precursors for ultrafiltration of water. **M.A. Hillmyer**
- 2:10 139.** Self-assembled block copolymer: Membrane protein nanosheets as high-performance membrane materials. **Y. Tu**, W. Song, T. Ren, R. Hickey, M. Kumar

- 2:35 140.** Gyroid thin-film composite membranes for ultrafiltration processes. **Q. Zhu**, P. Meyer, J.D. Moon, Y. Cheng, J. Koh, J. Kim, B.D. Freeman, C.J. Ellison, N.A. Lynd, C.G. Willson
- 3:00 141.** Developing super-tough ion exchange membranes for water and energy applications. **R. Sujanani**, M. Allen, Z.A. Page, D.R. Paul, B.D. Freeman
- 3:25** Intermission.
- 3:40 142.** Sugar-based magnetic hybrid nanoparticles for recovery of crude oil from aqueous environments. **M. Dong**, Y. Song, L. Su, J.A. Flores, H. Wang, D.K. Tran, K.L. Wooley
- 4:05 143.** Thermal conductive molecular hierarchical assemblies composed of filamentous viruses. **T. Sawada**, N. Ueda, Y. Murata, H. Marubayashi, S. Nojima, J. Morikawa, T. Serizawa
- 4:30 144.** Processes for gold recovery from electronic waste using porous porphyrin polymer and adsorbent regeneration. **J. Son**, C.T. Yavuz, Y. Hong, J. Chung, T. Nguyen, J. Han

SECTION B

Manchester Grand Hyatt San Diego
Cortez Hill C

Design, Synthesis & Engineering of Polypeptides for Biological & Biomedical Application

Polypeptides for Drug & Gene Delivery Applications

Cosponsored by POLY

J. Cheng, T. J. Deming, M. J. Vicent, *Organizers*
L. Yin, *Organizer, Presiding*
G. N. Tew, *Presiding*

- 1:00 145.** Amino acid and peptide functionalized unique molecular carriers for universal delivery of various RNAs. **Z. Guan**
- 1:30 146.** Poly(ethylene glycol)-polypeptide block copolymers for delivering nucleic acid-based therapeutics into brain. **K. Kataoka**
- 2:00 147.** Anti-cancer/anti-inflammation gene delivery via membrane-penetrating cationic helical polypeptides. H. Ye, Y. Li, C. Ge, **L. Yin**
- 2:30 148.** Redesigning cationic lytic peptides to promote the delivery of biomacromolecules into cell interiors. **S. Futaki**
- 3:00** Intermission.
- 3:20 149.** Intracellular antibody delivery via protein transduction domain mimics. **G.N. Tew**
- 3:50 150.** Robust polypeptide-based nanovehicles for controlled drug and gene delivery. X. Gu, M. Qiu, C. Deng, **Z. Zhong**

- 4:20 151.** Synthetic polypeptide polymers as simplified analogues of conjugated proteins. M. Nguyen, J. Stigliani, E. P. Arroni, L. Severac, F. Makni, J. Aujard-Catot, G. Pratviel, **C. Bonduelle**
- 4:40 152.** Synthesis of block copolymers of polyamides through ring-opening polymerization catalyzed by redox-switchable iron alkoxide complexes. **M. Thompson**, S. Gonsales, J. Byers

SECTION C

Manchester Grand Hyatt San Diego
Harbor H

PMSE Young Investigator Symposium

Financially supported by Tosoh Bioscience, LLC; IBM; Solvay Specialty Polymers USA, LLC; Royal Society of Chemistry; Jasco

A. P. Esser-Kahn, D. L. Watkins, *Organizers*
S. Alexander, *Presiding*

- 1:00** Introductory Remarks.
- 1:05 153.** New routes to sustainable polymeric materials. **G.W. Coates**
- 1:45 154.** Reversibly photocontrolled stress-relaxing networks. **J.A. Kalow**
- 2:15 155.** Polymer-based thermal diodes and switches. **Z. Tian**
- 2:45** Intermission.
- 3:00 156.** Hierarchical control of hydrogel properties with precise polymer microstructure. **A.M. Rosales**
- 3:30 157.** Understanding reaction-crystallization mechanism of porous coordination polymers for selected applications. **G. Giri**
- 4:00 158.** Withdrawn

SECTION D

Manchester Grand Hyatt San Diego
Harbor G

Journal of Polymer Science Innovation Award: Symposium in Honor of Patricia Dankers

Cosponsored by WCC
Financially supported by Wiley
J. Mahoney, *Organizer*
C. J. Hawker, *Organizer, Presiding*

- 1:30 159.** Evolution of dynamic supramolecular polymer networks for biomedicine. **T. Weil**
- 2:00 160.** Supramolecular affinity in dynamic hydrogel biomaterials. **M.J. Webber**
- 2:30 161.** Synthetic fibrous hydrogels: Responsive, adaptable, and highly biomimetic. **P.H. Kouwer**
- 3:00 162.** Chemical strategies for cell-instructive interfaces. **P. Jonkheijm**

- 3:30 163.** Designing dynamic hydrogels for tissue engineering. **M.B. Baker**
- 4:00 164.** Supramolecular polymerizations: Fundamental insights into adaptive biomaterials. **E.W. Meijer**
- 4:30 165.** Supramolecular polymeric materials as synthetic extracellular matrices: Importance of dynamics and robustness. **P.Y. Dankers**

SECTION E

Manchester Grand Hyatt San Diego
Hillcrest A

Unique & Complex Polymer Architectures

Materials

Cosponsored by POLY
K. C. Bentz, D. A. Savin, *Organizers*
K. A. Cavicchi, A. S. Veige, *Presiding*

- 1:30 166.** Engineering lubricating polymers under extreme conditions using polymer architecture. B. van Ravensteijn, R. Bou Zerdan, P.B. Corona, K.M. Weigandt, D. Seo, N. Cadirov, T. Watanabe, J. Gerbec, C.J. Hawker, J.N. Israelachvili, **M.E. Helgeson**
- 2:00 167.** Synthesis and properties of multiblock copolypeptide polyion complex hydrogels. **T.J. Deming**
- 2:30 168.** Effect of zone annealing on anisotropic nanoparticle reordering in polymer nanocomposites. **S. Kumar**
- 3:00** Intermission.
- 3:15 169.** Competing effects in the dynamics of soft nanoparticle polymer composites: Confinement vs. chain acceleration. S. Rostom, H. Martin, T. Saito, **M.D. Dadmun**
- 3:35 170.** Synthesis and characterization of soft and high grafting density nanoparticle. **L. Han**, T. White, K. Misichronis, P. Cao, M.D. Dadmun, T. Saito
- 3:55 171.** Lithium-ion conduction through salt-doped, high dispersity poly(styrene-*block*-ethylene oxide-*block*-styrene) lamellae. **H. Xu**, E. Greve, M.K. Mahanthappa
- 4:15 172.** Fabrication of high refractive index, infrared transmitting organically modified chalcogenide (ORMOCHALC) polymers. **D.A. Boyd**, V.Q. Nguyen, C.C. McClain, M.P. Hunt, C.C. Baker, J.D. Myers, W. Kim, J.S. Sanghera

SECTION F

Manchester Grand Hyatt San Diego
Cortez Hill A/B

Polymer Science & Engineering in Microelectronics

Q. Lin, Organizer

C. J. Ellison, Organizer, Presiding

C. J. Hawker, Presiding

- 1:30** **173.** Polymer fibrils, transport pathways, and stretchable electronics. **E. Reichmanis**
- 2:00** **174.** Poly(aldehydes): Phototriggerable polymers for transient devices. A. Engler, J. Jiang, M. Warner, C. Lo, **P. Kohl**
- 2:30** **175.** Advanced functional layer-by-layer assemblies containing MXenes and polyelectrolytes. **J.L. Lutkenhaus**, M. Radovic, M. Green, H. An
- 3:00** Intermission.
- 3:30** **176.** Polyether-based cryoprotectants for quantitative post-thaw recovery of mammalian cells. **N.A. Lynd**, A.A. Burkey, D. Harris, A.V. Hillsley, J. Baltzegar, D.Y. Zhang, N.J. Czarnecki, W. Sprague, A.M. Rosales
- 4:00** **177.** Mind the gap: Making materials with light. **Z.A. Page**
- 4:30** Concluding Remarks.

SECTION G

Manchester Grand Hyatt San Diego
Hillcrest B/C

Toughening of Networks & Gels through Molecular Design

Cosponsored by POLY

Financially supported by ACS Applied Polymer Materials

H. Chung, *Organizer*

C. Bowman, B. D. Vogt, *Organizers, Presiding*

- 1:00** **178.** Nonfouling zwitterionic polymeric elastomer. **S. Jiang**
- 1:30** **179.** Mechanomolecular engineering of tissue-like elastomers. **S. Sheyko**, M. Vantankhah-Varnosfaderani, D. Ivanov, A.V. Dobrynin
- 2:00** **180.** Toughening hydrogels through emulsion templating and triblock copolymer crosslinking. T. Zhang, **M.S. Silverstein**
- 2:20** **181.** Arylene-bridged silsesquioxane networks toughened by rigid particles. **B. Zhu**, D.E. Katsoulis

- 2:40** **182.** Development of tougher polymer composites through interfacial stress relaxation. **C. Bowman**, N. Sowan, L. Cox
- 3:10** **183.** Morphological considerations in the design of mechanically robust aerogels from engineering thermoplastics. **R.B. Moore**, S. Talley
- 3:30** **184.** Is toughening enough? Anti-fatigue-fracture hydrogels. X. Zhao, **S. Lin**
- 4:00** **185.** Structure evolution of supramolecular hydrogels during deformation and stress relaxation. **B.D. Vogt**, R.A. Weiss, C. Wang, C. Wiener
- 4:20** **186.** Spatiotemporal control of hydrogel mechanical properties through visible-light activation of viologen-based macrocrosslinkers. F. Solangi, A. Delawder, K. Liles, A. Natraj, **J.C. Barnes**
- 4:40** **187.** Self-healing yet selectively adhesive hydrogels by the self-assembly of amphiphilic random triblock copolymers. **T. Terashima**

Future of Biomacromolecules at a Crossroads of Polymer Science & Biology

Tissue Engineering

Sponsored by POLY, Cosponsored by BIOL, CARB, CELL, COLL, ENVR, MEDI, PHYS and PMSE

MONDAY EVENING – PMSE

SECTION A

San Diego Convention Center
TBD

Sci-Mix

T. J. Bunning, *Organizer*

8:00 - 10:00

37, 38. See Previous Listings.
295, 297, 298, 302, 304, 305, 307, 308, 309, 310, 311, 317, 322, 327, 328, 332, 336, 340, 345, 346, 347, 352, 354, 355, 359, 360, 361, 363, 368, 372, 375, 379, 380, 381, 382, 383, 384, 387, 388, 391, 394, 395, 420, 423, 443, 478, 479, 484, 502, 519, 524, 535, 537. See Subsequent Listings.

SECTION A

Manchester Grand Hyatt San Diego
Harbor I

Novel Polymeric Materials & Polymer-Based Processes for Energy-Efficient Treatment of Water & Resource Recovery

Energy-Efficient Water Purification & Resource Recovery

Cosponsored by ENVR

Financially supported by North American Membrane Society, Center for Materials for Water & Energy Systems (M-WET); Advanced Materials for Energy Water Systems Center (AMEWS); ACS Innovative Project Grant

S. B. Darling, Y. Ding, B. D. Freeman, E. Hatakeyama, W. A. Phillip, C. M. Stafford, *Organizers*

D. Bhattacharyya, *Organizer, Presiding*

M. Green, *Presiding*

- 8:25 Introductory Remarks.
- 8:30 **188.** Next generation poly(arylene ether sulfone) membranes: Integrating fouling resistance, chlorine tolerance, and water/salt permselectivity. **M. Green**, Y. Yang
- 9:10 **189.** Withdrawn
- 9:35 **190.** Polymer surface functionalization schemes for enhanced removal of heavy metal ions from aqueous solutions. **E. Barry**, J. Elam, S.B. Darling, V. Rozyyev
- 10:00 **191.** Oleo sponge: Advanced oil sorbent prepared using sequential infiltration synthesis. **J. Elam**, E. Barry, J. Libera, A.U. Mane, J.R. Avila, D. DeVitis, K. Van Dyke, S.B. Darling
- 10:25 Intermission.
- 10:40 **192.** Advanced supported ionic liquid (SIL) membranes for p electron cloud mediated separation of aromatics. **S.R. Wickramasinghe**
- 11:05 **193.** Novel amylopectin-graft-poly(methyl acrylate) solidifier for the containment and recovery of oil spills on water. F. Lopes Motta, S.R. Stoyanov, **J.B. Soares**
- 11:30 **194.** Catechol-containing hydrogels as bioinspired filters for water decontamination. **D. Mecerreyes**

SECTION B

Manchester Grand Hyatt San Diego
Cortez Hill C

Design, Synthesis & Engineering of Polypeptides for Biological & Biomedical Application

Bioengineering & Therapeutic Peptides

Cosponsored by POLY

J. Cheng, T. J. Deming, L. Yin, *Organizers*

M. J. Vicent, *Organizer, Presiding*

H. Lu, *Presiding*

- 8:00 **195.** Genetically encoded polypeptides that exhibit phase behavior and self-assemble across multiple length scales. **A. Chilkoti**
- 8:30 **196.** Adaptable protein-engineered hydrogels for organoid culture. **S.C. Heilshorn**
- 9:00 **197.** Investigation of the role of helix conformation in antifouling and low immunogenetic polypeptides. **H. Lu**
- 9:30 **198.** Genetic engineering of elastin-like polypeptides for cancer nanomedicine. **W. Gao**
- 10:00 Intermission.
- 10:20 **199.** Polypeptide-based conjugates as versatile therapeutics as single agents or in combination therapy. O. Zagorodko, F. Rodriguez-Otormin, J. Arroyo-Crespo, D. Chabonnier, A. Duro-Castano, A. Armiñan, **M.J. Vicent**
- 10:50 **200.** *In situ* self assembled biomaterials for bioimaging and therapeutics. **H. Wang**
- 11:20 **201.** Cationic α -polypeptoid polymers for biomedical applications. **A. Kargaard**, A. Heise
- 11:40 **202.** Injectable neuroprotective peptide hydrogels. **B. Sarkar**, X. Ma, P. Iglesias-Montoro, Z. Siddiqui, K. Kim, A.M. Agas, P. Nguyen, J. Haorah, V. Kumar

SECTION C

Manchester Grand Hyatt San Diego
Harbor H

PMSE Young Investigator Symposium

Financially supported by Tosoh Bioscience, LLC; IBM; Solvay Specialty Polymers USA, LLC; Royal Society of Chemistry; Jasco

A. P. Esser-Kahn, D. L. Watkins, *Organizers*

A. Anastasaki, *Presiding*

- 8:00 **203.** Self-immolative polymers: Designing structure, properties, and function. A. Rabiee Kenaree, Q. Sirianni, R. Yardley, B. Fan, **E.R. Gillies**
- 8:40 **204.** Supramolecular biomaterials: From fundamentals to advanced healthcare solutions. **E.A. Appel**
- 9:10 **205.** Solvent-induced self-assembly of triblock copolymers to create nanostructured hydrogels exhibiting plasmonic and photonic band gap properties. **R. Hickey**
- 9:40 Intermission.
- 10:00 **206.** Engineering the shape of macromolecules. D. Walsh, S. Dutta, C.E. Sing, **D. Guironnet**

- 10:30 207.** Dispersity effects in miktoarm star materials. **C.M. Bates**
- 11:00 208.** Versatile perfluorocarbon nanoemulsion theranostics stabilized by responsive poly(2-oxazoline) amphiphiles. **E.M. Sletten**

SECTION D

Manchester Grand Hyatt San Diego
Harbor G

Bioconjugate Chemistry & Lectureship Award: Symposium in Honor of Heather Maynard

Financially supported by Bioconjugate CHEMISTRY
C. G. England, E. Lavik, D. McDaniel, B. Smith, J. van Hest,
G. Zheng, *Organizers*
V. M. Rotello, *Organizer, Presiding*

- 9:00 209.** Penetration and eradication of multidrug-resistant bacterial biofilms using polymer and biopolymer-based nanomaterials. **V.M. Rotello**
- 9:30 210.** Epitope display and delivery using plant VLPs: Concept of prime-boost immunization. **N. Steinmetz**
- 10:00 211.** Ternary composite nanofibers containing chondroitin sulfate scavenge inflammatory chemokines from solution and prohibit squamous cell carcinoma migration. W. Boyle, W. Chen, A. Rodriguez, S. Linn, J. Tolar, K. Lozano, **T.M. Reineke**
- 10:30 212.** Development of peptide/protein conjugates from copper mediated living radical polymerisation. **D.M. Haddleton**
- 11:00 213.** Conjugation of polymers and small molecule drugs to proteins enhances therapeutic efficacy and delivery characteristics. **H.D. Maynard**

SECTION E

Manchester Grand Hyatt San Diego
Hillcrest A

Unique & Complex Polymer Architectures Synthesis & Bio

Cosponsored by POLY
K. C. Bentz, D. A. Savin, *Organizers*
D. A. Boyd, S. V. Orski, *Presiding*

- 8:30 214.** Silyl ketenes building blocks for complex molecules and polymers. Y. Xiang, S. Mitchell, **E. Pentzer**
- 9:00 215.** Use of photoredox-mediated ROMP to access unique polymer architectures. **A.J. Boydston**
- 9:30 216.** Catalytic synthesis and characterization of cyclic polyolefins including cyclic polypropylene. Z. Miao, D. Pal, W. Niu, T. Kubo, S. Gonsales, D.A. Savin, B.S. Sumerlin, **A.S. Veige**

- 10:00 217.** New polymeric materials based on element-blocks. **Y. Chujo**
- 10:20** Intermission.
- 10:35 218.** Enhanced thermal stability of cyclic polypeptoid thin films: Role of interfacially adsorbed chains. **D. Zhang**, N. Jiang
- 11:05 219.** ROMP polymers at biological interfaces. **J.K. Pokorski**
- 11:35 220.** Bundlemer grafts: Coiled-coil peptide-polymer conjugates. **N.I. Halaszynski**, G. Knappe, B.P. Sutherland, C.J. Kloxin

SECTION F

Manchester Grand Hyatt San Diego
Cortez Hill A/B

Innovations in Drug Delivery Systems: Recent Breakthroughs & New Approaches in Formulation, Drug Delivery Mechanisms & Advanced Delivery Systems Polymers for Drug Delivery

Financially supported by Bristol-Myers Squibb
S. Sridharan, *Organizer*
A. Kulshrestha, *Organizer, Presiding*
R. S. Bezwada, *Presiding*

- 8:30** Introductory Remarks.
- 8:35 221.** Development of poly(ester amide) particles for intra-articular drug delivery. **T. Gordon**, I.J. Villamagna, M.B. Hurtig, F. Beier, E.R. Gillies
- 9:00 222.** Thermo-sensitive block copolymers for the local delivery of antibiotics. **R. Yang**, M. Calabrese, B.D. Olsen, D.S. Kohane
- 9:25 223.** Comparison of linear and 4-arm star polyvinylpyrrolidone for aqueous binder jetting additive manufacturing of personalized dosage tablets. **E. Wilts**, D. Ma, Y. Bai, C.B. Williams, T.E. Long
- 9:50 224.** Methylated polysaccharides as low-immunogenic drug delivery system. **L. Pham**, s. Maiti, Z. Liang, S. Manna, J. Shen, A. Esser-Kahn, W. Du
- 10:15** Intermission.
- 10:25 225.** Nitric oxide-releasing polysaccharide hydrogels for treating periodontal disease. **E.S. Feura**, M.H. Schoenfisch
- 10:50 226.** Biodegradable pH-responsive polymeric nanoparticles for intracellular delivery of anticancer therapies. **E. Liatsi-Douvitsa**, A. Akhtar, A. Duro Castano, G. Battaglia
- 11:15 227.** Photoregulated delivery of anticancer drugs with cleavable polymer amphiphiles. **V. Brega**, F. Scaletti, X. Zhang, L. Wang, P. Li, Q. Xu, V.M. Rotello, S.W. Thomas

- 11:40 228.** Dual functional immunostimulatory polymeric prodrug carrier with pendent indoximod for enhanced cancer immunochemotherapy. **Z. Wan, S. Li**

SECTION G

Manchester Grand Hyatt San Diego
Hillcrest B/C

Toughening of Networks & Gels through Molecular Design

Cosponsored by POLY

Financially supported by ACS Applied Polymer Materials

C. Bowman, *Organizer*

H. Chung, B. D. Vogt, *Organizers, Presiding*

- 8:00** Introductory Remarks.
- 8:05 229.** Toughening anion exchange membranes. **M.A. Hickner**
- 8:35 230.** Shaping and structuring supramolecular gels: Beyond the inverted vial. **D.K. Smith**
- 8:55 231.** Ion-conductive and self-healable hydrogels based on an interpenetrating polymer network for a multimodal sensor system. **S. Shin, S. Hwang, D. Oh, J. Park**
- 9:15 232.** Designing corneal implants with supramolecular materials. **A. Feliciano, F. Ruitter, S. Giselbrecht, L. Moroni, P.Y. Dankers, C. van Blitterswijk, M.B. Baker**
- 9:35 233.** Synergistic dynamic covalent and noncovalent bonds for enhanced materials. **D. Konkolewicz, P. Chakma, B. Zhang, Z. Digby, E. Foster, J. Sparks**
- 9:55 234.** Engineering the mechanics of injectable environmentally responsive hydrogels. **T. Hoare**
- 10:25 235.** Quenched polyampholyte hydrogels: Low-temperature properties and energy device applications. **H. Chung, X. Li, T. La, H. Charaya**
- 10:45 236.** Role of topological defects in the mechanics of polymer networks. **B.D. Olsen, A. Arora, T. Lin, W. Zhou**
- 11:15 237.** Universal scaling behaviour during network formation in living polymerizations. **J.L. Mann, A.A. Smith, E.A. Appel**
- 11:35 238.** Architecturally tuning firmness of polymer networks. **A.N. Keith, M. Vantankhah-Varnosfaderani, A.V. Dobrynin, S. Sheyko**
- 11:55** Concluding Remarks.

Henkel Outstanding Graduate Research in Polymer Chemistry in Honor of Jovan Kamcev

Sponsored by POLY, Cosponsored by CHED and PMSE

Polymeric Materials for Water Purification

Sponsored by POLY, Cosponsored by PMSE

Polymeric Materials for Water Purification

Sponsored by POLY, Cosponsored by PMSE

TUESDAY AFTERNOON – PMSE

SECTION A

Manchester Grand Hyatt San Diego
Harbor I

Novel Polymeric Materials & Polymer-Based Processes for Energy-Efficient Treatment of Water & Resource Recovery

Energy-Efficient Water Purification & Resource Recovery

Cosponsored by ENVR

Financially supported by North American Membrane Society, Center for Materials for Water & Energy Systems (M-WET); Advanced Materials for Energy Water Systems Center (AMEWS); ACS Innovative Project Grant

D. Bhattacharyya, S. B. Darling, Y. Ding, B. D. Freeman, E. Hatakeyama, W. A. Phillip, C. M. Stafford, *Organizers*

I. C. Escobar, D. Miller, *Presiding*

- 1:25** Introductory Remarks.
- 1:30 239.** Design of hierarchical membranes for efficient oil/water separation and anti-oil fouling. **S. Yang**
- 2:10 240.** Pore functionalized membranes: Water applications and material science advances. **D. Bhattacharyya, H. Wan, A. Saad, S. Islam, A. Aher**
- 2:35 241.** Controlled post-assembly functionalization of nanoporous copolymer membranes that exhibit distinct multi-functionality. **J.R. Hoffman, A. Mikes, M. Loscocco, W.A. Phillip**
- 3:00 242.** Fabrication of reactive membranes with phosphorene-based pore fillers. **A. Mills, J. Eke, I.C. Escobar**
- 3:25** Intermission.
- 3:40 243.** Photothermal membrane distillation facilitated by a mussel-inspired polydopamine coating. **X. Wu, Q. Jiang, D. Ghim, S. Singamaneni, Y. Jun**
- 4:05 244.** Adsorption of organic micropollutants to polymer surfaces probed by second harmonic scattering laser spectroscopy. **D. Miller, W. Cole, H. Wei, S. Nguyen, C. Harris, R.J. Saykally**
- 4:30 245.** Long alkyl chain methacrylate copolymers as wax inhibitors for crude oil production. **M. Petr, R.P. Woodworth, S. Camacho, L. Rhodes, A.D. Hughes, S. Potisek, C.L. Jackson, P. Eastman, T. Fitzgibbons, B. Winniford, L. Reyes**

SECTION B

Manchester Grand Hyatt San Diego
Cortez Hill C

Design, Synthesis & Engineering of Polypeptides for Biological & Biomedical Application

Design & Applications of Functional Polypeptides

Cosponsored by POLY

J. Cheng, T. J. Deming, M. J. Vicent, L. Yin, *Organizers*

J. P. Schneider, R. Ulijn, *Presiding*

- 1:00** 246. Rechargeable antibacterial hydrogels from self-assembling peptides and molecular recognition. **J.P. Schneider**
- 1:30** 247. Expressing and characterizing EK fusion proteins. **S. Jiang**
- 2:00** 248. Metabolite-responsive peptide nanostructures. **R. Ulijn**
- 2:30** 249. Amicidin- α and amicidin- β : Amino acid block copolymers in development for prevention and treatment of infection in surgery and trauma. **M.P. Bevilacqua**, D.J. Huang, T.J. Deming
- 3:00** Intermission.
- 3:20** 250. Design and construction of functional peptide based materials for therapeutic and diagnostic applications. **X. Zhang**
- 3:50** 251. Rational design of nanocarrier for small molecule delivery. **T. Xu**, M. Lim, B. Jung
- 4:20** 252. Nanofibrous peptide hydrogels for modulating angiogenic responses of implanted polymeric scaffolds. Z. Siddiqui, B. Sarkar, K. Kim, R. Paul, A. Kumar, J. Yang, **V. Kumar**
- 4:40** 253. Peptide-graphene conjugates as biomaterials with structure-assembly control. **K. Eckhart**, S.A. Sydlik

SECTION C

Manchester Grand Hyatt San Diego
Harbor H

PMSE Young Investigator Symposium

Financially supported by Tosoh Bioscience, LLC; IBM; Solvay Specialty Polymers USA, LLC; Royal Society of Chemistry; Jasco

A. P. Esser-Kahn, D. L. Watkins, *Organizers*

Q. Michaudel, *Presiding*

- 1:00** 254. New synthetic polymers for the preparation of smart droplets and to enable autonomous processes. **T. Emrick**
- 1:40** 255. Synthesizing precise macromolecules through new pathways: Alkylborane initiation and functionalization-induced self-assembly. **A.J. Magenau**

- 2:10** Intermission.
- 2:30** 256. New opportunities in polymer synthesis using twisted amides. **W. Gutekunst**, M. Xu
- 3:00** 257. Modifying polymer properties through controlled hierarchical branching. **M. Zhong**, A. Le, M. Cao, R. Liang
- 3:30** 258. Stereoselective polymerization of vinyl ethers: New class of polar thermoplastics. **F.A. Leibfarth**
- 4:00** Concluding Remarks.

SECTION D

Manchester Grand Hyatt San Diego
Harbor G

Advances in Bioconjugate Materials for Biomedical Applications

Cosponsored by POLY

Financially supported by Bioconjugate Chemistry

C. G. England, E. Lavik, D. McDaniel, B. Smith, J. van Hest, *Organizers*

V. M. Rotello, G. Zheng, *Organizers, Presiding*

- 1:30** 259. Porphyrin nanoemulsion as a cancer theranostic platform. **G. Zheng**
- 1:55** 260. Nanoparticle probes for multimodality molecular imaging in living subjects. **J. Rao**
- 2:20** 261. Engineering personalized peptide-based cancer nanovaccines. H. Kakwere, H. Zhang, A. Kheirloom, **K. Ferrara**
- 2:45** 262. Avoiding the endosomal trap: Direct cytosolic delivery of nucleic acids and proteins (and CRISPR) through membrane fusion processes. **V.M. Rotello**
- 3:10** 263. Chemically functionalized macrophages as cell-based delivery tools for cancer. **M.E. Farkas**
- 3:25** Intermission.
- 3:40** 264. Interfacing mesoporous silicon nanoparticles with cells and tissues. **M.J. Sailor**
- 4:05** 265. See infrared via upconversion. **G. Han**
- 4:30** 266. Supramolecular “click” chemistry: Noncovalent approach to recognition specificity. **M.J. Webber**
- 4:45** 267. Platelet-delivered immunotherapies. **Z. Gu**

SECTION E

Manchester Grand Hyatt San Diego
Hillcrest A

Unique & Complex Polymer Architectures Synthesis & Bio

Cosponsored by POLY

K. C. Bentz, D. A. Savin, *Organizers*

P. J. Costanzo, D. Zhang, *Presiding*

- 1:30** 268. Designing protein-mimetic polymer architectures. **A. Knight**

- 2:00** **269.** Architectural control of isosorbide-based polyethers via ring-opening polymerization. D.J. Saxon, M. Nasiri, M. Mandal, S. Maduskar, P.J. Dauenhauer, C.J. Cramer, A. LaPointe, **T.M. Reineke**
- 2:30** **270.** Getting “lit” with polymers. **Z.A. Page**
- 3:00** Intermission.
- 3:15** **271.** Using bioinspired polypeptoids to understand how chain shape influences self-assembly. B. Yu, A. Patterson, E. Davidson, **R. Segalman**
- 3:45** **272.** Cyclic and supramolecular architectures via knotty templates. **R.C. Advincula**
- 4:15** **273.** Self-assembly behaviour of organic-inorganic hybrid triblock copolymer solid electrolytes. **S. Chakraborty**, G. Sethi, I. Villaluenga, N.P. Balsara

SECTION F

Manchester Grand Hyatt San Diego
Cortez Hill A/B

Innovations in Drug Delivery Systems: Recent Breakthroughs & New Approaches in Formulation, Drug Delivery Mechanisms & Advanced Delivery Systems

Bench to Bedside

Financially supported by Bristol-Myers Squibb

A. Kulshrestha, *Organizer*

S. Sridharan, *Organizer, Presiding*

R. Shah, *Presiding*

- 1:55** **274.** Patient tolerability with high-viscosity, large-volume subcutaneous infusions: Need for something different. **M. Huddleston**
- 2:20** **275.** Clinical translation of drug-delivery technologies: Case study in ocular delivery. **K. Nagapudi**
- 2:45** **276.** Designing successful amorphous solid dispersions. **I. Yates**
- 3:10** Intermission.
- 3:20** **277.** Parental drug delivery using *in situ* gelling PLGA system: Tuning release kinetics. **R. Shah**, S. Thati, Y. Zhu, N. Mathias
- 3:45** **278.** Polymers beyond PLGA for drug delivery and medical device applications. **R.S. Bezwada**, N. Srivastava
- 4:10** **279.** Absorbable polyurethanes for soft tissue and bone applications. **N. Srivastava**, R.S. Bezwada
- 4:35** **280.** Importance of particle surface energy in dry powder drug delivery modalities. **A.S. Narang**

SECTION G

Manchester Grand Hyatt San Diego
Hillcrest B/C

Toughening of Networks & Gels through Molecular Design

Cosponsored by POLY

Financially supported by ACS Applied Polymer Materials

C. Bowman, B. D. Vogt, *Organizers*

H. Chung, *Organizer, Presiding*

H. Zeng, *Presiding*

- 1:30** **281.** Developing bioinspired multifunctional gel adhesives through tunable intermolecular and surface interactions. **H. Zeng**
- 2:00** **282.** Mussel-inspired cellulose nanocomposite tough hydrogels with synergistic self-healing, adhesive, and strain-sensitive properties. **C. Shao**, J. Yang
- 2:20** **283.** Bio-inspired supramolecular interpenetrating networks: Impacts of supramolecular confinement on mechanics and stimuli-responsive behavior. **C.B. Thompson**, S. Chatterjee, L. Korley
- 2:40** **284.** Tailoring the mechanical properties of bioinspired amphiphilic polymer conetwork composites. **S.T. Velasquez**, D. Jang, L. Korley, N. Bruns
- 3:00** **285.** Kinetic trends in associative polymer networks. **J.A. Kalow**
- 3:30** **286.** Toughened graft copolymer blends from the accelerated thermal ring opening polymerization and crosslinking of benzoxazine monomers by end-group functionalized polymers. **D.A. Rider**
- 3:50** **287.** System-level structural control of self-assembled nanoparticle polymer composites. **R. Macfarlane**
- 4:10** **288.** Eutectic phase diagram of BDNPA and BDNPF. **A.S. Edgar**, D. Yang
- 4:30** **289.** Controlling viscoelasticity of phase change salogels via crosslinker geometry. **P. Karimineghlani**, S.A. Sukhishvili
- 4:50** **290.** Toughening block copolymer ion gels via installation of a photocoupled secondary network. **A.W. May**, T.S. Bailey
- 5:10** **291.** Self-reinforced hydrogels with hierarchical homocomposite molecular, nano-, and micro-scale networks. **A. Williams**, S. Roh, O.D. Velev

Biomacromolecules/Macromolecules Young Investigator Award

Sponsored by POLY, Cosponsored by PMSE

Polymeric Materials for Water Purification

Sponsored by POLY, Cosponsored by PMSE

Polymeric Materials for Water Purification

Sponsored by POLY, Cosponsored by PMSE

TUESDAY EVENING – PMSE

SECTION A

San Diego Convention Center

TBD

PMSE/POLY Poster Session

Advances in Bioconjugate Materials for Biomedical Applications

Cosponsored by POLY

T. J. Bunning, *Organizer*

5:00 - 7:00

292. Characterization and antibacterial activity of controlled silver nanoparticles biosynthesized using extract of *Gongronema latifolium*. **S.O. Aisida**, I. Ahmad, F. Ezema

SECTION A

San Diego Convention Center

TBD

PMSE/POLY Poster Session

Design, Synthesis & Engineering of Polypeptides for Biological & Biomedical Applications

Cosponsored by POLY

T. J. Bunning, *Organizer*

5:00 - 7:00

293. Peptide-functionalized biodegradable polymers for universal, safe, and efficient delivery of various RNAs. **D. Yang**, A. Eldredge, C. Hickey, H. Muradyan, Z. Guan

SECTION A

San Diego Convention Center

TBD

PMSE/POLY Poster Session

General Posters/New Concepts in Polymeric Materials

Cosponsored by POLY

T. J. Bunning, *Organizer*

5:00 - 7:00

294. Electrospun polymeric nanofibers incorporated with carbon nanofillers for water treatment applications. **A.K. Assaifan**, M. Luqman, M.O. Aijaz, N. Al Habis, H.F. Al-Harbi

295. Block copolymers containing stable radical and fluorinated blocks with long-range ordered morphologies prepared by anionic polymerization.

A. Cintora, H. Takano, M. Khurana, T. Hayakawa, C.K. Ober

296. Dielectric relaxation and conductivity studies on lyotropic liquid crystal mesophases of block copolymer/ionic liquid mixtures. **A. Bandegi**, M.M. Garcia, J. Banuelos, R. Foudazi

297. Antifouling properties of nitroxide modified surface active siloxane block copolymers. **A. Leonardi**, N. Duzen, C. Zhang, M.E. Barry, J.A. Finlay, N. Aldred, A.S. Clare, R.A. Segalman, C.K. Ober

298. Visualizing out of equilibrium behavior of polystyrene-block-poly(acrylic acid) (PS-PAA) self-assembled structures using liquid-phase electron microscopy. **A. Rizvi**, J.P. Patterson

299. Development of polymer nanoparticles adsorbing α -glucosidase for diabetes treatment. **A. Masuda**, H. Koide, H. Egami, Y. Hamashima, N. Oku, T. Asai

300. Hydrogel formation using thiol-functionalized lignosulfonate by thiol-ene click reaction. **B. Jeon**, J.A. Belgodere, J. Choe, S.A. Zamin, J.P. Jung, M. Kim

301. Synthesis and characterization of metal-containing polymers: Synthesis of organotin-containing synthetic nucleic acids from thymidine and their ability to inhibit human pancreatic and brain cancer cell lines. **C.E. Carraher**, J. Frank, M. Roner, L. Chen, Z.M. Rabinowitz, L. Miller, S. Jafri, A.H. Patel, F. Mosca, P. Slawek, P. Thaker, A. Zamora, F. Russell, F. Fox IV, Y. Rigaud

302. Ratiometric pH imaging with a dendritic CEST MRI contrast agent. **C.J. Kombala**, M.D. Pagel

303. Salicylic acid based biodegradable, biocompatible poly(anhydride esters) for bone regeneration applications. **C. Kulkarni**, D. Graves, K.E. Uhrich

304. Design and fabrication of a pilot-scale desktop polymer melt processing system. **D.M. Wirth**, Y. Zheng, J.K. Pokorski

305. Novel liquid crystalline brush-like copolymers for photonic properties from visible to near-infrared spectrum. **D. Ndaya**, R. Bosire, R. Kasi

306. Synthesis and self-assembly of dendrimer-b-poly(N-isopropylacrylamide) block copolymers containing folates for applications in biosensors and drug delivery systems. **D.L. Bertuzzi**, C. Ornelas, B.D. Olsen

307. New eco-friendly phosphorus organic polymers as gas storage media. **D. Ahmed**

308. PIFPC-01: Photo-induced fluorinated polymer coating for the protection of OLEDs and electronics against redox reactions. **D. Alamo**, K.R. Cruz, W.

- Yaseen, K. Bodenstedt, S. Li, S.B. Marpu, M.A. Omary
- 309.** Effect of polymer conformation on the immunogenicity of the protein-polymer conjugates. **E. Davis**, J.K. Pokorski
- 310.** Investigation of P3HT photo-degradation for solar applications. **E.J. Abraham**, **M. Al-Sheeb**, **T. Kubbar**, K. Kakosimos, M. Al-Hashimi
- 311.** Tuning the lower critical solution temperature of oligoethylene substituted polycaprolactones. **E.L. Calubaquib**, M.C. Stefan
- 312.** Preparation of polymer-grafted nanoparticles for designing 2D superlattices and arrays. **F.H. Käfer**, D. Wu, C.K. Ober
- 313.** Synthesis of organotin polymers from the HIV drug lamivudine (3TC) and their ability to inhibit the Zika virus. **F. Mosca**, P. Slawek, **C.E. Carraher**, M. Roner, L. Miller, J.E. Haky
- 314.** Polycarbonates with pendent selenonium: Preparation and property. L. Yu, **F. Du**, Z. Li
- 315.** Tuning the molecular weight of polymeric amphiphiles as a tool to access micelles with a wide range of enzymatic degradation rates. **G. Slor**, R.J. Amir
- 316.** π Conjugate polymer-cored sea urchin-structured chaperones for inhibition of amyloid β -protein aggregation and cytotoxicity. **G. Hao**
- 317.** Metal ion binding and oxidation behavior of linear synthetic polyphenols. **H. Hlushko**, R. Hlushko, T.M. Kelly, R. Wang, D. Korouski, S.A. Sukhishvili
- 318.** Self-organization of hydrophilic-hydrophobic π -conjugated diblock copolymers: Investigation of solvent effect. **H. Sasaki**, M. Yoshizawa-Fujita, Y. Takeoka, M. Rikukawa
- 319.** Green synthesis and toxicity of nanoparticle attached-electrospun nanofiber. **H. Yip**, M. Calzado Delgado, K. Yeung
- 320.** Development of a plastic antibody that captures vascular endothelial growth factor (VEGF) for anticancer therapy. **H. Koide**, Y. Hoshino, Y. Nishimura, Y. Miura, N. Oku, K.J. Shea, T. Asai
- 321.** Adjustable 3D elastomeric cavities for tumor spheroid culture and *in situ* analyses. **H. An**, H. Kim, K. TaeHo, J. Song, I. Choi
- 322.** Polydiacetylene-liquid crystalline copolymers as a route to optically active stimuli-responsive materials. **I. Martin**
- 323.** Injectable biodegradable gelatin-methacrylate/ β tricalcium phosphate composite for the repair of bone defects. **I. Kwon**
- 324.** Catalase mimicking nanopods targeting tumor adaption to hypoxia potentiate image-guided photothermal therapy. **I. Park**, K. Cherukula, Y. Lee
- 325.** Molecularly engineered photomotility of untethered soft robots. **J. Kim**, J. Jeon, J. Lee, S. Rajamanickam, Y. Kim, M. Cho, J. Youk, J. Wie
- 326.** 3D printing curable particulate composites: Effects of glycerin on the cure kinetics of hydroxyl-terminated polybutadiene binders (HTPB). **J. Strutton**, J. McCollum, S.T. Iacono, J. Mates
- 327.** Drug/sensor migration in multilayer polymeric nanoparticles. **J. Samonina**
- 328.** Increased flexibility in polyimide aerogel substrates for conformal, lightweight antennas. **J. Cashman**, B.N. Nguyen, B. Dosa, M. Meador
- 329.** Brain and pancreatic cancer inhibition by group 4 metallocene polymers from gabapentin. **J. Frank**, **C.E. Carraher**, M. Roner, Z.M. Rabinowitz
- 330.** Preparation of flexible silicone rubber nanocomposite foams with high absorption and effective electromagnetic shielding by supercritical CO₂. **J. Yang**, X. Liao, J. Li, W. Tang, G. Wang, G. Li
- 331.** Evaporative crystallization of drug with limited air flow for preparation of uniformly aligned composite crystals. **J. Seo**, J. Lee
- 332.** Microwave-assisted aqueous RAFT polymerization of cationic monomers. **J.G. Schellinger**, J. Tran, A. Ennis, W. Sherwin, T. Luu, A. Masgumbol
- 333.** Rational molecular design of sulfur copolymers toward ultra negative triboelectric materials. **J. Lee**, K. Kim, M. Choi, J. Jeon, Y. Lee, M. Lee, J. Wie
- 334.** *In vitro* and *in vivo* evaluation of thermally grafted biomembrane mimic polymer on silicone surface. **J. Kim**, S. Kang, S. Kim, M. Wufue, Y. Kim, X. Jin, J. Park, Y. Lee, T. Choi
- 335.** Engineering cell surfaces via PET-RAFT for a durable, functional synthetic skin. **J. Hochberg**, J.K. Pokorski
- 336.** Poly(methyl methacrylate) functionalized nanocrystal quantum dots for suspension in luminescent solar concentrators. **K. Koch**, M. Plummer, D.A. Rider
- 337.** Bioluminescent silk microparticles. **K. Hausken**, A. Murphy
- 338.** Effect of fumed silica on the mechanical properties of graphene oxide/aminopropyl terminated polydimethylsiloxane elastomers. **K. Ha**, **S. Mun**, **C.J. Ellison**
- 339.** Synthesis and evaluation of polythiophene-silica particles by surface grafting (III) effect of reaction conditions on surface grafting. **K. Koizumi**, M. Yoshizawa-Fujita, Y. Takeoka, M. Rikukawa
- 340.** Towards processable MOFs through polymer/MOF hybrid materials. **K.S. Barcus**

- 341.** Colorimetric voltmeter using Fe_3O_4 @ SiO_2 nanoparticles as an overpotential alarm system for zinc-air battery. **L. Zheng**, T.N. Tran, D. Zhalmuratova, H. Chung
- 342.** Design and set-up of a low-cost electrospinning equipment: Study of working parameters using HPMC nanofibers. **M. Calzado Delgado**, M. Guerrero-Perez, K. Yeung
- 343.** Preparation of porous materials using biodegradable polymers and application to scaffold materials: Differentiation-induction of poly(L-lactic acid) monolith. **M. Mukai**, M. Yoshizawa-Fujita, Y. Takeoka, M. Rikukawa
- 344.** Cellulose fiber network as reinforcement of thermoplastic films. **M.F. Flores**, L. Cordeiro, A.A. Curvelo
- 345.** Ultrafast photophysics of polarons and bipolarons in doped semiconducting polymers. **M.G. Voss**, D.T. Scholes, J. Challa, S.H. Tolbert, B.J. Schwartz
- 346.** Oxygen nanosensors for brain imaging. **M. Zhuang**, H. Liang, N. Manu, J. Kapur, C.L. Fraser
- 347.** Photoswitching in poly(2-oxazoline) nanoreactors. **M. Kuepfert**, P. Qu, M. Weck
- 348.** Synthesis of hydrophilic-hydrophobic diblock copolymers and surface properties evaluation on solid substrates: Evaluation of particle morphology. **M. Ayane**, M. Yoshizawa-Fujita, Y. Takeoka, M. Rikukawa
- 349.** Morphological effect for cellular uptake of torpedo-shaped peptidic nanocapsule. **M. Ueda**, Y. Ito
- 350.** Temperature-responsive and size-dependent drug release via lipid domain of peptide-lipid hybrid vesicle. **M. Ueda**, M. Rahman, Y. Ito
- 351.** Fabrication of nylon 6,6 grafted graphene-carbon nanotube hybrids for the reinforcement of nylon 6,6 composites. **M. Kim**, D. Kim, E. Choi, C. Kim
- 352.** Absorbable tissue adhesives. **N. Srivastava**, R.S. Bezwada
- 353.** Absorbable polyurethanes from functionalized phenylalanine. **N. Srivastava**, R.S. Bezwada
- 354.** Fast, absorbable PDS (PDS Rapide) polymers for biomedical applications. **N. Srivastava**, R.S. Bezwada
- 355.** Absorbable polyurethanes from functionalized tyrosine. **N. Srivastava**, R.S. Bezwada
- 356.** Mechanical stability of fluoroethylene vinyl ether polyurethane films blended with a soft macrodiol subjected to weathering. **N. Weise**, I. Long, A.E. Mera, J.H. Wynne
- 357.** Ethylene scavenger based on organoclay modified n-octyltriethoxysilane. **N. Rangsiwutisak**, **H. Manuspiya**
- 358.** Performance of graphene oxide-modified nanofiltration membrane in an ozone membrane reactor for treatment and removal of endocrine disrupting compounds. Y. Li, **O.V. Ezeh**, K. Yeung
- 359.** Expansion and solvation of poly(vinyl alcohol) chains: Lithium salt hydrate vs. water as a solvent. **P. Karimineghlani**, J. Zheng, Y. Hu, S.A. Sukhishvili
- 360.** Synthesis, characterization, and study of citric and trans-aconitic acid based biodegradable polyesters. **P.P. Pham**, N.A. Hermes
- 361.** 3D printing of rubber toughened epoxy with tunable mechanical properties and shape memory behavior. **Q. Chen**, R.C. Advincula
- 362.** Improving permeability and antifouling properties of polyethersulfone composite ultrafiltration membranes by incorporation of partially unzipped carbon nanotubes. **S. Kong**, H. Seo, H. Shin, K. Jung, M. Kim, J. Lee
- 363.** Designing dye incorporated polymeric architectures for stimuli-responsive function. **S. Vaidya**, M. Sharma, C. Bruckner, R. Kasi
- 364.** Mild condition produced m-PBI with various types of membranes. **S. Nam**
- 365.** Alkaline anion exchange membrane fuel cell application of PEEK polymer electrolyte membrane with imidazolium. **S. Nam**
- 366.** Flexible and conductive MXene-polymer nanocomposite films. D. Kim, H. Kim, Y. Yeo, S. Lee, C. Koo, **S. Cho**
- 367.** Post-UV initiated cross-linking of thermally cured EVA encapsulant in solar panels. **S. Kaur**, C. Savich, E. Stoikou
- 368.** Tuning the hydrophilicity in porous membranes for water filtration formed by self-assembled ABC linear terpolymers. **S. Antoine**, Z. Geng, C.J. Hawker, V. Ganesan, R.A. Segalman
- 369.** Reconstructing device architecture of organic photodiode using etalon-electrode to realize color filter free image sensor. **S. Yoon**, S. Kim, J. Kim, S. Hassan, D. Chung
- 370.** Poly(N-isopropylacrylamide) hydrogel/polydimethylsiloxane composites for novel water flow systems. **S. Lee**, J. Lee
- 371.** Effect of macromolecular chain movement induced by high pressure CO_2 on the crystalline nucleation and spherulites growth of polylactic acid. **S. Li**, X. Liao, W. Han, Z. Yan, J. Li, Q. Yang, G. Li
- 372.** Controlled release of cationic amphiphile antimicrobials. **S. Song**, K.E. Uhrich

- 373.** Fabrication of novel organic-inorganic perovskites using p-conjugated polymers: Effect of cation types and polymer introductions. **S. Shimizu**, M. Yoshizawa-Fujita, Y. Takeoka, M. Rikukawa
- 374.** 1,3-Oxathiolane-2-thione-based photosensitive polymeric system to create multi-chemical surface functionalities. **S. An**, Y. Song, M. Kim
- 375.** Electrostatically varied grafted copolymers for enhancing multivalent ion rejection for nanofiltration. **S. Aguilar**, S. Bustillos, S. Xue, W.H. Mak, C. Ji, E. Rao, B. McVerry, R.B. Kaner
- 376.** Poly(2-methacryloyloxyethyl phosphorylcholine) covalent grafting can reduce bacterial adhesion and host-inflammatory reaction on the surface of Gore-Tex implants. **S. Kang**, Y. Jin, D. Choi, J. Seo, H. Jin, Y. Lee
- 377.** Realization of red-selective organic photodiode based on newly synthesized phenanthrocarbazole-diketopyrrolopyrrole copolymer. **S. Hassan**, S. Yoon, M. Kang, **J. Cho**, Y. Kim, D. Chung
- 378.** Fundamental study of swelling mechanism by carbon dioxide in PEBAX 2533 membrane for gas separation. **T. Park**, E. Chung
- 379.** Graphitization and strength of annealed silks and polymer fibers. **T. Dugger**, S. Sarkar, S. Correa-Garhwal, M. Shishebour, M. Zhernenkov, Y. Zhang, G. Kolhatkar, R. Mohan, A. Lubio Cervantes, A. Ruediger, P. Zavattieri, C. Hayashi, D.J. Kisailus
- 380.** Fluorescence measurement of macromolecules with broad dispersities. **T.A. Swift**
- 381.** Two-dimensional polythiophene composites for thermoelectric applications. **T. Meng**
- 382.** Modular materials for molecular electronics and targeted therapeutics. **T.A. Su**
- 383.** Diffraction-based method to evaluate enzymatic degradation of poly(lactic acid) films. **V. Salgado**, A. Elias, K. Harris
- 384.** Controlling functionality of layer-by-layer assembled upper critical solution temperature micelles. **V. Albright**, A. Aliakseyeu, J. Ankner, S.A. Sukhishvili
- 385.** DNA-driven nanomachines for drug and nitric oxide delivery. **W. Kim**, H. Park
- 386.** Surface modification of PDMS surface by poly(acrylic acid) micropatterns to suppress foreign body reaction against PDMS implants. J. Lee, B. Shin, Y. Choy, C. Heo, **W. Koh**
- 387.** Molecular design strategies for mechanochemically active polymers. **X. Hu**, T. Zeng, M.E. McFadden, R. Barber, M.J. Robb
- 388.** Achieving flat-on crystals and blocking ionic conduction in polycarbonate/poly(vinylidene fluoride) multilayer films. **X. Chen**, H. Huang, E. Baer, L. Zhu
- 389.** Development of apoptosis-inducing polypeptide via simultaneous mitochondrial membrane disruption and Ca²⁺ delivery. J. Ha, **Y. Kim**
- 390.** Dual pH/temperature-responsive injectable hydrogels in protection and sustained release of oncolytic adenovirus for tumor therapy. **Y. Li**
- 391.** Polarizing nonpolar polymers with poly(N-isopropylacrylamide) in nonpolar alkanes. **Y. Fu**, D.E. Bergbreiter, S. Madrahimov
- 392.** Fabrication of mechanically robust hollow fiber membranes with tailored pore structure by thermally assisted dry-wet phase inversion for osmotic process applications. **Y. Cho**, S. Kim, H. Park, Y. Park
- 393.** Peptide-mediated sinonasal delivery of therapeutic reagents for effective inhibition of epithelial to mesenchymal transition in nasal epithelium. **Y. Kim**, S. Hwang, S. Kang, H. Shin, Y. Lee
- 394.** Lewis pair-mediated ring-opening polymerization of cyclic disulfides: Building high molar mass polymers with dynamic s-s bonds. **Y. Liu**, Y. Jia, Q. Wu, J.S. Moore
- 395.** Remotely actuated liquid crystal elastomers. T. VanVolkenburg, K. Ohiri, M. Hagedon, E. Whitewhite, **Z. Xia**

SECTION A

San Diego Convention Center

TBD

PMSE/POLY Poster Session

Novel Polymeric Materials & Polymer-Based Processes for Energy Efficient Treatment of Water & Resource Recovery

Cosponsored by POLY

T. J. Bunning, *Organizer*

5:00 - 7:00

396. Withdrawn

SECTION A
San Diego Convention Center
TBD

PMSE/POLY Poster Session

Toughening of Networks & Gels through Molecular Design

Cosponsored by POLY
T. J. Bunning, *Organizer*

5:00 - 7:00

397. New vitrimer design via direct silyl ether metathesis reaction. **C. Tretbar**, J. Neal, Z. Guan
398. Ionically cross-linked silk microfibers/alginate tough composite hydrogels with hierarchical structures. **L. Meng**, J. Yang, C. Shao
399. Adaptive structures via additive manufacturing of stimuli-responsive polymers. **Q. Zhou**, F. Gardea, S.A. Sukhishvili

Future of Biomacromolecules at a Crossroads of Polymer Science & Biology

Sponsored by POLY, Cosponsored by BIOL, CARB, CELL, COLL, ENVR, MEDI, PHYS and PMSE

Polymeric Materials for Water Purification

Sponsored by POLY, Cosponsored by PMSE

Polymeric Materials for Water Purification

Sponsored by POLY, Cosponsored by PMSE

WEDNESDAY MORNING – PMSE

SECTION A
Manchester Grand Hyatt San Diego
Harbor I

Novel Polymeric Materials & Polymer-Based Processes for Energy-Efficient Treatment of Water & Resource Recovery

Nanomaterials for Separations

Cosponsored by ENVR
Financially supported by North American Membrane Society, Center for Materials for Water & Energy Systems (M-WET); Advanced Materials for Energy Water Systems Center (AMEWS); ACS Innovative Project Grant
D. Bhattacharyya, S. B. Darling, Y. Ding, E. Hatakeyama, W. A. Phillip, C. M. Stafford, *Organizers*
B. D. Freeman, *Organizer, Presiding*
J. Kamcev, *Presiding*

8:25 Introductory Remarks.

- 8:30 400. Multifunctional nanocomposite coatings for desalination and water purification. **Q. Li**
- 9:10 401. Functionalized porous aromatic frameworks for rapid boron removal from aqueous solutions. **J. Kamcev**, M.K. Taylor, J.R. Long
- 9:35 402. Porphyrin organic frameworks for photothermally enhanced water evaporation. **Z. Xia**, R. Waldman, Z. Chen, H. Yang, Y. Zhao, C. Zhang, S. Patel, S.B. Darling
- 10:00 403. Metal organic framework mixed matrix membranes for monovalent separations. **T. Dilenschneider**, K. Reimund, B.D. Freeman, H. Wang
- 10:25 Intermission.
- 10:40 404. Fe-Pd-embedded graphene oxide-based catalytic membranes for removal of perfluoroalkyl substances and chlorinated organics from water. **A. Aher**, D. Bhattacharyya
- 11:05 405. Chicken feathers/graphene oxide based adsorbent for water purification. **M. Zubair**, **R. Syamaladevi Mohandas**, **A. Ullah**
- 11:30 406. Porous porphyrin polymer for precious metal capture. **Y. Hong**, D. Thirion, S. Subramanian, C.T. Yavuz

SECTION B
Manchester Grand Hyatt San Diego
Cortez Hill C

Design, Synthesis & Engineering of Polypeptides for Biological & Biomedical Application

Design & Studies of Functional Polypeptide Materials

Cosponsored by POLY
J. Cheng, T. J. Deming, M. J. Vicent, L. Yin, *Organizers*
J. A. Baccile, A. Kros, *Presiding*

- 8:00 407. Structure-property relationships of oligonucleotide polyelectrolyte complex micelles. **M. Lueckheide**, J. Viereg, **M.V. Tirrell**
- 8:30 408. Skin-elastin copolymers for biomedical utility. **D.L. Kaplan**
- 9:00 409. One peptide for them all? Stabilization of gold nanoparticles of different sizes by a common peptide amphiphile. **A. Kros**
- 9:30 410. Polypeptide-based polymersomes for crossing the blood brain barrier. **G. Battaglia**
- 10:00 Intermission.
- 10:20 411. Peptide-mediated surface deposition of polymers and nanoparticles. **H.A. Klok**
- 10:50 412. How to build atomically defined nanostructures from sequence-defined peptoid polymers. **S. Xuan**, X. Jiang, R.K. Spencer, N.P. Balsara, **R.N. Zuckermann**

- 11:20 **413.** Stimuli-responsive polypeptide-based nanoconstructs. **A. Duro Castano**, L. Rodriguez-Arco, L. Ruiz-Perez, C. De Pace, G. Battaglia
- 11:40 **414.** Visualizing mechanical stress in artificial protein hydrogels. **J.A. Baccile**, D.A. Tirrell

SECTION C

Manchester Grand Hyatt San Diego
Bankers Hill

General Papers/New Concepts in Polymeric Materials

T. J. Bunning, *Organizer*

E. Camerino, C. Gorin, *Presiding*

- 9:00 **415.** Synthesis and exploration of extended silyl based cross-linked networks that disassemble in the presence of specific stimuli. **E. Camerino**, G. Daniels, J.H. Wynne, E. Iezzi
- 9:20 **416.** Bioinspired mechanical reinforcement of HMX/TATB based polymer bonded explosives via *in situ* polymerization of dopamine. **C. Lin**, Z. Yang, J. Liu, F. Gong, L. Pan, J. Li, S. Guo
- 9:40 **417.** Synthesis and self-assembly of poly(styrene-*b*-solketal acrylate) linear and bottlebrush block copolymers. **D.M. Smith**, D. Yu, T.P. Russell, J. Rzyayev
- 10:00 Intermission.
- 10:20 **418.** Morphology and unusual crystallization behavior in diblock copolymer/homopolymer blends. **C. Chu**, G. Chen
- 10:40 **419.** Sliding crosslinker enabled highly stretchable elastomer. **Q. Zhang**
- 11:00 **420.** Advanced polymer materials for 3D printing. **C. Gorin**
- 11:20 **421.** Dynamic single-ion-conductive network as a stable lithium metal artificial solid electrolyte interphase in carbonate electrolyte. **D.G. Mackanic**, Z. Yu, Y. Cui, Z. Bao

SECTION D

Manchester Grand Hyatt San Diego
Hillcrest A

General Papers/New Concepts in Polymeric Materials

T. J. Bunning, *Organizer*

F. Solangi, E. B. Trigg, *Presiding*

- 9:00 **422.** Chemical kinetics and segmental relaxation within and between dynamic polymer networks. **D. Wang**
- 9:20 **423.** Development of liquid crystalline thermosets for additive manufacturing. **E.B. Trigg**, H. Koerner

- 9:40 **424.** Using hydrogels to create a biodegradable bioelectronic device. **E. Hall**, M. Geoghegan, M. Grell, R. Cameron
- 10:00 Intermission.
- 10:20 **425.** Bio-inspired mechanically adaptive nanocomposites. **Y. Zhang**, **N. Pon**, S.J. Rowan
- 10:40 **426.** Bioinspired semitransparent silver nanowires conductor based on vein network with excellent electromechanical and photothermal properties. **C. Zhu**, Y. Qiang
- 11:00 **427.** Transient mechanochromic response and stereochemical effects of spiropyran copolymers. **F. Kempe**, O. Brügner, L. Metzler, M. Walter, M. Sommer
- 11:20 **428.** Oligoviologen-based photo-redox actuating hydrogels. **F. Solangi**, K. Liles, A. Delawder, N.D. Colley, M. Palmquist, J.C. Barnes

SECTION E

Manchester Grand Hyatt San Diego
Hillcrest B

Unique & Complex Polymer Architectures

Assembly

Cosponsored by POLY

K. C. Bentz, D. A. Savin, *Organizers*

A. Knight, Z. A. Page, *Presiding*

- 8:30 **429.** Breaking parallel orientation of rods toward diverse supramolecular structures. **R. Zhang**, S.Z. Cheng
- 8:50 **430.** Programmable fabrication of sub-micron bent pillar structures enabled by photo-reconfigurable azopolymer. **W. Jo**, J. Choi, H. Kang, H. Kim
- 9:10 **431.** Bottlebrush elastomers as tissue-mimetic dielectric actuators. **V. Karimkhani**, M. Vantankhah-Varnosfaderani, E. Dashtimoghadam, B.J. Morgan, A.N. Keith, A.V. Dobrynin, S. Sheyko
- 9:30 Intermission.
- 9:45 **432.** Injectable elastomers with tunable (tissue-mimetic) mechanical properties. **M. Vatankhah Varnosfaderani**, E. Dashtimoghadam, X. Hu, A.N. Keith, A.V. Dobrynin, S. Sheyko
- 10:05 **433.** Tunable transient polymer networks via Lewis pair interactions. F. Vidal, **F. Jäkle**
- 10:25 **434.** Self-assembly and dielectric properties of mesogen-free liquid crystalline poly(oxypropylene)s with *n*-alkylsulfonyl side chains. **M. Kwok**, B.T. Seymour, R. Li, B. Zhao, L. Zhu
- 10:45 **435.** Highly branched, self-condensing vinyl polymerisation via reversible addition-fragmentation chain transfer with a comparatively high initiator loading: Review of material properties. **T.A. Swift**, S. Rimmer

SECTION F

Manchester Grand Hyatt San Diego
Cortez Hill A/B

Innovations in Drug Delivery Systems: Recent Breakthroughs & New Approaches in Formulation, Drug Delivery Mechanisms & Advanced Delivery Systems

Polymers for Biomedical Applications

Financially supported by Bristol-Myers Squibb

A. Kulshrestha, *Organizer*

S. Sridharan, *Organizer, Presiding*

K. Nagapudi, *Presiding*

- 9:00 436. Peptomicelles in tuberculosis therapy. **M. Barz**
- 9:25 437. Bottlebrush polymers with chiral sidechains: Synthesis and biomedical applications. **H. Nguyen**, Y. Jiang, J.C. Barnes, N.J. Oldenhuis, W. Wang, M. Golder, J.A. Johnson
- 9:50 438. Polymersomes for biotransformation applications. **A. Schmidt**, J. Leroux
- 10:15 439. Polymeric artificial organelles containing an enzyme mimic. **C. Ade**, E. Brodzkij, B. Stadler
- 10:40 440. Hydrogel-based delivery of enzymes to mitigate infection and facilitate bone regeneration in critical-sized segmental bone defects. **P.P. Kalelkar**, C.T. Johnson, A. Garcia
- 11:05 441. Radiation-grafting of poly(N-vinylimidazole) onto cotton gauzes to produce antibacterial medical devices. **L.A. Camacho Cruz**, E. Bucio

SECTION G

Manchester Grand Hyatt San Diego
Hillcrest C

General Papers/New Concepts in Polymeric Materials

T. J. Bunning, *Organizer*

J. J. Benkoski, H. Lopez Hernandez, *Presiding*

- 9:00 442. Triggerable, solid-state depolymerization of bulk thermoformable cyclic poly(phthalaldehyde). **H. Lopez Hernandez**, A.M. Feinberg, E. Lloyd, S. White, N.R. Sottos, J.S. Moore
- 9:20 443. Withdrawn
- 9:40 Intermission.
- 10:00 444. Linear and star-shaped PCL block copolymer nano-assemblies in drug delivery. **M. Malhotra**, M. Jayakannan
- 10:20 445. Novel surface modifying amphiphilic additives (SMAAs) with varying architecture: Effect on fouling-release properties of siloxane-polyurethane (SiPU) fouling-release coatings. **J.R. Benda**

- 10:40 446. Ionenes 2.0: Convergence of high-performance polymers with ionic liquids. **J.E. Bara**, I. Kammakam, K.E. O'Hara
- 11:00 447. Microfluidic 3-D printing of hierarchically structured biomaterials for myocardial tissue constructs. **J.J. Benkoski**, J. Fite, A. Freeman, D. Trigg, M. Abraham, J. Afzal

Materials Advances in Nanocellulose Research for Engineered Functionality

Sponsored by CELL, Cosponsored by PMSE and POLY

Future of Biomacromolecules at a Crossroads of Polymer Science & Biology

Delivery Systems

Sponsored by POLY, Cosponsored by BIOL, CARB, CELL, COLL, ENVR, MEDI, PHYS and PMSE

Polymeric Materials for Water Purification

Sponsored by POLY, Cosponsored by PMSE

Polymeric Materials for Water Purification

Sponsored by POLY, Cosponsored by PMSE

WEDNESDAY AFTERNOON – PMSE

SECTION A

Manchester Grand Hyatt San Diego
Harbor I

Novel Polymeric Materials & Polymer-Based Processes for Energy-Efficient Treatment of Water & Resource Recovery

Nanomaterials for Separations

Cosponsored by ENVR

Financially supported by North American Membrane Society, Center for Materials for Water & Energy Systems (M-WET); Advanced Materials for Energy Water Systems Center (AMEWS); ACS Innovative Project Grant D. Bhattacharyya, Y. Ding, B. D. Freeman, E. Hatakeyama, W. A. Phillip, C. M. Stafford, *Organizers*
S. B. Darling, *Organizer, Presiding*
O. Coronell, *Presiding*

- 1:25 Introductory Remarks.

- 1:30 448.** Peptide amphiphiles for phosphate recovery. W.C. Fowler, **M.V. Tirrell**
- 2:10 449.** Highly efficient carcinogenic bromate removal from water by a cationic covalent organic framework. **T. Skorjanc**, D. Shetty, F. Gandara, L. Ali, A. Trabolsi
- 2:35 450.** Energetically efficient, electrochemically tunable affinity separation using multicomponent polymeric nanostructures for water treatment. **X. Mao**, G.C. Rutledge, T. Hatton
- 3:00 451.** Combining polymeric structures with metal oxides for advanced water treatment. **R. Waldman**, H. Yang, D. Mandia, S. Sankaranarayanan, A.B. Martinson, J. Elam, S.B. Darling
- 3:25** Intermission.
- 3:40 452.** Highly conductive, low-cost, and durable graphene composite membrane with multi-purpose application. **J. Hutfles**, J. Pellegrino
- 4:05 453.** Porous polymer adsorbents for chromium VI removal from water resources. **Z. Abbasian Chaleshtari**, R. Foudazi
- 4:30 454.** Novel metal–organic brush membranes (MOBs) for organic solvent nanofiltration. **P. Ramesh**, W. Xu, M. Yu, G. Belfort

SECTION B

Manchester Grand Hyatt San Diego
Cortez Hill C

Design, Synthesis & Engineering of Polypeptides for Biological & Biomedical Application

Design of Functional Peptides & Polypeptides

Cosponsored by POLY

J. Cheng, T. J. Deming, M. J. Vicent, L. Yin, *Organizers*
Y. Jiang, Z. Song, *Presiding*

- 1:00 455.** Dispersity as a design parameter for polypeptide and polypeptide based biomaterials. N. Gangloff, C. Schlutt, S. Forster, **R. Luxenhofer**
- 1:30 456.** Star-shaped polypeptides as efficient nanocarriers for gene delivery in bone regeneration. R. Murphy, D. Walsh, F. O'Brien, S. Cryan, **A. Heise**
- 2:00 457.** Antimicrobial amino acid polymers as synthetic mimics of host defense peptide. **R. Liu**, Y. Wu, Y. Qian
- 2:30 458.** Cell penetration profiling for biotherapeutics. **J. Kritzer**
- 3:00** Intermission.
- 3:20 459.** Polypept(o)ides: From controlled polymer synthesis to functional systems for diagnosis and therapy. **M. Barz**
- 3:50 460.** End-sealed high aspect ratio hollow nanotubes encapsulating an anticancer drug: Torpedo-shaped peptidic nanocapsules. **Y. Ito**

- 4:20 461.** Tuning helix-coil transition profile of synthetic polypeptides. **Z. Song**, J. Cheng
- 4:40 462.** Selective killing of *Helicobacter pylori* with pH-responsive antimicrobial polypeptides. **Y. Jiang**, M. Xiong, Y. Bao, L. Chen, J. Cheng

SECTION C

Manchester Grand Hyatt San Diego
Bankers Hill

General Papers/New Concepts in Polymeric Materials

T. J. Bunning, *Organizer*

M. A. Luzuriaga, K. Nomura, *Presiding*

- 1:30 463.** Analysis of mechanical and cytotoxic properties of emulsion-templated macroporous-mesoporous polyurea gels. **K. Mawhinney**, N. Yazdani, M. Kimel, R. Willits, S.C. Jana
- 1:50 464.** Improving the recyclability of PET/PE mixed waste streams. **K. Nomura**, X. Peng, H. Kim, K. Jin, H. Kim, A.F. Bratton, K.M. Miller, C.J. Ellison
- 2:10 465.** Multilayer coextrusion production of tunable bioresorbable polyester fibers for tissue engineering. **K. Van de Voorde**, J.K. Pokorski, L. Korley
- 2:30** Intermission.
- 2:50 466.** Enhanced immunogenic response of biomimetic mineralized vaccines. **M.A. Luzuriaga**, R.P. Welch, J.J. Gassensmith
- 3:10 467.** Improving neural differentiation of embryonic stem cells via glycosaminoglycans-mimicking scaffold with nanogold coating. S. Zhang, **L. Wang**, H. Chen
- 3:30 468.** Bio-inspired design of mechanochromisms via surface engineering. S. Zeng, R. Li, D. Zhang, **L. Sun**
- 3:50 469.** Conjugated polythiophene/polyisocyanide hybrid biomimetic hydrogels with enhanced red light-activated ROS production. **H. Yuan**, C. Xing, A.E. Rowan, Y. Zhan, P.H. Kouwer

SECTION D

Manchester Grand Hyatt San Diego
Hillcrest A

General Papers/New Concepts in Polymeric Materials

T. J. Bunning, *Organizer*

M. J. Derry, N. Kang, *Presiding*

- 1:30 470.** Large-scale simulation of nonequilibrium network phases for battery electrolytes. **M. Mueller**, L. Schneider

- 1:50 471.** RAFT dispersion polymerization of glycidyl methacrylate for the synthesis of epoxy-functional block copolymer nanoparticles in mineral oil. P.J. Docherty, **M.J. Derry**, S.P. Armes
- 2:10 472.** Materials visually responsive to physical stimuli. **M. Humphries**
- 2:30** Intermission.
- 2:50 473.** Aromatic modification of helical polypeptides for efficient *in vitro* and *in vivo* gene delivery. **N. Zheng**
- 3:10 474.** Quantitative study on the interphase of elastomer nanocomposites. **M. Tian**, C. Tian, G. Chu, C. Miao, Y. Lu, N. Ning, L. Zhang
- 3:30 475.** Nanoporous films with controllable porosity and pore morphologies. **N. Kang**, J. Pang, M. Li, E.E. Leonhardt, H. Zhou, G. Sun, P. Trefonas, K.L. Wooley
- 3:50 476.** Room-temperature synthesis of Zn–Co–based zeolitic imidazolate frameworks with hollow structure. **B. YAO**, H. Doan, V. Ting, Z. Dong

SECTION E

Manchester Grand Hyatt San Diego
Hillcrest B

General Papers/New Concepts in Polymeric Materials

T. J. Bunning, *Organizer*

P. Arias-Monje, A. Mroz, *Presiding*

- 1:30 477.** Direct numerical estimates of the shear modulus of Gaussian polymer networks and their exact theoretical description. **A. Gusev**
- 1:50 478.** Synthesis and analysis of photodegradable polyurethanes with poly (propylene glycol) and nitro-benzene derivatives. **A. Mroz**, S. Spain, P. Fairclough
- 2:10 479.** One-pot synthesis of polar olefinic diblock copolymers via MILRad polymerization. **A.C. Keyes**, E. Harth
- 2:30 480.** Mimicking ‘J-shaped’ and anisotropic stress-strain behavior of human aorta by fabric-reinforced elastomer composites. **D. Zhalmuratova**, T. La, D. Nobes, C. Kim, D. Freed, H. Chung
- 2:50** Intermission.
- 3:10 481.** Novel design of hierarchically structured poly(e-caprolactone)-based blend fibers by facile solvent vapor annealing treatment. **B. Li**, A.J. Bauer
- 3:30 482.** Nanoporous liquid crystalline polymers: Utilizing magnetic anisotropy in designing functional materials. **R. Bosire**, D. Ndaya, R. Kasi
- 3:50 483.** Superhydrophilic fibrous materials via nanofluid modification. **L. Lao**, L. Fu, g. qi, E.P. Giannelis, J. Fan

- 4:10 484.** Noncovalent ordered wrapping of poly(methyl methacrylate) on single-wall carbon nanotubes and its effect on macroscopic-continuous polymer composite fibers. **P. Arias-Monje**, A. Bakhtiari Davijani, M. Lu, J. Ramachandran, S. Kumar

SECTION F

Manchester Grand Hyatt San Diego
Cortez Hill A/B

Innovations in Drug Delivery Systems: Recent Breakthroughs & New Approaches in Formulation, Drug Delivery Mechanisms & Advanced Delivery Systems

Nanoscience in Drug Delivery

Financially supported by Bristol-Myers Squibb

S. Sridharan, *Organizer*

A. Kulshrestha, *Organizer, Presiding*

R. Shah, *Presiding*

- 1:30 485.** Self-assembled supramolecular polymers for next-generation nanoparticle-based combination drug delivery. X. Li, R. Li, A. Delawder, **J.C. Barnes**
- 1:55 486.** Pirfenidone NPs modulate TGFβ1- SMAD expression and attenuate EMT in lung cancer cell line. **R. Kulshrestha**, A. Singh, A. Pandey, N. Tyagi, S. Sharma, A. Bahl, S. Bansal, A. Dinda
- 2:20 487.** Novel ultra-high capacity nanoformulations of extremely hydrophobic drugs and their evaluation in 3D cancer models. H. Malik, J. Schreiner, S. Kendl, M. Lübtow, M. Kroiß, **R. Luxenhofer**
- 2:45 488.** Engineered HDL-mimetic nanoparticles synergize therapeutic effects on the cancer stem-like cell population in sonic hedgehog medulloblastoma. **J. Kim**, A. Dey, A. Malhotra, S. Ahn, J. Liu, Y.J. Sei, A.M. Kenney, T.J. MacDonald, Y. Kim
- 3:10 489.** Stimuli-responsive biodegradable polymer nanohydrogels for biomedical application. Y. Li, Z. Zhang, Y. Ding, **C. Wang**

SECTION G

Manchester Grand Hyatt San Diego
Hillcrest C

General Papers/New Concepts in Polymeric Materials

T. J. Bunning, *Organizer*

Q. Fu, P. Shieh, *Presiding*

- 1:30 490.** Endowing materials with degradability. **P. Shieh**, W. Zhang, J.A. Johnson

THURSDAY MORNING – PMSE

SECTION A

Manchester Grand Hyatt San Diego
Coronado A

Novel Polymeric Materials & Polymer-Based Processes for Energy-Efficient Treatment of Water & Resource Recovery Gas Separation Membranes

Cosponsored by ENVR

Financially supported by North American Membrane Society, Center for Materials for Water & Energy Systems (M-WET); Advanced Materials for Energy Water Systems Center (AMEWS); ACS Innovative Project Grant D. Bhattacharyya, S. B. Darling, Y. Ding, E. Hatakeyama, W. A. Phillip, C. M. Stafford, *Organizers* B. D. Freeman, *Organizer, Presiding*

8:25 Introductory Remarks.

8:30 **497.** Novel gas separation constructs from polymer-grafted nanoparticles. **S. Kumar**

9:10 **498.** ROMPs and CANALS: New approaches to design microporous polymers for gas separations. **F. Benedetti**, Y. He, H.W. Lai, S. Lin, A.X. Wu, Z. Jin, Y. Teo, H. Ye, C. Liu, Y. Zhao, T.A. Van Voorhis, M. De Angelis, Y. Xia, T.M. Swager, Z. Smith

9:35 **499.** Propane/propylene separation mechanism through Ag-X type zeolite membrane. **M. Matsukata**, N. Fujimaki, M. Sakai

10:00 **500.** Gas separations important to the water/energy nexus. **B.D. Freeman**

SECTION B

Manchester Grand Hyatt San Diego
Cortez Hill C

General Papers/New Concepts in Polymeric Materials

T. J. Bunning, *Organizer*

S. Förster, S. Rajabpour, *Presiding*

9:00 **501.** Reactive polymer-based dsRNA detection as a diagnostic platform for viral infection. S. Kim, J. Ku, J. Park, Y. Kim, **S. Li**

9:20 **502.** Unveiling graphene role in pan/graphene composite fiber: Combination of atomistic scale simulation and experimental characterization. **S. Rajabpour**, Z. Gao, M. Kowalik, J. Zhu, X. Li, A.C. Van Duin

9:40 **503.** Synthesis of Cu nanoparticles decorated reduced graphene oxide and its role in tailoring the electrical character of percolative polymer composites. **T. Hussain**, I. Saeed, A. Mujahid

- 1:50 **491.** Improving the thermal stability of thin film composite membranes by modifying the structure of the selective layer. **P. Karami**, B. Khorshidi, M. Sadrzadeh, J.B. Soares
- 2:10 **492.** Developing high-performance PA 11/cellulose nanocomposites for industrial-scale melt processing. **P. Venkatraman**, A. Gohn, A.M. Rhoades, J. Foster
- 2:30 Intermission.
- 2:50 **493.** pH-Responsive amphiphilic polymeric oleonic acid prodrug nanoparticles encapsulating 10-hydroxycamptothecin for combined chemotherapy. **Y. Wang**, P. Zhu, G. Li, S. Zhu, K. Liu, Y. Liu, J. He, J. Lei
- 3:10 **494.** Universal smart antibacterial surfaces with regenerability and multifunctionality. **Q. Yu**
- 3:30 **495.** Continuous assembly of a polymer on a metal-organic framework. **Q. Fu**

Future of Biomacromolecules at a Crossroads of Polymer Science & Biology

Biomaterials

Sponsored by POLY, Cosponsored by BIOL, CARB, CELL, COLL, ENVR, MEDI, PHYS and PMSE

Polymeric Materials for Water Purification

Sponsored by POLY, Cosponsored by PMSE

WEDNESDAY EVENING – PMSE

SECTION A

Manchester Grand Hyatt San Diego
Harbor A-E

PMSE/POLY Plenary Lecture & Awards Symposium

Cosponsored by POLY

M. Becker, S. E. Morgan, *Organizers, Presiding*

5:30 Reception.

6:00 **496.** Ion solubility, diffusivity, and transport in charged polymer membranes. **B.D. Freeman**

6:40 Award Presentation.

7:00 Reception.

- 10:00 Intermission.
- 10:20 **504.** 3D printing PLGA scaffolds following chemical modification for cartilage and bone tissue regeneration. **S. Lee**
- 10:40 **505.** Degradable thermoset fibers containing renewable carbohydrate-derived diol subunits. **S. Kim**, C. Lau, L.M. Lillie, W.B. Tolman, T.M. Reineke, C.J. Ellison
- 11:00 **506.** Enhanced mechanical reactivity of mechanophore-linked nanocomposites. **T. Kim**, C. Lamuta, H. Kim, C. Leal, J.S. Moore, S. White, N.R. Sottos
- 11:20 **507.** High-brilliance neutron beams for spatially and time-resolved *in situ* investigations of polymeric and biological materials. H. Frielinghaus, **S. Förster**

SECTION C

Manchester Grand Hyatt San Diego
Bankers Hill

General Papers/New Concepts in Polymeric Materials

T. J. Bunning, *Organizer*

V. R. Feig, W. Young, *Presiding*

- 9:00 **508.** Tuning dynamics of wrinkling surfaces. S. Zeng, R. Li, D. Zhang, **L. Sun**
- 9:20 **509.** Micelles postmodified with cell penetrating peptides for efficient gene delivery in plants. **T. Miyamoto**, K. Tsuchiya, K. Numata
- 9:40 **510.** Electrochemical patterning of tissue-mimetic conductive hydrogels. **V.R. Feig**, H. Tran, M. Lee, K. Liu, Z. Huang, Z. Bao
- 10:00 Intermission.
- 10:20 **511.** Novel synthesis method of PVA/HPMC nanofibers resistant in aqueous media for their use in drug delivery. **M. Calzado Delgado**, M. Guerrero-Perez, K. Yeung
- 10:40 **512.** Phase behavior of mixed polymer brushes grown from ultra-thin coatings. **W. Wei**, T. Kim, B. Ayyakkalai, S. Hur, P. Gopalan
- 11:00 **513.** Analysis of gel fraction and swell ratio of polyacrylic copolymers using asymmetric flow field flow fractionation. **W. Young**, L. Bai, L. Leal, J. Koenig, S. Golden, S. Zhang
- 11:20 **514.** Main-chain donor-acceptor conjugated polymers by “click” chemistry. **W. Huang**

SECTION D

Manchester Grand Hyatt San Diego
Hillcrest A

General Papers/New Concepts in Polymeric Materials

T. J. Bunning, *Organizer*

X. Yao, Y. Zheng, *Presiding*

- 9:00 **515.** Relationship between gas solubility/diffusivity and dielectric property under high temperatures and pressures. **X. Yao**, L. Schadler, H. Park, P. Lee
- 9:20 **516.** Heparin-mimicking polymers modified material surfaces: Preparation and blood interaction studies. X. Chen, S. Jin, **X. Liu**, H. Chen
- 9:40 **517.** Effects of polymer-grafted graphene oxide and polymer-grafted thermally reduced graphene oxide on the volume shrinkage, mechanical properties, and thermal conductivities of cured vinyl ester resins. **Y. Huang**, T. Chang, Y. Lin, Y. Chen, W. Lin
- 10:00 Intermission.
- 10:20 **518.** Electrically conductive polymer/rGO nanocomposite films at ambient temperature via miniemulsion polymerization using GO as surfactant. **Y. Fadil**, V. Agarwal, F. Jasinski, S. Thickett, H. Minami, P.B. Zetterlund
- 10:40 **519.** Processing methods for protein-polymer composites. **Y. Zheng**, C. Wang, D.M. Wirth, N. Steinmetz, J.K. Pokorski

SECTION E

Manchester Grand Hyatt San Diego
Hillcrest B

General Papers/New Concepts in Polymeric Materials

T. J. Bunning, *Organizer*

Z. Aytac, Y. Liu, *Presiding*

- 9:00 **520.** Layered polymer-based devices for detecting volatile organic compounds. **Y. Zhang**, **M. Serpe**
- 9:20 **521.** Regulating force-activated ring opening of aliphatic cyclobutenes. **Y. Liu**, Y. Jia, J.S. Moore
- 9:40 Intermission.
- 10:00 **522.** Electrospun gelatin nanofibers encapsulating ciprofloxacin/cyclodextrin inclusion complex as a fast-dissolving drug delivery system. **Z. Aytac**, S. Ipek, I. Erol, E. Durgun, T. Uyar
- 10:20 **523.** Enhancing the processability of hybrid filled-type thermally conductive polycarbonate composites. **Z. Yu**, J.H. Wang, Y. Bai, Y. Li
- 10:40 **524.** Spiropyran for impact strain sensing. V. Alphonse, K. Ott, E. Lloyd, **Z. Xia**

- 11:00 525. Polymeric acidoCEST MRI contrast agent for imaging tumor extracellular pH. **C.J. Kombala**, M.D. Pagel

SECTION F

Manchester Grand Hyatt San Diego
Hillcrest D

General Papers/New Concepts in Polymeric Materials

T. J. Bunning, *Organizer*

B. D. Almquist, F. Zhang, *Presiding*

- 9:00 526. Harnessing cellular traction forces to enable cell-selective delivery of biologics. A. Stejskalová, N. Oliva, F. England, **B.D. Almquist**
- 9:20 527. Improving functionality and targeting capabilities of polymeric micelles. **B. Grim**, M. Green
- 9:40 528. Tissue-adaptive bottlebrush networks. **E. Dashtimoghadam**, M. Vantankhah-Varnosfaderani, D. Zhang, F. Fahimipour, S. Sheyko
- 10:00 Intermission.
- 10:20 529. Degradable polyphosphoester-based nanoparticles carrying silver-based antimicrobials for the treatment of bacterial infections. **F. Zhang**, Q. Chen, K.N. Shah, R. Li, J.A. Smolen, C.L. Cannon, K.L. Wooley
- 10:40 530. Supramolecular hydrogels: Complex rheological behavior and its impact on drug delivery. **H. Lopez Hernandez**, E.A. Appel
- 11:00 531. Effect of pH on chitosan-tripolyphosphate nanoparticles for oral drug delivery in a model digestive system. **J.M. Patterson**, K. Milligan, C. Winstead
- 11:20 532. Site-specific grafting from strategy improves both activity and stability of insulin-trehalose glycopolymer conjugate. **K.M. Messina**, H.D. Maynard

SECTION G

Manchester Grand Hyatt San Diego
Hillcrest C

General Papers/New Concepts in Polymeric Materials

T. J. Bunning, *Organizer*

A. Sarkar, Y. Yang, *Presiding*

- 9:00 533. Broader range of tunable persistent micelle templates: Homopolymer swelling approach. **A. Sarkar**, M. Stefik
- 9:20 534. Conjugation of polynorbornene to cell surfaces. **D. Church**, J.K. Pokorski
- 9:40 535. Hydrogels from crosslinked bottlebrush polymers. **F. Jia**, R. Macfarlane
- 10:00 536. Systematically controlled decomposition mechanism in phosphorus flame retardants by precise molecular architecture: P-O vs. P-N. **J.C. Markwart**, A. Battig, B. Schartel, F. Wurm
- 10:20 Intermission.
- 10:40 537. Compartmentalized nanoreactors for one-pot redox-driven deracemizations. **P. Qu**, M. Kuepfert, S. Jockusch, M. Weck
- 11:00 538. Dynamic ureas with fast and pH-independent hydrolytic kinetics. **Y. Yang**, K. Cai, H. Ying, J. Cheng
- 11:20 539. Evaluation of the Hofmeister series with color-tunable poly(N-isopropylacrylamide) microgel-based etalons. **W. Carvalho**, **M. Serpe**

Materials Advances in Nanocellulose Research for Engineered Functionality

Sponsored by CELL, Cosponsored by PMSE and POLY

Polymeric Materials for Water Purification

Sponsored by POLY, Cosponsored by PMSE

Polymeric Materials for Water Purification

Sponsored by POLY, Cosponsored by PMSE

POLY

DIVISION OF POLYMER CHEMISTRY

T. Epps, B. Helms and H. Brown, *Program Chairs*

SUNDAY MORNING – POLY

SECTION A

Manchester Grand Hyatt San Diego
Hillcrest B

Polymerization-Induced Nanostructural Transitions

S. P. Armes, A. J. Magenau, *Organizers*
R. Hickey, *Organizer, Presiding*
M. Seo, *Presiding*

- 8:00** 1. High throughput and solution phase TEM for discovery of new pisa reaction manifolds. **N.C. Gianneschi**, M.A. Touve, A. Figg, D. Wright, C. Park, J. Cantlon, B.S. Sumerlin
- 8:30** 2. Accelerated polymerization-induced self-assembly using automated continuous-flow reactors. **N. Warren**
- 8:50** 3. How do diblock copolymer micelles form during polymerization-induced self-assembly?. **M.J. Derry**, O. Mykhaylyk, A.J. Ryan, S.P. Armes
- 9:10** 4. RAFT dispersion polymerization in silicone oil. **M.J. Rymaruk**, S.J. Hunter, C. O'Brien, S. Brown, C. Williams, S.P. Armes
- 9:30** 5. Synthesis of amphiphilic block copolymers in RAFT aqueous emulsion polymerization: From block copolymer nanoparticles towards surfactant-free latexes. **M. Lansalot**, J. Lesage de la Haye, E. Velasquez, I. Chaduc, B. Ebeling, M. Fuentes-Exposito, J. Delorme, C. Bergerbit, V. Monteil, F. D'Agosto
- 10:00** Intermission.
- 10:20** 6. Self-templating surface-initiated polymerization for fabrication of conjugated polymer brushes. **S. Zapotoczny**, K. Wolski, M. Szuwarzynski, A. Gruskiewicz, G. Grzes, A.J. Wojcik, M. Slowikowska, J. Rokita
- 10:40** 7. Polymerization-induced self-assembly of bottlebrush-like polymers. **S. Häkkinen**, J. Tanaka, R. Garcia Maset, S. Perrier

- 11:00** 8. Controlled polymerization of ethylene and potential applications to polymerization induced self-assembly. **F. D'Agosto**, A. Wolpers, C. Bergerbit, F. Baffie, M. Lansalot, V. Monteil, N. Baulu, C. Boisson
- 11:30** 9. Using wavelength orthogonality for successive photoinduced polymerization-induced self-assembly (PISA), photo-crosslinking, and disassembly. **C. Boyer**

SECTION B

Manchester Grand Hyatt San Diego
Coronado D

Paul Flory's "Statistical Mechanics of Chain Molecules: The 50th Anniversary of Polymer Chemistry"

History & Principles of Statistical Mechanics of Chain Molecules

A. E. Tonelli, *Organizer*
G. D. Patterson, *Organizer, Presiding*
D. Y. Yoon, *Presiding*

- 8:00** 10. History of the development of the concept of molecular rotational states. **G.D. Patterson**
- 8:30** 11. Paul Flory's "statistical mechanics of chain molecules" in China. **D. Wu**, Y. Xu
- 9:00** 12. Chemistry, physics, and biology meet. **U.W. Suter**
- 9:30** Intermission.
- 9:45** 13. Statistical mechanics of chain molecules in nematic melts of semiflexible polymers and thin polymer films. **D.Y. Yoon**
- 10:15** 14. Structure-property relationships of green polymers, unraveled by *ab initio*, RIS, and periodic density functional theory calculations. **Y. Sasanuma**
- 10:45** 15. Influences of *Statistical Mechanics of Chain Molecules* on atomistic materials simulation software. **D. Rigby**

SECTION C

Manchester Grand Hyatt San Diego
Promenade A/B

Eco-Friendly Polymerization

C. Boyer, D. Konkolewicz, *Organizers*

A. Anastasaki, P. B. Zetterlund, *Presiding*

- 8:00** 16. Oxygen tolerant Cu-mediated RDRP. **E. Liarou**, A. Anastasaki, R. Whitfield, D.M. Haddleton
- 8:20** 17. Stereocontrolled cationic polymerization of vinyl ethers. **T.P. Varner**, A. Teator, Z. Wickens, E.N. Jacobsen, F.A. Leibfarth
- 8:40** 18. Rapid and efficient RAFT polymerization using enzymes under mild conditions. **D. Konkolewicz**, A. Danielson, C.T. Kozuszek, J. Bornstein, D. Bailey Van-Kuren, R.C. Page
- 9:00** 19. Multiblock copolymer synthesis and nanoparticle engineering in environmentally friendly aqueous-based emulsion systems. T. Guimaraes, M. Khan, G. Clothier, H. Minami, G. Moad, S. Perrier, **P.B. Zetterlund**
- 9:30** 20. Using oxygen for photocontrolled/living radical polymerization in water. J. Yeow, **C. Boyer**
- 10:00** Intermission.
- 10:30** 21. Metal-free living cationic polymerization based on degenerative chain-transfer mechanism. **M. Uchiyama**, K. Satoh, M. Kamigaito
- 11:00** 22. Controlled/living polymerization of renewable styrenes for novel functional bio-based polymers. **K. Satoh**
- 11:30** 23. What happens in the dark in organic and aqueous media? Assessing the temporal control of photo-mediated radical polymerizations. **A. Anastasaki**, N. Dolinski, C.J. Hawker

SECTION D

Manchester Grand Hyatt San Diego
Mission Beach A/B

Characterization of Plastics in Aquatic Environments

Cosponsored by ANYL, BIOL, CEI, ENVR, I&EC, PMSE and PRES

Financially supported by NIST; BASF

S. V. Orski, M. A. Pasquinelli, *Organizers*

R. T. Mathers, *Organizer, Presiding*

- 8:00** Introductory Remarks.
- 8:10** 24. Transport and characterization of microplastics in inland waterways. J.A. Czuba, **J.R. Barone**
- 8:40** 25. Tracking microplastics to their source: Analytical techniques for characterizing weathered polymers. **P. Potter**, Q. Birch, P. Pinto, S.R. Al-Abed
- 9:00** 26. Analytical approach for the identification

and quantification of microplastic particles by a combination of particle analysis with FTIR and Raman microscopy. **F. Fischer**, J. Brandt, L. Bittrich, A. Käppler, D. Fischer, K. Eichhorn

- 9:20** 27. Quantification and characterisation of nanoplastics generated from the fragmentation of microplastic in water. **J. Lee**, M. Enfrin, L.F. Dumeé Intermission.
- 9:50** 28. Plastic degradation: How stabilizing additives affect plastics in aquatic environments. **K.M. Knauer**
- 10:20** 29. Low-temperature decomposition on thermoplastic and ocean contamination derived from debris plastic. **K. Saïdo**, H. Kimukai, **K. Koizumi**, Y. Koderä, K. Yamada, S. Chung, B. Kwon, T. Hiaki
- 10:50** 30. Hydrophobicity influences degradation of ocean plastics. **R.T. Mathers**

SECTION E

Manchester Grand Hyatt San Diego
Mission Beach C

General Topics: New Synthesis & Characterization of Polymers

B. Barkakaty, D. Garcia, *Organizers*

B. Hu, A. V. Zhukhovitskiy, *Presiding*

- 8:00** 31. Synthesis of new flame retardant polymers via olefin metathesis. **E. Kovacs**, F. Domahidy, L. Trif, G. Turczel, R. Tuba
- 8:20** 32. Mild polymerization methods for the synthesis of modular fluoropolymers. **J. Jaye**, E.M. Sletten
- 8:40** 33. Controlled and quasi-living carbene polymerization initiated by dinuclear palladium complexes. **A.V. Zhukhovitskiy**, I. Kobylanskiy, A. Thomas, A.M. Evans, C. Delaney, N.C. Flanders, S.E. Denmark, W.R. Dichtel, D. Toste
- 9:00** 34. Chain-growth polymerization of alkenyl boronates: Synthesis of conventionally inaccessible polymers based on replaceable side chain. **T. Nishikawa**, M. Ouchi
- 9:20** 35. Utilising the inbuilt feeding mechanism of emulsion polymerisation to improve RAFT control: Applications to methacrylate monomers. **R. Richardson**, G. Moad, P.B. Zetterlund, S. Perrier
- 9:40** 36. Exploiting the orthogonality of cationic and radical RAFT polymerization for the synthesis of bottlebrush polymers. **J. Tanaka**, W. You
- 10:00** 37. Organocatalytic ring-opening copolymerization of 3S,6S-dimethylmorpholine-2,5-dione and L-lactide: Route towards isolated α -amino acid moieties along the polylactide chain. **T. Kivijärvi**, D. Pappalardo, P. Olsen, A.F. Wistrand

- 10:20** 38. Synthesis of bottlebrushes from PGMA-PVDMA block copolymers. **B. Hu**, N. Borodinov, R. Kumar, S. Retterer, B.S. Lokitz
- 10:40** 39. Polymerization induced phase separation of methyl methacrylate and Trommsdorff effect. **Y. Suzuki**, Y. Shinagawa, K. Fukao, A. Matsumoto
- 11:00** 40. Versatile synthesis of well-defined AIE-active polymers via Cu(0)-mediated RDRP. **C. Ma**, D.M. Haddleton, A.M. Eissa
- 11:20** 41. Tailored monomers for backbone degradable polymers by ring-opening metathesis polymerization. **P. Shieh**, J.A. Johnson
- 11:40** 42. Developing a simple and versatile route to amphiphilic polymethacrylates: Catalytic chain transfer polymerisation (CCTP) coupled with post-polymerisation modification. **J. Abi Saleh**, G. Patias, J.S. Town, A. Wemyss, A. Eissa, A. Shegiwal, D.M. Haddleton

Emulsification & Encapsulation by Soft Matter Techniques

Engineering of Emulsification & Encapsulation

Sponsored by PMSE, Cosponsored by POLY

SUNDAY AFTERNOON – POLY

SECTION A

Manchester Grand Hyatt San Diego
Hillcrest B

Polymerization-Induced Nanostructural Transitions

S. P. Armes, R. Hickey, *Organizers*
A. J. Magenau, *Organizer, Presiding*
N. J. Penfold, *Presiding*

- 1:00** 43. Polymerization induced microphase separation approaches to nanostructured materials for electrochemical, optical, and water applications. **M.A. Hillmyer**
- 1:30** 44. Size-dependent transport in porous polymer membranes via polymerization-induced microphase separation: Pushing the limit of domain size control. **M. Seo**
- 2:00** 45. Static and *in situ* morphology characterization of polymeric materials created using polymerization-induced nanostructural transitions. **R. Hickey**
- 2:30** 46. Polymerization-induced self-assembly for membrane technology. **M. Semsarilar**
- 3:00** Intermission.

- 3:30** 47. Dictating the evolution of morphology in PISA. G. Scheutz, C. Figg, R.N. Carmean, K.C. Bentz, D.A. Savin, M.A. Touve, N.C. Gianneschi, **B.S. Sumerlin**
- 4:00** 48. How much hydrophobicity is necessary for polymerization induced self assembly (PISA)? **R.T. Mathers**
- 4:30** 49. Steering PISA toward the fiber morphology. G. Mellot, L. Bouteiller, F. Stoffelbach, **J. Rieger**

SECTION B

Manchester Grand Hyatt San Diego
Coronado D

Paul Flory's "Statistical Mechanics of Chain Molecules: The 50th Anniversary of Polymer Chemistry"

Biological Applications of the Rotational Isomeric State Paradigm

G. D. Patterson, A. E. Tonelli, *Organizers*
R. L. Jernigan, W. K. Olson, *Presiding*

- 1:00** 50. Empirical energies and intramolecular bond and sequence correlations. **R.L. Jernigan**
- 1:30** 51. α -Helix-sense inversion of polypeptides triggered by the side chain conformation. **A. Abe, H. Furuya**
- 2:00** 52. Chromosome organization through Flory's insights. **D. Thirumalai**
- 2:30** Intermission.
- 2:45** 53. Insights into DNA and chromatin from realistic treatment of the double helix. **W.K. Olson**
- 3:15** 54. Applications of basic ideas of statistical mechanics of chain molecules to proteins. **A. Kloczkowski, R.L. Jernigan**
- 3:45** 55. Multi-scale modeling of the nanomechanics of microtubule filaments. **R.I. Dima**

SECTION C

Manchester Grand Hyatt San Diego
Promenade A/B

Eco-Friendly Polymerization

C. Boyer, *Organizer*
D. Konkolewicz, *Organizer, Presiding*
S. Perrier, *Presiding*

- 1:00** 56. Aqueous photoiniferter polymerizations. M.B. Sims, R.N. Carmean, C. Figg, G. Scheutz, T. Kubo, **B.S. Sumerlin**
- 1:30** 57. *Ab initio* RAFT emulsion polymerization using low molar mass RAFT agents to form low dispersity polymers. S.J. Stace, J. Vanderspikken, S. Howard, G. Li, B.W. Muir, C.M. Fellows, D.J. Keddie, **G. Moad**

- 2:00 58. Transition-metal-free photopolymerization of pi-conjugated polymers. **J.A. Kalow**
- 2:30 59. RAFT polymerisation: From yellow to green. **S. Perrier**
- 3:00 Intermission.
- 3:30 60. Copper mediated living radical polymerisation in the presence of oxygen. **D.M. Haddleton**, E. Liarou
- 4:00 61. Designing thermally stable organocatalyst for high temperature polymerization and depolymerizations. C. Jehanno, A.P. Dove, **H. Sardon**
- 4:20 62. Cationic polymerization in emulsion: New catalysts for enhanced polymer synthesis. **F. Ganachaud**, S.V. Kostjuk, I. Vasilenko
- 4:40 63. Supported lanthanide catalysts: Role of the grafting on the stereochemical outcome of β -butyrolactone ROP reaction. **A. Bathellier**, C. Dinoi, I. Del Rosal, L. Maron

SECTION D

Manchester Grand Hyatt San Diego
Mission Beach A/B

Characterization of Plastics in Aquatic Environments

Cosponsored by ANYL, BIOL, CEI, ENVR, I&EC, PMSE and PRES

Financially supported by NIST; BASF

R. T. Mathers, M. A. Pasquinelli, *Organizers*

S. V. Orski, *Organizer, Presiding*

- 1:00 64. In-depth look at polymer identification of Hawaiian plastic marine debris: Inter-laboratory comparison of different methods. **J. Lynch**, A. Deshpande, W. Weatherford, R. Wagner, K.C. Brignac, K. Page, M.R. Jung, N. Lascelles, D. Freeman, D. Drayton, C. King
- 1:30 65. Microplastics quantification in complex environment samples using combined solvent extraction and pyrolysis gas chromatography-mass spectrometry. **E. Okoffo**, F. Ribeiro, S. O'Brien, J. O'Brien, M. Gallen, K. Thomas
- 1:50 66. Ingested micronizing plastic particle compositions and size distributions within stranded post-hatchling sea turtles. **E.M. White**, S. Clark, C. Manire, B. Crawford, S. Wang, J.J. Locklin, B. Ritchie
- 2:20 Intermission.
- 2:50 67. Quantitative chemical, thermal, and molecular mass measurements of recovered ocean plastics. **S.V. Orski**, V. Rodriguez C., G. Kenlaw, K. Beers
- 3:20 68. Electrokinetic focusing, sorting, and separation of microplastics by serial faradaic ion concentration polarization. **C. Davies**, R.M. Crooks

- 3:40 69. Characterization of plastics in aquatic environments: Panel discussion. J.R. Barone, **K. Beers**, K.M. Knauer, J. Lee, E.M. White

SECTION E

Manchester Grand Hyatt San Diego
Mission Beach C

General Topics: New Synthesis & Characterization of Polymers

B. Barkakaty, D. Garcia, *Organizers*

Y. Li, M. J. Young, *Presiding*

- 1:00 70. Copolymer microstructure determination by tandem mass spectrometry. **J.S. Town**
- 1:20 71. Fast measurements of hydrodynamic radii and intrinsic viscosity measurements of polymers via diffusion NMR. **T.A. Swift**
- 1:40 72. Advanced size-exclusion chromatography and field-flow fractionation for characterization of complex synthetic polymers. **Y. Li**, M. Bashir, D.M. Meunier
- 2:00 73. Investigating the kinetics and structure of network formation in UV-photopolymerizable starch nanogel network hydrogels using very small angle neutron scattering (vSANS). **M.J. Majcher**
- 2:20 74. Fabrication of polymer-coated thiol-reactive magnetic nanoparticles for cellular targeting. **A. Sanyal**
- 2:40 75. Transient self-assembled polymeric contrast agents for superfine cerebrovasculature MR imaging. **A. Mahara**, S. Saito, Y. Hsu, T. Yamaoka
- 3:00 76. Tuning material properties: CO₂-selective terpolymerizations from β -butyrolactone, epoxides and CO₂ and their kinetic, thermal and mechanical characterization. **S. Kernbichl**, B. Rieger
- 3:20 77. Interior of amylopectin in solution probed by fluorescence, molecular mechanics optimizations, dynamic light scattering, and viscosity. **J. Duhamel**, L. Lu
- 3:40 78. Nanophase separation of high χ , low N block copolymers by photoinduced, copper-mediated ATRP, achieving sub-2 nm domains at half-pitch. **E.K. Hancox**, E. Liarou, G.R. Jones, J.S. Town, P. Topham, D.M. Haddleton
- 4:00 79. Two-dimensional, sandwich-like porous polymers and their potential in energy field. **X. Zhuang**
- 4:20 80. Enzymatic route for the synthesis of norcamphor lactone and its polymerization for applications as thermo-sensitive networks. **W. Farhat**, A. Stamm, A. Biundo, L. Fogelström, E. Malmström, P. Syrén

- 4:40 **81.** Designing “sweet nanoparticles” as a novel strategy to combat antibiotic-resistant bacteria. **M. Al-Ali**, B.C. Benicewicz, A. Decho, S.L. Witcher

Design, Synthesis & Engineering of Polypeptides for Biological & Biomedical Application

Self-Assembly & Engineering of Functional Polypeptides

Sponsored by PMSE, Cosponsored by POLY

Emulsification & Encapsulation by Soft Matter Techniques

Conventional & Non-conventional Multiphase Systems

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MONDAY MORNING

SECTION A

Manchester Grand Hyatt San Diego
Golden Hill A/B

Polymerization-Induced Nanostructural Transitions

S. P. Armes, R. Hickey, A. J. Magenau, *Organizers*
B. Jones, R. T. Mathers, *Presiding*

- 8:00 **82.** *In situ* spectroscopic studies of highly transparent nanoparticle dispersions enable assessment of trithiocarbonate chain-end fidelity during RAFT dispersion polymerization in non-polar media. **S.P. Armes**
- 8:30 **83.** Metal-catalyzed polymerization-induced self-assembly. **S. Jimaja**, D. Taton, R.K. O'Reilly, A.P. Dove
- 8:50 **84.** Nanostructure synthesis by ring-opening metathesis polymerization-induced self-assembly. **J. Foster**, S. Varlas, L.A. Arkinstall, R. Keogh, R.K. O'Reilly
- 9:10 **85.** RAFT aqueous emulsion polymerization of 2-methoxyethyl methacrylate. **E.E. Brotherton**, F.L. Hatton, A.A. Cockram, S.P. Armes
- 9:30 **86.** One-pot synthesis of functional micelles and vesicles. F.H. Sobotta, **J.C. Brendel**
- 10:00 Intermission.
- 10:30 **87.** Using PISA to create functional nanostructures. **R.K. O'Reilly**, J. Foster
- 11:00 **88.** Accessing unusual morphologies via polymerization-induced self-assembly. **Z. An**, F. Lv, P. Wu
- 11:30 **89.** Artificial biomembrane models using giant vesicles prepared by photo NMP-induced self-assembly. **E. Yoshida**

SECTION B

Manchester Grand Hyatt San Diego
Coronado D

Paul Flory's “Statistical Mechanics of Chain Molecules: The 50th Anniversary of Polymer Chemistry”

G. D. Patterson, A. E. Tonelli, *Organizers*
H. W. Spiess, A. E. Tonelli, *Presiding*

- 8:00 **90.** Multiscale computational approaches for building realistic molecular models of self-organized co-oligomers in select solvents. **C. Atilgan**
- 8:30 **91.** Allosteric interactions in biological macromolecules. **t. haliloglu**
- 9:00 **92.** Turn ENM into a timer and sizer of biomacromolecular functional dynamics. **L.W. Yang**, J. Chan, H. Lin, K. Takemura, K. Chang, Y. Chang, J. Yasumasa, A. Kitao
- 9:30 Intermission.
- 9:45 **93.** Role of conformation of side groups in supramolecular organization of materials for organic electronics. **H.W. Spiess**
- 10:15 **94.** Using Flory's view of conformational populations to probe polymer mixing. **J.L. White**
- 10:45 **95.** Characterizing the overall molecular architectures of synthetic polymers requires Flory's *Statistical Mechanics of Chain Molecules*. **A.E. Tonelli**

SECTION C

Manchester Grand Hyatt San Diego
Promenade A/B

Eco-Friendly Polymerization

D. Konkolewicz, *Organizer*
C. Boyer, *Organizer, Presiding*
T. Junkers, *Presiding*

- 8:00 **96.** Highly efficient aminolysis process for polycarbonate recycling. **C. Wu**, Y. Huang, S. Dai, R. Jeng
- 8:20 **97.** Bio-based recyclable block copolymers from limonene oxide and CO₂. **L. Pena Carrodeguas**, C.K. Williams
- 8:40 **98.** Bio-based reprocessable polyhydroxyurethane networks: Full recovery of cross-link density with three concurrent dynamic chemistries. **X. Chen**, S. Hu, J.M. Torkelson

- 9:00 **99.** Reprocessable polymer networks exhibiting full crosslink density recovery after recycling: Three eco-friendly alternatives to conventional thermosets based on dynamic covalent bonds. **J.M. Torkelson**, L. Li, X. Chen, K. Jin
- 9:30 **100.** Room-temperature polymerization in concentrated emulsion gels with no solvents. **F.D. Blum**, T. Zhang, G. Xu
- 10:00 Intermission.
- 10:30 **101.** Selective or living organopolymerization of a six-five bicyclic lactone to produce fully recyclable polyesters. **R.M. Cywar**, J. Zhu, E.Y. Chen
- 10:50 **102.** Designing plastics for the circular economy. **P. Christensen**, A. Scheuermann, K. Loeffler, B. Helms
- 11:10 **103.** Sustainable solventless approach to fabricate porous polymer membranes. **N. Movsesian**, G. Dianat, M. Gupta
- 11:30 **104.** Biobased monomer synthesis and their sustainable radical polymerization. **T. Junkers**

SECTION D

Manchester Grand Hyatt San Diego
Mission Beach A/B

Future of Biomacromolecules at a Crossroads of Polymer Science & Biology

Synthetic Cells

Cosponsored by BIOL, CARB, CELL, COLL, ENVR, MEDI, PHYS and PMSE

A. Albertsson, S. Percec, *Organizers*

K. S. Anseth, T. J. Deming, *Presiding*

- 8:00 Introductory Remarks.
- 8:10 **105.** Searching for the early events of life with sequence-defined unimolecular components based on bio-renewable materials. **V. Percec**
- 8:40 **106.** Designing biomacromolecular materials with tailored (poly)peptide conjugates. K.L. Kiick, **M.L. Klein**, K. Elokely, E. Gianti, V. Carnevale
- 9:10 **107.** Biomimetic polymer-based self-assemblies: Future directions towards functional biomaterials. **S. Lecommandoux**
- 9:40 Intermission.
- 10:00 **108.** Materials made of synthetic polysaccharides. **P.H. Seeberger**
- 10:30 **109.** Molecular intelligence: Rise of polymeric nanomachines. **D.A. Wilson**
- 10:55 **110.** Responsive nanocapsules and synthetic multicompartment as cell mimics. **B. Voit**, D. Appelhans, X. Liu, X. Wang
- 11:25 **111.** Polymer nanostructures for bioapplications: From stem cells enrichment to drug delivery. **M. Monteiro**

SECTION E

Manchester Grand Hyatt San Diego
Mission Beach C

General Topics: New Synthesis & Characterization of Polymers

B. Barkakaty, D. Garcia, *Organizers*

A. M. Alb, D. C. McLeod, *Presiding*

- 8:00 **112.** Enhanced toughness and water resistance of polyamide 11 copolymers with dimer acids derived from waste vegetable oil. **M. Park**, S. Lee, A. Kim, J. Shin, Y. Kim
- 8:20 **113.** *In situ* SAXS studies during aqueous emulsion polymerisation. **A. Czajka**, S.P. Armes
- 8:40 **114.** Competitive effects of synthesis parameters on polymer chain architecture and behavior under changes in environmental conditions. **A.M. Alb**
- 9:00 **115.** Effect of fluorinated monomer incorporation on backbone of polyimide aerogel matrix. **S.L. Vivod**, M. Meador
- 9:20 **116.** Evaluation of drug release from bottlebrush and brush-arm star polymers. **S.L. Kristufek**, H.V. Nguyen, J.A. Johnson
- 9:40 **117.** Controlled self-assembly of amphiphilic polymers: Design strategies for precision nanostructure materials. **T. Terashima**
- 10:00 **118.** Ion gels by self-assembly of triblock copolymer/ionic liquid/monomer mixtures. **A. Bandegi**, J. Banuelos, R. Foudazi
- 10:20 **119.** Synthesis of hydrogen-bonded 2-D polymers. **D.C. McLeod**, R.H. Lambeth
- 10:40 **120.** Synthesis of 2-oxazoline ethylenimine copolymers possessing complex architectures. **T. Floyd**, S. Perrier
- 11:00 **121.** Macromolecular engineering of fluoropolymers. V. Bouad, M. Guerre, C. Totée, B.M. Ameduri, S. Banerjee, C. Detrembleur, A. Debuigne, G. Silly, R. Poli, **V. Admiral**
- 11:20 **122.** Temperature-directed morphology transformation method to produce well-defined complex multifunctional polymer particles. **V. Bobrin**, S. Chen, Z. Jia, M. Monteiro

Design, Synthesis & Engineering of Polypeptides for Biological & Biomedical Application

Design & Synthesis of Polypeptide Materials

Sponsored by PMSE, Cosponsored by POLY

Unique & Complex Polymer Architectures Networks

Sponsored by PMSE, Cosponsored by POLY

2019 ACS International Award for Research in Agrochemicals: Advances in the Physiology & Biochemistry of Insect Control

Sponsored by AGRO, Cosponsored by AGFD, BIOL, MEDI, POLY and PROF

Emulsification & Encapsulation by Soft Matter Techniques

Polymerization-Induced Self Emulsification & Encapsulation

Sponsored by PMSE, Cosponsored by POLY

MONDAY AFTERNOON – POLY

SECTION A

Manchester Grand Hyatt San Diego
Golden Hill A/B

Polymerization-Induced Nanostructural Transitions

S. P. Armes, R. Hickey, A. J. Magenau, *Organizers*
J. C. Brendel, M. J. Derry, *Presiding*

- 1:00** **123.** Combining crystallization-driven and polymerization-induced self-assembly: Scale-up of uniform and hierarchical polymeric nano- and microparticles. **I. Manners**
- 1:30** **124.** Exploiting metathesis depolymerization of polybutadiene for responsive materials: From block polymer self-assembly to modification of elastomers. **B. Jones**
- 2:00** **125.** Inducing block copolymer self-assembly through functionalization. **A.J. Magenau**
- 2:30** **126.** Deprotection-induced glycopolymer self-assembly (DISA) for nanostructure construction and immunological applications. **G. Chen**
- 3:00** Intermission.
- 3:20** **127.** Dynamic covalent bonds to design and morph materials from the nanoscale up. **D. Konkolewicz**, S. Wanasinghe, P. Chakma, A. Thompson, E. Schreiber, J. Sparks
- 3:50** **128.** Formation mechanism of polyethylene nanofibers produced via polymerization in confinement. **V. Karimkhani**, V. Haddadi-Asl, T. Mahmoudi, E. Zhuravlev, A. Gharachorlou, M. Vantankhah-Varnosfaderani, C. Schick, F.J. Stadler
- 4:10** **129.** *In situ* SAXS studies during RAFT aqueous dispersion polymerisation. **A. Czajka**, S.P. Armes
- 4:30** **130.** *In situ* SAXS studies during RAFT aqueous emulsion polymerization. **S.P. Armes**

SECTION B

Manchester Grand Hyatt San Diego
Coronado D

Paul Flory's "Statistical Mechanics of Chain Molecules: The 50th Anniversary of Polymer Chemistry"

G. D. Patterson, A. E. Tonelli, *Organizers*
B. E. Eichinger, C. Wu, *Presiding*

- 1:00** **131.** Depolymerization of polymeric sulfur. T. Kemper, E. Wimmer, **B.E. Eichinger**
- 1:30** **132.** Universal scaling of phase diagrams of polymer solutions. **C. Wu**
- 2:00** **133.** Intramolecular and intermolecular interactions in semicrystalline polymers. **T. Miyoshi**
- 2:30** Intermission.
- 2:45** **134.** Conformational dynamics play critical role in protein evolution. **S. Ozkan**
- 3:15** **135.** Multiscale modeling of protein unfolding and translocation in the degradation pathway. **G. Stan**
- 3:45** **136.** Effective interactions between nano-particles mediated by dense polymer systems and the Flory's theorem. **A. Chervanyov**
- 4:15** **137.** Conformational analysis, RIS models, and chain dimensions of chemically substituted polycarbonates and polyesters using rotational isomeric state theory. **U. Natarajan**

SECTION C

Manchester Grand Hyatt San Diego
Promenade A/B

Eco-Friendly Polymerization

C. Boyer, D. Konkolewicz, *Organizers*
R. B. Grubbs, E. Harth, *Presiding*

- 1:00** **138.** Towards fully renewable polymeric materials: Block copolymers from bio-based monomers. **T. Chen**, L. Pena Carrodegua, C.K. Williams
- 1:20** **139.** 4-Hydroxyproline-derived sustainable polythioesters: Controlled ring-opening polymerization, complete recyclability, and facile functionalization. **H. Lu**
- 2:00** **140.** Facile ring-opening metathesis polymerization toward bioplastics and ionomer membranes. **C. Tang**
- 2:30** **141.** Polymer networks in the nano- and micro-scale from renewable resources. **E. Harth**, E. Ordóñez, B. Loftin
- 3:00** Intermission.
- 3:30** **142.** Toward sustainable polymerization of carbonyl compounds. **R.B. Grubbs**

- 4:00** **143.** Poly(methyl caprolactone)s as a soft, renewable, and degradable polyesters for next-generation sustainable materials. **M.A. Hillmyer**
- 4:30** **144.** One-pot terminal functionalization of polypeptides by protease-catalyzed chemoenzymatic polymerization. **K. Tsuchiya, K. Numata**

SECTION D

Manchester Grand Hyatt San Diego
Mission Beach A/B

Future of Biomacromolecules at a Crossroads of Polymer Science & Biology

Tissue Engineering

Cosponsored by BIOL, CARB, CELL, COLL, ENVR, MEDI, PHYS and PMSE

A. Albertsson, S. Percec, *Organizers*

H. A. Klok, M. Monteiro, *Presiding*

- 1:00** **145.** Photoresponsive hydrogels to study cell-matrix interactions and mechanobiology. **K.S. Anseth**
- 1:30** **146.** Nano- and microfabricated hydrogels for regenerative engineering. **A. Khademhosseini**
- 2:00** **147.** Printable and structured dynamic hydrogels for tissue engineering and biosensing. **T. Hoare**
- 2:25** Intermission.
- 2:40** **148.** Designing fiber-based, degradable 3D porous scaffolds suitable for soft tissue engineering. **A.F. Wistrand, T. Fuoco, A. Ahlinder**
- 3:15** **149.** Biodegradable thermogels and their biomedical applications. **B. Jeong, H. Lee, S. Um**
- 3:40** **150.** Glycosaminoglycan hydrogels and nanogels having smart biomimetic functions for biomedical applications. **R. Auzely-Velty**
- 4:05** **151.** Polymers with distinctive anticancer mechanism that inhibits tumor metastasis and mitigates drug resistance. **Y. Yang, C. Yang, N. Park, J. Hedrick**

SECTION E

Manchester Grand Hyatt San Diego
Mission Beach C

Industrial Innovations in Polymer Science

S. M. Ramirez, L. M. Stratton, *Organizers, Presiding*

- 1:00** **152.** Renewable superabsorbent polymers (bio-SAP) enabled by renewable acrylic acid (bio-AA), produced via the dehydration of lactic acid or its derivatives. **D.I. Collias, J. Godlewski, J. Velasquez, P. Dziezok, M. Kehrler, J. Nagengast, J. Kadar, N. Taccardi, J. Albert, P. Wasserscheid**

- 1:30** **153.** Machine learning approaches to predicting Hansen solubility parameters for polymers. **A.J. Guenther**
- 2:00** **154.** Dodecanedioic acid program, lessons for future bio-based commodity chemicals. **J. Laplaza**
- 2:30** **155.** Development of polymeric lubricants and surfactants using catalytic chain transfer polymerization. **G. Patias, A. Wemyss, S. Efstathiou, J. Abi Saleh, J.S. Town, A. Shegiwal, P. O'Hora, T. Smith, D.M. Haddleton**
- 3:00** Intermission.
- 3:15** **156.** Nanofabrication and surface chemistry for genetic analysis systems. **A. Brown**
- 4:00** **157.** Novel MEMS/polymer lab-on-a-chip for detection of cancer biomarkers. **J.P. Hinestrosa, T. Harris, A. MacLyman, R. Turner, S. Conradson, R. Krishnan**
- 4:30** **158.** Designing polymers and adhesives for wearable devices and point-of-care diagnostic applications. **M. Allen, T. Gordon, C. Nolen, D.E. Herr**

Design, Synthesis & Engineering of Polypeptides for Biological & Biomedical Application

Polypeptides for Drug & Gene Delivery Applications

Sponsored by PMSE, Cosponsored by POLY

Unique & Complex Polymer Architectures Materials

Sponsored by PMSE, Cosponsored by POLY

Plastics in Aquatic Environments, Part II: Transport, Fate & Global Impacts

Sponsored by ENVR, Cosponsored by POLY

Toughening of Networks & Gels through Molecular Design

Sponsored by PMSE, Cosponsored by POLY

SECTION A

San Diego Convention Center
TBD

Sci-Mix

T. H. Epps, *Organizer*

8:00 - 10:00

17, 42. See Previous Listings.
176, 217, 221, 239, 241, 242, 243, 245, 247, 248,
249, 251, 254, 255, 256, 257, 258, 260, 263, 265,
266, 267, 268, 269, 270, 275, 277, 281, 283, 284,
287, 288, 319, 366, 377. See Subsequent Listings.

TUESDAY MORNING – POLY

SECTION A

Manchester Grand Hyatt San Diego
Golden Hill A/B

Polymers for Defense Applications

R. H. Lambeth, T. Pruyn, A. M. Savage, *Organizers*

P. Zarras, *Organizer, Presiding*

- 8:00 159. Polymer-grafted cellulose nanocrystals as functional materials. **S.J. Rowan**
- 8:30 160. Magneto-rheology for tunable structural design. **T.L. Thornell**, J.A. Jefcoat, Z.B. McClelland, R.D. Moser, T.S. Rushing
- 8:50 161. Force-decoupled strategies in mechanochemically active polymers. **M.J. Robb**
- 9:10 162. Polymer design for use in broad army operational environments. **R. Mrozek**
- 9:35 163. Crosslinked and shape-memory polyimides with phenylethynyl pendants for programmed enhancement in T_g and modulus. **L. Tan**, D.H. Wang, Z. Yu
- 10:00 Intermission.
- 10:20 164. Controllable shape-morphing in polymers with living and non-living components. **T.H. Ware**, L. Rivera-Tarazona, C. Ambulo
- 10:50 165. Mechanically robust 3D-printed silica part: Binder development for binder jet 3D printing. **L. Han**, D. Gilmer, M. Lehmann, A. Kisliuk, D. Siddel, D. Goldsby, A. Elliott, T. Saito
- 11:10 166. Identifying key properties in determining additive manufacturing potential of reactive composites. **J. McCollum**, M. Knott, S.T. Iacono, J. Mates
- 11:30 167. Polymer and nanomaterials in 3D printing: Towards high-performance and military applications. **R.C. Advincula**

SECTION B

Manchester Grand Hyatt San Diego
Coronado D

Henkel Outstanding Graduate Research in Polymer Chemistry in Honor of Jovan Kamcev

Cosponsored by CHED and PMSE

Financially supported by Henkel Corporation

M. K. Mahanthappa, *Organizer, Presiding*

B. D. Freeman, *Presiding*

- 8:00 168. Single-ion doping and homopolymer blending approaches to improved ion-transport in block polymer electrolyte materials. **T.H. Epps**
- 8:30 169. Construction of a universal chemical potential that captures the Dusek-Tanaka collapse of swollen hydrogels. **G. Manning**
- 9:00 170. Using bioinspired polypeptoids to make functional anti-fouling surfaces. **R.A. Segalman**, M.E. Barry
- 9:30 Intermission.
- 9:55 171. Theory for diffusional transport of water through RO membranes. **D.R. Paul**
- 10:25 172. New porous network polymers for metal ion separations and water purification. J. Kamcev, A. Uliana, D. Shin, S. Lee, K. Colwell, M.K. Taylor, K. Chakarawet, S. Demir, G. Barin, N. Brune, N. Jarenwattananon, H. Furukawa, J. Van Humbeck, J.A. Reimer, D.K. Shuh, C.J. Chang, **J.R. Long**
- 10:55 Award Presentation.
- 11:00 173. Ion partitioning and transport in ion exchange membranes: Importance of counter-ion condensation. **J. Kamcev**, G. Manning, D.R. Paul, B.D. Freeman

SECTION C

Manchester Grand Hyatt San Diego
Promenade A/B

Eco-Friendly Polymerization

C. Boyer, D. Konkolewicz, *Organizers*

M. Cunningham, T. P. Varner, *Presiding*

- 8:00 174. Inverse vulcanised sulfur polymers for functional materials. **J.A. Smith**, J.M. Chalker, T. Hasell
- 8:20 175. Depolymerization enabled by a combination of tensile force and radical abstraction. **M.T. Robo**, P.M. Zimmerman
- 8:40 176. Striding towards a sustainable world via combination of agricultural and energy production waste streams: Biocomposites of elemental sulfur and lignin. **M.K. Mahappu Koralalage**, A.G. Tennyson, R.C. Smith

- 9:00** **177.** Synthetic optimization of hydrogels and nanogels used for animal feed and agricultural applications. **H.D. Maynard**
- 9:30** **178.** Ionic fluorogels as innovative sorbents for PFAS remediation from residential water supplies. **F.A. Leibfarth, E. Kumarasamy**
- 10:00** Intermission.
- 10:30** **179.** Thermal and mechanical properties of recyclable high sulfur content copolymers utilizing a bioderived monomer. **T. Thiounn, E.K. Kibler, E.W. Lyles, A.G. Tennyson, R.C. Smith**
- 10:50** **180.** Synergistic combination of agricultural and energy waste products yielding durable, sustainable composites of sulfur and cellulose. **M.K. Lauer, A.G. Tennyson, R.C. Smith**
- 11:10** **181.** Interpenetrating network-reinforced sulfur composites. **R.C. Smith, A.G. Tennyson**
- 11:30** **182.** Microsuspension polymerization of styrene using cellulose nanocrystals as Pickering emulsifiers. **J. Glasing, P. Champagne, P.G. Jessop, M.F. Cunningham**

SECTION D

Manchester Grand Hyatt San Diego
Mission Beach A/B

Polymeric Materials for Water Purification

Cosponsored by PMSE

Financially supported by NSF, ACS Publications, Journal of Membrane Science, Membrane Technology Research
E. Dawson, B. D. Freeman, L. E. Katz, N. A. Lynd, R. A. Segalman, *Organizers*
N. Lynd, *Presiding*

- 8:00** Introductory Remarks.
- 8:05** **183.** Interactions of solutes and polymer membrane surfaces in complex waters: From adsorption to nucleation and crystal growth. **L.E. Katz**
- 8:50** **184.** Polymers of intrinsic microporosity: Selective membrane permeation for purification. **K. Fruehauf, K.J. Shea**
- 9:20** **185.** Sustainable hydrogel-base materials for capture and storage of excessive liquid water through ring-opening copolymerization with biobased materials and carbon dioxide. **D.K. Tran, T.M. Folsom, G.A. Bhat, Y. Wang, D.J. Darensbourg, K.L. Wooley**
- 9:50** Intermission.
- 10:20** **186.** Programming hydration water with complex surfaces: Role of interfacial water dynamics. **J.I. Monroe, A. Schrader, S. Han, M. Shell**

- 11:05** **187.** Dynamic properties of water and salt ions in self-assembled morphologies of block copolymers. **D. Aryal, R. Samanta, M. Howard, T. Truskett, V. Ganesan**

SECTION E

Manchester Grand Hyatt San Diego
Mission Beach C

Young Industrial Polymer Scientist Award in Honor of Jason Roland

C. Farrell, *Organizer*

J. M. DeSimone, *Organizer, Presiding*

- 8:00** Introductory Remarks.
- 8:05** **188.** PRINT technology for particle design and engineering. **B.W. Maynor**
- 8:35** **189.** VolCat: Catalytic depolymerization process for the chemical recycling of PET. **R.D. Allen**
- 9:05** **190.** 3D-printed ion exchange membranes. **M.A. Hickner**
- 9:35** Intermission.
- 10:00** **191.** Relationships between chemistry, design, and process using 3D printing with carbon's digital light synthesis technology. **S.J. Mecham, R. Zhang, C. Caudill, K. Illiadis, R. Pinschmidt, R. Januszewicz, J. Perry, S. Tian, A. Redmann, T.A. Osswald, J.M. Desimone**
- 10:30** **192.** 3D-printable, resorbable elastomers for use in soft tissue engineering. **M. Becker**
- 11:00** **193.** Integral design of soft robots via stereolithography and CLIP. **R. Shepherd**
- 11:30** **194.** Production redefined: Carbon's novel digital light synthesis platform. **J.P. Rolland**

Design, Synthesis & Engineering of Polypeptides for Biological & Biomedical Application

Bioengineering & Therapeutic Peptides

Sponsored by PMSE, Cosponsored by POLY

Unique & Complex Polymer Architectures Synthesis & Bio

Sponsored by PMSE, Cosponsored by POLY

Toughening of Networks & Gels through Molecular Design

Sponsored by PMSE, Cosponsored by POLY

SECTION A

Manchester Grand Hyatt San Diego
Golden Hill A/B

Polymers for Defense Applications

R. H. Lambeth, T. Pruyn, A. M. Savage, *Organizers*
P. Zarras, *Organizer, Presiding*

- 1:00** **195.** Surface segregating coating additives for self-decontamination applications. **J.H. Wynne**, J. Lundin, S. Giles, B.T. Rasley
- 1:25** **196.** High-performance hybrids at the extreme limits of molecular-scale confinement. **R. Dauskardt**
- 1:50** **197.** Chemical protective coatings for improved surface decontamination. **A.P. Malanoski**, B.J. Johnson, B.J. Melde, M.H. Moore
- 2:10** **198.** Effect of chemical purity on measurement of agent resistance and decontamination performance for materials. **T.P. Pearl**, M.J. Varady, J.P. Myers, M.L. Sheahy, M.J. Chesebrough, J.L. Ruth, J.C. Piesen, B.A. Mantooth
- 2:30** **199.** Designing durable coatings with low surface adhesion for mitigation of fouling and ice adhesion. **D.C. Webster**
- 3:00** Intermission.
- 3:20** **200.** Dry adhesive and self-healing boronic ester polymers. **J.J. Cash**
- 3:40** **201.** Smart corrosion-inhibiting coatings based on novel conductive polymers and reactive monomers. **P. Zarras**, J.D. Stenger-Smith, R. Quintana, L. Baldwin, A.M. Hughes, J.E. Baca, M. Tesfahun
- 4:00** **202.** Sticking like barnacles: Unraveling and mimicking a natural adhesive. **C. So**, K. Fears, E.A. Yates, L.A. Estrella, D. Leary, J. Schultzhaus, C. Spillmann, K.J. Wahl
- 4:20** **203.** Catechol-functionalized acrylates and methacrylates: Comonomer influence on adhesive properties. **J.A. Orlicki**, M.A. Bartucci, S. Radzinski, D. Flanagan, J.L. Lenhart
- 4:40** **204.** Atomistic simulations of adsorption of bioinspired oligomers on a model metal oxide surface in aqueous conditions. **I. Yeh**, J.L. Lenhart, J.A. Orlicki, C.B. Rinderspacher

SECTION B

Manchester Grand Hyatt San Diego
Coronado D

Biomacromolecules/Macromolecules Young Investigator Award

Cosponsored by PMSE
P. Majumder, *Organizer*
A. Albertsson, M. A. Hillmyer, S. J. Rowan, *Presiding*

- 1:00** Introductory Remarks.
- 1:05** **205.** Enabling polymer synthesis, assembly, and function through the power of natural products. **T.M. Reineke**
- 1:30** **206.** Peptide/protein conjugates from copper mediated living radical polymerisation. **D.M. Haddleton**
- 1:55** **207.** Nanoparticles to stabilize and release therapeutic proteins and peptides. **H.D. Maynard**
- 2:20** **208.** Degradable vinyl materials for biomedical applications from controlled radical ring-opening copolymerization. **J. Nicolas**
- 2:50** Intermission.
- 3:05** **209.** Bioinspired complex coacervate-based adhesives. **M. Kamperman**
- 3:30** **210.** Investigating the role of sequence-defined charges on the solution self-assemblies of discrete amphiphilic peptoid oligomers. **D. Zhang**
- 3:55** **211.** Power of molecular precision in designing polymeric amphiphiles. **R.J. Amir**
- 4:20** **212.** Precision polymer particles powered by polyelectrolytes and amphiphilic polymers. **I.K. Voets**
- 4:50** Concluding Remarks.

SECTION C

Manchester Grand Hyatt San Diego
Promenade A/B

General Topics: New Synthesis & Characterization of Polymers

B. Barkakaty, D. Garcia, *Organizers*
T. Chi, R. M. Pankow, *Presiding*

- 1:00** **213.** Withdrawn
- 1:20** **214.** Patterning surface-initiated polymer growth by an electrochemical redox switch. **M. Qi**, H. Zhang, Q. Dong, D. Wang, J.A. Byers
- 1:40** **215.** Synthesis and characterization of thioxanthone-based photoinitiators for two-photon controllable nanolithographic printing. **T. Chi**, P. Somer, D.A. Wilcox, V. Iyer, R. Le, J.J. Gengler, M. Ferdinandus, C. Liebig, L. Pan, X. Xu, B.W. Boudouris

- 2:00** **216.** Open-to-air and additive-free photocontrolled radical polymerization of acrylates and acrylamides. **J.R. Lamb**, J.A. Johnson
- 2:20** **217.** Networks of polymers linked by photo-redox-active metal-organic cages as multi-state switchable catalytic materials. **N.J. Oldenhuis**, K. Qin, J.A. Johnson
- 2:40** **218.** Bifuran polyesters: Preparation, properties, and monomer synthesis. **T.P. Kainulainen**, J. Sirviö, T.I. Hukka, J.P. Heiskanen
- 3:00** **219.** Hydrolysable DMAEA and DMAEMA copolymers for RNA delivery: Influence of composition and architecture on binding efficiency and release of RNA. **F. Burgevin**, S. Perrier
- 3:20** **220.** Sustainable methods for the preparation of conjugated polymers using direct arylation polymerization (DARp). **R.M. Pankow**, B.C. Thompson
- 3:40** **221.** Utilization of multiple cloning site as a versatile platform for DNA triblock copolymer. **J. Shin**, S. Li
- 4:00** **222.** PET-RAFT polymerization under near-infrared light by using silver phosphate as the photocatalyst. **J. Jiang**, **G. Ye**
- 4:20** **223.** Exploring the behavior of bimetallic organonickel complexes in the controlled synthesis of π -conjugated polymers. **J. Buenaflor**, C.K. Luscombe

SECTION D

Manchester Grand Hyatt San Diego
Mission Beach A/B

Polymeric Materials for Water Purification

Cosponsored by PMSE

Financially supported by NSF, ACS Publications, Journal of Membrane Science, Membrane Technology Research
E. Dawson, B. D. Freeman, L. E. Katz, N. A. Lynd, R. A. Segalman, *Organizers*
C. Liu, *Presiding*

- 1:00** **224.** Hierarchically porous, hypercrosslinked, emulsion-templated polymers: Water purification and absorption. S. Israel, **M.S. Silverstein**
- 1:45** **225.** Zwitterionic poly(arylene ether sulfone) (PAES) copolymers: Synthesis and fundamental properties for desalination membranes. **Y. Yang**, M. Green
- 2:15** **226.** Relationship between structure and performances of poly(methylalkyldiallyl ammonium chloride). **X. Jia**, X. Zhang, Y. Zhang
- 2:45** Intermission.
- 3:15** **227.** Precise nanoporous membranes from self-assembled materials: Progress towards the promise. **C. Osuji**, X. Feng, Q. Imran, Y. Zhang,

L. Sixdenier, X. Lu, G. Kaufman, U. Gabinet, K. Kawabata, M. Elimelech

- 4:00** **228.** Novel approach to boron removal in produced water by an integrated electro dialysis-nanofiltration system using selective membranes. **M.R. Landsman**, M. Chwatko, R.A. Segalman, N.A. Lynd, D.F. Lawler, L.E. Katz
- 4:30** **229.** Network polymerization of epoxides to yield compositionally-controlled polyether-based membranes. **M. Chwatko**, C. Rodriguez, B.D. Freeman, N.A. Lynd

SECTION E

Manchester Grand Hyatt San Diego
Mission Beach C

General Topics: New Synthesis & Characterization of Polymers

B. Barkakaty, D. Garcia, *Organizers*

D. G. Mackanic, A. H. Westlie, *Presiding*

- 1:00** **230.** Characterization of sub-unit cell morphology in tubular network block copolymers. **E.L. Thomas**, X. Feng, C. Burke, I. Prasad, A. Reddy, G. Grason
- 1:20** **231.** Synthesis of functional bottlebrush copolymers. **A. Sood**, J. Rzaev
- 1:40** **232.** Multiple sensitive and intelligent detachable thermosetting polymer based on dynamic disulfide linkages. **L. Zhou**
- 2:00** **233.** Catalyzed chemical synthesis of uncommon or unnatural polyhydroxyalkanoates. **A.H. Westlie**, X. Tang, E.Y. Chen
- 2:20** **234.** Stimuli-responsive polyurethanes that rapidly degrade via intramolecular cyclization. **E. Morado**, S.C. Zimmerman
- 2:40** **235.** Decoupling of mechanical properties and ionic conductivity in supramolecular stretchable battery materials. **D.G. Mackanic**, Y. Cui, Z. Bao
- 3:00** **236.** Construction of polyphosphoramidates with acid-triggered backbone degradation. **H. Wang**, M. Dong, R. Li, K.L. Wooley

Design, Synthesis & Engineering of Polypeptides for Biological & Biomedical Application

Design & Applications of Functional Polypeptides

Sponsored by PMSE, Cosponsored by POLY

Advances in Bioconjugate Materials for Biomedical Applications

Sponsored by PMSE, Cosponsored by POLY

Unique & Complex Polymer Architectures

Synthesis & Bio

Sponsored by PMSE, Cosponsored by POLY

Toughening of Networks & Gels through Molecular Design

Sponsored by PMSE, Cosponsored by POLY

TUESDAY EVENING – POLY

SECTION A

San Diego Convention Center
TBD

Eco-Friendly Polymerization

C. Boyer, D. Konkolewicz, *Organizers*

5:00 - 7:00

237. Copolymers of elemental sulfur and fatty acids. **A.D. Smith**, A.G. Tennyson

238. Synthesis and properties of novel biodegradable polyurethanes using polycaprolacton diol and diisocyanates. **H. Kouzai**, Y. Awagakubo

SECTION A

San Diego Convention Center
TBD

Future of Biomacromolecules at a Crossroads of Polymer Science & Biology

Cosponsored by BIOL, CARB, CELL, COLL, ENVR, MEDI, PHYS and PMSE

A. Albertsson, S. Percec, *Organizers*

5:00 - 7:00

239. Diselenide-containing polymer with light-induced cytotoxicity. **C. Sun**

240. Graphene oxide-conjugated polymer hybrid materials for calmodulin sensing. **C. Xing**, X. Bao, H. Yuan, D. Gao

241. Diffraction-like methodologies discover encoded biological recognition in bicomponent cell membrane mimics. **M. Young**, C. Rodriguez-Emmenegger, Q. Xiao, N. Yu. Kostina, M.L. Klein, V. Percec

SECTION A

San Diego Convention Center
TBD

General Topics: New Synthesis & Characterization of Polymers

D. Garcia, *Organizer*

5:00 - 7:00

242. Synthesis and characterization of amphiphilic graft copolymers prepared by organocatalyzed transesterification of terpene-containing reagents. **J.R. Hughes**, P.M. Iovine

243. Synthesis and characterization of block-brush arm star polymers. **L. Costa**, P. Shieh, J.A. Johnson

244. Synthesis of fully conjugated copolymers based on N-alkyl-bisthiazole-dicarboximide. **M. Comi Bonachi**, M. Al-Hashimi

245. Syntheses of eugenol based copolymers applying thiol-ene reactions. **L.T. Reilly**, M.J. Miri

246. Synthesis and analysis of thermo-reversible Diels-Alder reaction between bismaleimide moiety and furan moiety. **Y. Kim**, K. Park, H. Park, T. Lee

247. Mechanochemical synthesis: Solvent effects on helicity of conducting polymers. **W.H. Mak**, C. Lin, R.B. Kaner

248. Quasi-living polymerization of dienes and polar vinyl monomers catalyzed by a discrete neodymium phosphate complex. **J.O. Cue**, R. Kularatne, Y. Ren, M.C. Biewer, M.C. Stefan

249. Synthesis of sustainable polycarbonates and controlling the glass transition temperature: Towards simultaneous biomass-upcycling and CO₂ conversion. **E. Choi**, C. Song

250. Co-oligomerizations of 2,5-dibromo-1,1-disubstituted-3,4-diphenyl-siloles with 4,4'-(hexafluoroisopropylidene)diphenol or 4,4'-biphenol and their characteristics. **J.W. Lim**, **Y.T. Park**

251. Ring opening metathesis polymerization-derived sulfur functionalized polyolefins. **S. Podiyanachari**, U. Gandra, I. Kulai, A. Hlil, S. Al-Meer, M. Al-Hashimi, H.S. Bazzi

252. Withdrawn

253. Enhancement of poly(2-ethylhexyl methacrylate) by photo crosslinking. **J. Dodge**, B. Gordon, L.M. Stratton

254. Alternating sequence copolymer consisting solely of acrylamide units: Strategic monomer design and sequence driven properties. **Y. Kametani**, M. Ouchi

255. Combining controlled Suzuki-Miyaura cross coupling polymerization and controlled radical polymerization for the synthesis of conjugated rod-coil copolymers. **S. Huber**, S. Mecking

256. Light-responsive CO-release from polymer synthesized via ring opening metathesis polymerization (ROMP). **U. Gandra**, A. Sinopoli, S. Zaric, M. Sohail, S. Almeer, M. Al-Hashimi, H.S. Bazzi

257. Withdrawn

258. Antioxidant sunscreen polymers through click modification of polybutadienes with s-tetrazines. **R. Nanayakkara**, W. Sun, R. Bagge, D.A. Loy

259. Structure-activity relationship studies of antimicrobial poly-(guanylurea) for overcoming drug resistance. **M.M. Miranda**, T. Annamalai, Y. Tse-Dinh, J. Moon

260. Antifouling strategies of biodegradable polyurethane for implantable biomedical devices. **H. Wang**, S. Fattahpour, D. Christiansen, G. Cheng

261. Thermo-responsive poly(*N*-vinyl caprolactam) (PVCL)-based drug carriers for controlled drug release. **D. Choi**, J. Moon, J. Eom, Y. Roh, Q. Truong Hoang, K. Bong, M. Shim

262. Enzymatically degradable self-reporting micellar nanocarriers. **M. Green Buzhor**, R.J. Amir

263. Glycosylated polypeptide bottlebrushes. **Z. Clauss**, A. Schlirf, N. Wright, S. Saini, J. Kramer

264. Ethylene glycol-based highly conductive PEDOT:PSS dispersion and silver nanowire hybrid film for transparent electrode. **S. Kim**, D. Park, S. Lee

265. Growth mechanism of PEDOT-SiO₂ hybrid thin films via vapour phase polymerization. **K.A. Nodora**, J. Yim

266. Preparation of a stretchable PEDOT-thermoplastic polyurethane hybrid via *in situ* vapor phase polymerization and its application as strain sensor. **C. Palicpic**, P. Losaria, J. Yim

267. Self-assembly of rigid polymers into nanostructures. **S. Jimaja**, D. Taton, R.K. O'Reilly, A.P. Dove

268. ROPISA: Ring-opening polymerization induced self-assembly. **P.J. Hurst**, J.P. Patterson

269. Aqueous dispersions of polyethylene and ethylene-copolymers and their clay nanocomposites from free-radical dispersion polymerization. **T. Morgen**, S. Mecking

270. End group analysis of poly(3-hexylthiophene) from halogenated monomers and their potential application for bis-end-functionalization. **M. Talukder**, M.C. Biewer, M.C. Stefan

271. Tough and recyclable polyesters by ring-opening polymerization of benzo-thia-caprolactones. L. Li, F. Du, **Z. Li**

272. Semitransparent superhydrophobic surface with improved mechanical durability. **Y. Park**, H. Lim

273. Thiazole-based conjugated ryleneimides copolymers as unipolar semiconductors. **S. Attar**, J.

Kim, D. Sredojevic, A. Kalin, S. Banerjee, L. Fang, M. Yoon, M. Al-Hashimi

274. Epoxidation of soybean oil utilizing dioxirane intermediates generated from oxone. **R.A. Setien**, D.C. Webster

275. Robust pernigraniline salt-like oligomers featuring ladder type constitution and Pauli paramagnetism. **X. Ji**, H. Xie, Y. Zou, L. Fang

276. Kinetic studies of random copolymerization of various methacrylate and acrylamide monomers by Cu(0)-mediated reversible deactivation radical polymerization. **J. Kim**, J. Choe, K. Paeng, M. Kim

277. Smart polymeric sensors for healthcare applications. **S. Efstathiou**, A. Wemyss, R. Hand, G. Kirby, D.M. Haddleton

278. Research at a primarily undergraduate institution: Conjugated polymer-peptide hybrid materials. **A. Murphy**, E. James, T. Blatz, T.J. Albin, M. Fry, L. Jenkins, Z. Pollard, H. Pan, T. Kowalczyk, R. Santen

279. Organic chemistry as an inspiration for new methods in polymer synthesis. **W. Gutekunst**

280. Fabrication of polymeric nanofiber and its application for the removal of heavy metals from industrial waste water. **A. Okewole**

SECTION A

San Diego Convention Center
TBD

Polymeric Materials for Water Purification

Cosponsored by PMSE

Financially supported by NSF, ACS Publications, Journal of Membrane Science, Membrane Technology Research E. Dawson, B. D. Freeman, L. E. Katz, N. A. Lynd, R. A. Segalman, *Organizers*

5:00 - 7:00

281. Novel living polymer/bacteria composites for bioremediation. **M. Mafi**, A. Greiner

282. Crown ether functionalized bottlebrush polymers for selective lithium capturing. **S. Zhao**, S. Warnock, C.M. Bates, M.M. Abu-Omar

283. Polyolefin functionalization towards biphasic separation of transition metals. **I. Kulai**, D. Chouikhi, D.E. Bergbreiter, M. Al-Hashimi, H.S. Bazzi

284. Harnessing magnetic anisotropy in designing functional materials for use as liquid crystalline polymers. **R. Bosire**, D. Ndaya, R. Kasi

285. Cellulosic microparticles for removal of organic pollutants in water. **M. Hossen**, S. Sultana, M. Mason

SECTION A
San Diego Convention Center
TBD

Polymers for Defense Applications

R. H. Lambeth, T. Pruyn, A. M. Savage, P. Zarras, *Organizers*

5:00 - 7:00

- 286.** Insect repellent release from coaxial electrospun fibers. **J.J. Ryan**, J.A. Orlicki, J.H. Wynne, J. Lundin
- 287.** Epoxy group analysis through titroprocessor. **S. Bommakanti**
- 288.** Synthesis, characterization, and cure kinetics study of carborane containing cyanate esters with excellent thermal stability. **S. Goyal**, M. Forrester, M.W. Lee, E.W. Cochran
- 289.** Synthesis and characterization of metallo-supramolecular nanocomposites. **A.M. Savage**, F.L. Beyer
- 290.** Induced alignment of core liquids by confinement from coaxial electrospinning. **M.J. Bertocchi**, R. Casalini, D.C. Ratchford, J.H. Wynne, J. Lundin

Plastics in Aquatic Environments, Part II: Transport, Fate & Global Impacts

Sponsored by ENVR, Cosponsored by POLY

PMSE/POLY Poster Session

Advances in Bioconjugate Materials for Biomedical Applications

Sponsored by PMSE, Cosponsored by POLY

PMSE/POLY Poster Session

Design, Synthesis & Engineering of Polypeptides for Biological & Biomedical Applications

Sponsored by PMSE, Cosponsored by POLY

PMSE/POLY Poster Session

General Posters/New Concepts in Polymeric Materials

Sponsored by PMSE, Cosponsored by POLY

PMSE/POLY Poster Session

Novel Polymeric Materials & Polymer-Based Processes for Energy Efficient Treatment of Water & Resource Recovery

Sponsored by PMSE, Cosponsored by POLY

PMSE/POLY Poster Session

Toughening of Networks & Gels through Molecular Design

Sponsored by PMSE, Cosponsored by POLY

WEDNESDAY MORNING

SECTION A
Manchester Grand Hyatt San Diego
Golden Hill A/B

Polymers for Defense Applications

R. H. Lambeth, T. Pruyn, P. Zarras, *Organizers*
A. M. Savage, *Organizer, Presiding*

- 8:00** **291.** Hydroxide conducting block copolymers. **Y.A. Elabd**
- 8:30** **292.** Emulsion-templated monolithic encapsulation of inorganic and organic phase change materials: Thermal energy storage and release. **L. Weinstock**, R.A. Sanguramath, I. Berezovska, N. Rosen, K. Kapilov-Buchman, E. Ovidia, R. Mor Yosef, E. Tuval, I. Moshe, A. Miller, A. Picciotto, **M.S. Silverstein**
- 8:50** **293.** Conductance variability in non-conjugated polymers: Memristors in neuromorphic applications. **S.H. Foulger**
- 9:10** **294.** High polymers of intrinsic microporosity: New class of high-temperature, low-loss dielectrics for electronic applications. **Z. Zhang**, K. Premasiri, X. Gao, **L. Zhu**
- 9:30** **295.** Role of functionalized nanoclay particles on the diffusion of military fuels through collapsible fuel storage tanks. **J.M. Sloan**, D. Flanagan
- 9:50** Intermission.
- 10:15** **296.** Diverse polymeric architectures from perfluoropyridine as a chemoselective scaffold for additive manufacturing. **C.A. Corley**, K. Stewart, N. Weeks, A. Peloquin, A.R. Jennings, **S.T. Iacono**
- 10:40** **297.** Additive-manufactured stochastic polyimide foam for low-density and low-loss electronic architectures. **H. Liu**, J. Hardin, J. Berrigan
- 11:00** **298.** Microwave-assisted polyarylene synthesis and characterization for advanced materials. **S.M. Budy**, D.Y. Son
- 11:20** **299.** Influence of monomer polarity on the mechanical properties of ring opening metathesis polymers. **N.T. Tran**, T. Long, C. Busch, K. Masser, J.L. Lenhart, D. Knorr
- 11:40** **300.** Hygromorphic films of sulfonylated poly(2,6-dimethyl-1,4-phenylene oxide) derivatives. **D.H. Wang**, B. Treml, L. Zhu, R.A. Vaia, L. Tan

SECTION B

Manchester Grand Hyatt San Diego
Harbor H

Herman F. Mark Award in Honor of Nicholas Peppas

M. Grunlan, *Organizer, Presiding*

- 8:00 Introductory Remarks.
- 8:05 **301.** Hyperloaded poly(2-oxazoline) micelles as drug carriers for cancer therapy. **A.V. Kabanov**
- 8:30 **302.** Electrostatic polymer systems for nanoparticle targeting of cells and tissues. **P.T. Hammond**
- 8:55 **303.** Functional integration of covalent and supramolecular polymers. **S.I. Stupp**
- 9:20 **304.** Ten puzzles of the airway surface layer. **M. Rubinstein**
- 9:45 Intermission.
- 10:05 **305.** Biorecognition: Bridge from self-assembled hydrogels to drug-free macromolecular therapeutics. **J. Kopecek**, J. Yang, L. Li, J. Wang
- 10:30 **306.** Designing polymeric biomaterials with spatiotemporal control for directing stem cell behavior. **J.L. Holloway**
- 10:55 **307.** Gel-like nature of cartilage polymers. **F. Horkay**
- 11:20 **308.** Reexamining the swelling and deformation theories of ionic, stimuli-responsive networks, and gels. **N. Peppas**, N.R. Richbourg

SECTION C

Manchester Grand Hyatt San Diego
Promenade A/B

Future of Biomacromolecules at a Crossroads of Polymer Science & Biology

Delivery Systems

Cosponsored by BIOL, CARB, CELL, COLL, ENVR, MEDI, PHYS and PMSE

A. Albertsson, S. Percec, *Organizers*

S. Lecommandoux, D. A. Wilson, *Presiding*

- 8:00 **309.** Self-assembled supramolecular nanosystems for smart targeted therapy of cancer. **K. Kataoka**
- 8:30 **310.** Thermosensitive polyplexes for nucleic acid delivery. L. Fliervoet, **T. Vermonden**
- 8:55 **311.** Rationally-designed polypeptides based on structural proteins. **K. Numata**
- 9:20 Intermission.
- 9:35 **312.** Bioresponsive polymersomes as an emerging platform for targeted tumor therapy. Y. Wei, W. Gu, H. Sun, F. Meng, **Z. Zhong**
- 10:05 **313.** Phosphonium biomaterials: From antibiotics

to ionic hydrogels. T. Cuthbert, T. Harrison, B. Hisey, P.J. Ragogna, **E.R. Gillies**

- 10:30 **314.** Withdrawn
- 10:55 **315.** Synthesis of antimicrobial polymers: Effect of polymer composition and architecture. P. Judzewitsch, E. Wong, **C. Boyer**
- 11:20 **316.** Use of poly(methionine sulfoxide) to impart cell and tissue compatibility in degradable biomaterials. **T.J. Deming**

SECTION D

Manchester Grand Hyatt San Diego
Mission Beach A/B

Polymeric Materials for Water Purification

Cosponsored by PMSE

Financially supported by NSF, ACS Publications, Journal of Membrane Science, Membrane Technology Research
E. Dawson, B. D. Freeman, L. E. Katz, N. A. Lynd, R. A. Segalman, *Organizers*
M. Chwatko, *Presiding*

- 8:00 **317.** Advancing conductivity-permselectivity tradeoff of ion-exchange membranes with sulfonated CNT nanocomposites. **H. Fan**, Y. Huang, N. Yip
- 8:30 **318.** Controlling water and ion transport in hydrated polymer membranes via chemical functionality. Y. Ji, H. Luo, K. Chang, **G.M. Geise**
- 9:15 **319.** Self-healable membrane coatings with selective wettability. B. Shrestha, M. Ezazi, **G. Kwon**
- 9:45 Intermission.
- 10:15 **320.** Structural and transport properties of membranes in high-salinity desalination using cascading osmotically mediated reverse osmosis. **X. Chen**, C. Boo, N. Yip
- 11:00 **321.** Design and syntheses of bio-based exotic amino acid derived cationic polyamide for the application of water treatment. **J. Phanthuwongpakdee**, S. Dwivedi, K. Takada, S. Babel, T. Kaneko
- 11:30 **322.** Membrane hydrophilicity tuning by the functional additives with different molecular architectures. **Y. Jiang**, Y. Zhang, B. Chen, X. Zhu

SECTION E

Manchester Grand Hyatt San Diego
Mission Beach C

DSM Graduate Student Award

J. J. Van Gorp, *Organizer*

R. A. Vanbenthem, *Organizer, Presiding*

C. J. Hawker, *Presiding*

- 8:00 Introductory Remarks.

- 8:05 323.** DSM science and technology award for graduate students: Polymers for a sustainable future. M. Remmers, **R.A. Vanbenthem**
- 8:15 324.** Recyclable cross-linked polyurethanes. **D.J. Fortman**
- 8:45 325.** Tailoring vinyl-addition polynorbornenes for advanced CO₂ separation membranes: High T_g glasses that behave like rubbers. **C. Maroon**, J. Townsend, K.R. Gmernicki, D. Harrigan, B.J. Sundell, J.A. Lawrence III, S.M. Mahurin, K.D. Vogiatzis, B.K. Long
- 9:15 326.** Polymers for a sustainable future: Controlling and benefitting from polymer degradation via hydrolytic, oxidative, and biological pathways during production, use, and end of life. **J.J. Van Gorp**
- 9:45** Intermission.
- 10:00 327.** Organocatalyzed atom transfer radical polymerization: Sustainable polymer synthesis. **B. McCarthy**, G. Miyake
- 10:30 328.** Compositionally controlled heterocopolymers using old and new aluminum-based catalysts. **M. Chwatko**, C. Rodriguez, R.C. Ferrier, N.A. Lynd
- 11:00 329.** Programming functions by combining supramolecular and covalent polymers with renewable resources. **V. Percec**

Materials Advances in Nanocellulose Research for Engineered Functionality

Sponsored by CELL, Cosponsored by PMSE and POLY

Design, Synthesis & Engineering of Polypeptides for Biological & Biomedical Application

Design & Studies of Functional Polypeptide Materials

Sponsored by PMSE, Cosponsored by POLY

Unique & Complex Polymer Architectures Assembly

Sponsored by PMSE, Cosponsored by POLY

WEDNESDAY AFTERNOON – POLY

SECTION A

Manchester Grand Hyatt San Diego
Golden Hill A/B

Polymers for Defense Applications

T. Pruy, A. M. Savage, P. Zarras, *Organizers*
R. H. Lambeth, *Organizer, Presiding*
K. Waters, *Presiding*

- 1:00 330.** Synthesis of hybrid organic-inorganic boron-containing polymers for high temperature applications. **J. Heckler**, T.L. Pruy
- 1:20 331.** Improved synthesis and properties of two-dimensional covalent organic frameworks. **W.R. Dichtel**
- 1:50 332.** Oriented free-standing films of two-dimensional covalent organic frameworks. **E. Egap**
- 2:20 333.** Screening 2D COF containing databases for 2D polymers with advantageous mechanical properties using first principles methods. **K. Waters**, E. Sandoz-Rosado, J. Andzelm, E. Wetzel
- 2:40 334.** Enhanced polymer compatibility via modification of metal-organic frameworks for enhanced chemical biological protection. **G.W. Peterson**, T.H. Epps
- 3:00** Intermission.
- 3:20 335.** Design and applications of hydrogen bonding interactions in 2D covalent organic frameworks. **R. Smaldone**
- 3:50 336.** Synthesis and processing of high-strength and high-toughness 2-D covalent organic frameworks. M.G. Barnes, D. Zhu, Q. Fang, J. Liang, M. Rahman, A. Kumar, P. Ajayan, J. Lou, **R. Verduzco**
- 4:20 337.** Efforts toward hydrogen-bonded 2D polymers. **R.H. Lambeth**
- 4:40 338.** Interface and mechanical property relationships in a simple polymeric composite. **S. Manni**, J. Mares, T. Kosta, M. Nixon

SECTION B

Manchester Grand Hyatt San Diego
Harbor H

Overberger International Prize in Honor of Kenneth Wagner

R. M. Laine, J. Pollak, *Organizers*
J. Kim, *Presiding*

- 1:00 339.** New catalysts and processes for organocatalytic polymerization: From chemistry to biology. **R.M. Waymouth**
- 1:30 340.** Functional nanomaterials from single polymer chains. **E.B. Berda**
- 2:00 341.** 3D structure of grain boundaries in tubular network block copolymers. **X. Feng**, H. Guo, E.L. Thomas
- 2:30 342.** Admet polymerization via microwave irradiation. **T.W. Gaines**, K. Williams, K.B. Wagener, G. Rojas
- 3:00 343.** Poly (ethylene-2,2'-bifuran-5,5'-dicarboxylate): Biosourced high performance polyester. **S.R. Turner**, H.E. Edling, H. Sun, D.A. Schiraldi, E.E. Paschke

- 3:30 **344.** Synthesis of polymers with designed structures. **R.H. Grubbs**
- 4:00 **345.** Bulk polycondensation creating high melting aliphatic polysulfones. **J. Pribyl, K.B. Wagener**

SECTION C

Manchester Grand Hyatt San Diego
Promenade A/B

Future of Biomacromolecules at a Crossroads of Polymer Science & Biology

Biomaterials

Cosponsored by BIOL, CARB, CELL, COLL, ENVR, MEDI, PHYS and PMSE

A. Albertsson, *Organizer*
S. Percec, *Organizer, Presiding*
A. F. Wistrand, *Presiding*

- 1:00 **346.** Discovering biomaterials for low-temperature stabilisation of biologics. **M.I. Gibson**
- 1:30 **347.** Bottom-up strategies for recovery and valorization of biomacromolecules. **U. Edlund, N. Wahlström, M. Sterner**
- 1:55 Intermission.
- 2:10 **348.** Designing for degradation: Utilizing topology, architecture, and stoichiometry to control polymer degradation *in vivo*. **M. Becker**
- 2:50 **349.** L-amino acid based polymeric biomaterial platform. **M. Jayakannan**
- 3:20 **350.** 3D printing of degradable materials for the development of medical devices. **A.P. Dove**
- 3:45 **351.** Nucleoporin-like proteins and bioinspired gels. **B.D. Olsen, Y. Yang, D. Mai**
- 4:10 **352.** Surface engineering living cells. **H.A. Klok**
- 4:40 Concluding Remarks.

SECTION D

Manchester Grand Hyatt San Diego
Mission Beach A/B

Polymeric Materials for Water Purification

Cosponsored by PMSE

Financially supported by NSF, ACS Publications, Journal of Membrane Science, Membrane Technology Research
E. Dawson, B. D. Freeman, L. E. Katz, R. A. Segalman, *Organizers*
N. A. Lynd, *Presiding*

- 1:00 **353.** Polymerization in nanoconfinement of soft templates for making ultrafiltration membranes. **S. Qavi, A. Lindsay, M.A. Firestone, R. Foudazi**
- 1:30 **354.** Expanding the functionality of nanostructured polymeric membranes through

- additive manufacturing. **W.A. Phillip**
- 2:15 **355.** Impact of polymer microstructure on flocculation and dewatering performance: Case of Canadian oil sands tailings. **V. Vajihinejad, J.B. Soares**
- 2:45 Intermission.
- 3:15 **356.** Half-wave rectified alternating current electrochemical method for uranium extraction by amidoxime electrode. **C. Liu**
- 4:00 **357.** Highly chlorine-tolerant desalination membranes by solvent-free melt processing. **H. Oh, B.D. Freeman, D.R. Paul**

Design, Synthesis & Engineering of Polypeptides for Biological & Biomedical Application

Design of Functional Peptides & Polypeptides

Sponsored by PMSE, Cosponsored by POLY

WEDNESDAY EVENING – POLY

PMSE/POLY Plenary Lecture & Awards Symposium

Sponsored by PMSE, Cosponsored by POLY

THURSDAY MORNING – POLY

SECTION A

Manchester Grand Hyatt San Diego
Golden Hill A/B

Polymers for Defense Applications

R. H. Lambeth, A. M. Savage, P. Zarras, *Organizers*
T. Pruyn, *Organizer, Presiding*

- 8:00 **358.** Fluorescent, polymer-encapsulated nanocrystals for digital microfluidics applications. **N.P. Godman, U.N. Tohgha, C. Jarnagin**
- 8:20 **359.** Electrochromic fabric devices: Next generation material for adaptive camouflage. **R. Daniels, S. Sinha, O. Yassin, M. Baczkowski, G. Sotzing**
- 8:40 **360.** Molecular modeling of polycyanurates to predict thermophysical properties. **L. Moore, N. Redeker, K.B. Ghiassi**
- 9:00 **361.** Surface passivation of aluminum nanoparticles with novel perfluoroalkyl carboxylic acids for improved processability of 3D-printable fluoropolymer composites. **N.J. Weeks, E. Gazmin, J. Mates, J. McCollum, S.T. Iacono**
- 9:20 **362.** Sensing study of nitro-explosives using

General Topics: New Synthesis &
Characterization of PolymersB. Barkakaty, D. Garcia, *Organizers*
J. E. Bara, S. Percec, *Presiding*

- 8:00** 374. Chemical synthesis of crystalline poly(hydroxyalkanoate)s from cyclic diolides. **X. Tang**, E.Y. Chen
- 8:20** 375. Segmented ionene nanocomposites. **M. Wang**, M. Green
- 8:40** 376. Zwitterionic polyurethanes with tunable surface and bulk properties. **H. Wang**, Y. Hu, D. Lynch, M. Young, S. Li, H. Cong, F. Xu, G. Cheng
- 9:00** 377. Alkaline poly(ionic liquids) with methylpyrrolidinium, methylpiperidinium, methylazepanium, methylazocanium, and methylazonanium cations. **R. Sun**, Y.A. Elabd
- 9:20** 378. Synthesis of bottlebrush polymers with quaternary ammonium macromonomers for anti-marine fouling. **H. Senkum**, W. Gramlich
- 9:40** 379. Withdrawn
- 10:00** 380. Anionic ionenes: Synthesis of “main-chain” polyanions for diverse applications. **J.E. Bara**, P. Rupa, I. Kammakakam, K.E. O'Hara
- 10:20** 381. Rare-earth metal-mediated synthesis of radical-containing poly(dialkyl vinylphosphonates): Novel materials for battery systems. **T.M. Pehl**, B. Rieger
- 10:40** 382. Synergistic effect of sulfur and chalcogen atoms on the enhanced refractive indices of polyimides. **H. Kim**, H. Ko, N. You
- 11:00** 383. Functionalization of chitosan oligomers: Towards bio-based products with new functionalities. **G. David**
- 11:20** 384. β -keto adipic acid as a platform molecule. **N.A. Rorrer**, S. Notonier, B. Knott, B.A. Black, G. Schmidt, C.W. Johnson, D. Salvachua, S. Nicholson, A. Carpenter, M.J. Bidy, G. Glenn, A.P. Klamczynski, K.J. Ramirez, D. Peterson, M.F. Crowley, W. Hart-Cooper, G. Beckham

FRET pair of fluorescent copolymers. **V. Kumar**, S. Satapathi

- 9:40** 363. Selective catalyst deactivation for high-temperature resin systems. **R. Blanski**, T.S. Haddad, J.A. Boatz, K.B. Ghiassi
- 10:00** Intermission.
- 10:30** 364. Force-dependent color generation using a multifunctional mechanophore. **M.E. McFadden**, M.J. Robb
- 10:50** 365. Mechanically activated fluorescence in polymer matrix composites. **M. Wang**, M. Green
- 11:10** 366. Design of polymeric additives to modify properties of marine coatings to combat biofouling. **A. Rahimi**, D.C. Webster

SECTION B

Manchester Grand Hyatt San Diego
Coronado DGeneral Topics: New Synthesis &
Characterization of PolymersB. Barkakaty, D. Garcia, *Organizers*
J. Brantley, D. Walsh, *Presiding*

- 8:00** 367. Biobased degradable PE-like polymers with precisely spaced vitamin C groups by acyclic diene metathesis polymerization. **O. Suraeva**, C. Champanhac, F. Wurm, i. Lieberwirth
- 8:20** 368. All for aluminum: Single-component, main group element mediated group transfer polymerization. **M. Weger**, B. Rieger
- 8:40** 369. Metallocarbene-containing polymers: New directions in metallopolymer science. **J. Brantley**, B. Wilson
- 9:00** 370. Polyisobutylene chain-end modification via organocatalytic nucleophilic conjugate additions. **I. Kulai**, T. Malinski, D.E. Bergbreiter, M. Al-Hashimi, H.S. Bazzi
- 9:20** 371. Unexpected synthesis of segmented poly(hydroxyurea–urethane)s from dicyclic carbonates and diamines by organocatalysis. A. Bossion, D. Taton, **H. Sardon**
- 9:40** 372. Catalytic incorporation of polyolefins into functionalized (polar and non-polar) block copolymers. **D. Walsh**, T. Yan, D. Guironnet
- 10:00** 373. Exploiting Lewis pair polymerization to overcome challenges in chemo- and stereoselectivity. **M.L. McGraw**, E.Y. Chen

SECTION D
Manchester Grand Hyatt San Diego
Mission Beach A/B

Polymeric Materials for Water Purification

Cosponsored by PMSE

Financially supported by NSF, ACS Publications, Journal of Membrane Science, Membrane Technology Research

E. Dawson, B. D. Freeman, L. E. Katz, N. A. Lynd, R. A.

Segalman, *Organizers*

H. Oh, *Presiding*

- 8:00** **385.** Effect of inorganic salts on the apparent viscosity of P(DAC-AM). T. Chen, L. Zhang, **Y. Zhang**
- 8:30** **386.** Carbon dioxide switchable polymers as draw agents for forward osmosis. S. Ellis, A. Cormier, P. Champagne, P.G. Jessop, **M.F. Cunningham**
- 9:15** **387.** Removal of volatile organic pollutants from water by nanoporous crystalline polymer materials. **C. Daniel**, G. Guerra
- 9:45** **388.** Superhydrophobic polymers for oil and water separation and filtration. **R.C. Advincula**

Materials Advances in Nanocellulose Research for Engineered Functionality

Sponsored by CELL, Cosponsored by PMSE and POLY

PRES

PRESIDENTIAL EVENTS

SUNDAY MORNING – PRES

Characterization of Plastics in Aquatic Environments

Sponsored by POLY, Cosponsored by ANYL, BIOL, CEI, ENVR, I&EC, PMSE and PRES

Chemistry of Water Reuse Processes Toward Water Sustainability

Sponsored by ENVR, Cosponsored by AGRO and PRES

Chemistry of Water Reuse Processes Toward Water Sustainability

Sponsored by ENVR, Cosponsored by AGRO and PRES

Water, Health, & Environmental Justice in Marginalized Communities

(A) Toxic Chemicals in Water; & (B) Sanitation & Wastewater Resource Recovery Technologies

Sponsored by ENVR, Cosponsored by CMA and PRES

SUNDAY AFTERNOON – PRES

150 Years of the Periodic Table

Sponsored by HIST, Cosponsored by CINF, INOR and PRES

Chemistry & Water: Opening Session

Sponsored by MPPG, Cosponsored by CEI, ENVR and PRES

Characterization of Plastics in Aquatic Environments

Sponsored by POLY, Cosponsored by ANYL, BIOL, CEI, ENVR, I&EC, PMSE and PRES

Chemistry of Water Reuse Processes Toward Water Sustainability

Sponsored by ENVR, Cosponsored by AGRO and PRES

Water, Health, & Environmental Justice in Marginalized Communities

Socio-Cultural & Economic Dimensions of Water & Health

Sponsored by ENVR, Cosponsored by CMA and PRES

MONDAY MORNING – PRES

150 Years of the Periodic Table

Sponsored by HIST, Cosponsored by CINF, INOR and PRES

Chemistry of Water Reuse Processes Toward Water Sustainability

Sponsored by ENVR, Cosponsored by AGRO and PRES

MONDAY AFTERNOON – PRES

150 Years of the Periodic Table

Sponsored by HIST, Cosponsored by CINF, INOR and PRES

Leadership Development: The ACS Commitment Now & for the Future

Sponsored by BMGT, Cosponsored by PRES

Water Scarcity: Challenges for Agriculture

Sponsored by AGRO, Cosponsored by ENVR and PRES

Water Scarcity: Challenges for Agriculture

Sponsored by AGRO, Cosponsored by ENVR and PRES

Chemistry of Water Reuse Processes Toward Water Sustainability

Sponsored by ENVR, Cosponsored by AGRO and PRES

TUESDAY MORNING – PRES

GSSPC: From Oceans to Clouds: The Environmental Chemistry of Water

Sponsored by CHED, Cosponsored by PRES

Chemistry of Water Reuse Processes Toward Water Sustainability

Sponsored by ENVR, Cosponsored by AGRO and PRES

Connecting Safety, Education, Training & Productivity in Analytical Laboratories

Sponsored by ANYL, Cosponsored by CCS, CHAS, CINF and PRES

TUESDAY AFTERNOON – PRES

SECTION A

San Diego Convention Center
Room 5A

Chemistry of Disasters

Cosponsored by CCS, CHAS and I&EC

J. M. Pickel, Organizer, Presiding

- 1:00** Introductory Remarks.
- 1:05** **1.** Post-earthquake lab spill assessment. **R. Furr**, K. Creed
- 1:35** **2.** Wildfire and water quality: Updates on research following the Camp Fire in Paradise, California. **J. Webster**
- 2:05** **3.** Importance of science in responding to large-scale drinking water contamination disasters: Wildfires, chemical spills, and more. **A.J. Whelton**
- 2:35** **4.** Wildfire disaster preparedness for Lawrence Berkley National Laboratory. **M. Neitzel**
- 3:05** Intermission.
- 3:20** **5.** Planning to protect people, the planet and processes when disasters strike in a chemical manufacturing environment. **A.S. Hinkle**
- 3:50** **6.** Anthropology of disaster. **R.M. Izzo**
- 4:20** **7.** Preventing chemical security events. **M.E. Mulcahy**
- 4:50** **8.** Two years after Harvey: Arkema Crosby, TX flooding. **E. Tilles**

Collaborating for the Greater Good: What Works & What Doesn't

Sponsored by BMGT, Cosponsored by PRES

GSSPC: From Oceans to Clouds: The Environmental Chemistry of Water

Sponsored by CHED, Cosponsored by PRES

TUESDAY EVENING – PRES

Chemistry of Water Reuse Processes Toward Water Sustainability

Sponsored by ENVR, Cosponsored by AGRO and PRES

Water, Health, & Environmental Justice in Marginalized Communities

Sponsored by ENVR, Cosponsored by CMA and PRES

WEDNESDAY AFTERNOON – PRES

Keeping Water Safe

Sponsored by I&EC, Cosponsored by CHAS and PRES

THURSDAY MORNING – PRES

Remediation of Wastewater from Energy Usage

Sponsored by ENFL, Cosponsored by PRES

PROF

DIVISION OF PROFESSIONAL RELATIONS

R. Libby, *Program Chair*

SUNDAY AFTERNOON – PROF

Chemical Angel Network

Chemists Investing in Chemical Companies

Sponsored by BMGT, Cosponsored by PROF and SCHB

Division of Chemical Health & Safety Awards

Sponsored by CHAS, Cosponsored by PROF

MONDAY MORNING – PROF

SECTION A

Hilton San Diego Bayfront
Indigo 202 B

When Chemists Go to Washington: 45 Years of the ACS Public Policy Fellowships

Cosponsored by SCHB

R. E. Forslund, K. M. Kuhn, C. Trupp Gil, *Organizers*

- 8:30 Introductory Remarks.
- 8:35 1. Science and public policy: Career choices and social responsibility. **D.L. Garin**
- 8:55 2. Hill reaction: How a year on Capitol Hill changed me...and my life. **N.E. Noonan**
- 9:15 3. Career unwound: Road less traveled. **A.M. Boccanfuso**
- 9:35 4. Show me the money: Lessons learned working for the U.S. Senate Budget Committee. **K.M. Omberg**
- 9:55 Intermission.
- 10:05 5. In defense of being nontraditional: Building a career that plays to my strengths. **C.W. Avery**
- 10:25 6. A science policy course for undergraduates, or “What I did after my sabbatical”. **L.E. Pence**
- 10:45 7. ACS Science Policy Fellowship: Experience beyond expectations. **S.H. DeLuca**
- 11:05 8. How to apply for an ACS Public Policy Fellowship. **C. Trupp Gil**
- 11:25 Concluding Remarks.

Getting your First Industrial Job

Sponsored by YCC, Cosponsored by PROF

Women Make COMP

Sponsored by COMP, Cosponsored by PROF and WCC

2019 ACS International Award for Research in Agrochemicals: Advances in the Physiology & Biochemistry of Insect Control

Sponsored by AGRO, Cosponsored by AGFD, BIOL, MEDI, POLY and PROF

2019 ACS International Award for Research in Agrochemicals: Advances in the Physiology & Biochemistry of Insect Control

Sponsored by AGRO, Cosponsored by AGFD, BIOL, MEDI, POLY and PROF

MONDAY AFTERNOON – PROF

2019 ACS International Award for Research in Agrochemicals: Advances in the Physiology & Biochemistry of Insect Control

Sponsored by AGRO, Cosponsored by AGFD, BIOL, MEDI and PROF

Women Make COMP

Sponsored by COMP, Cosponsored by PROF and WCC

MONDAY EVENING – PROF

SECTION A San Diego Convention Center TBD

Sci-Mix

R. Libby, *Organizer*

8:00 - 10:00

9. Live-tweeting the academic meeting: Challenges and opportunities. **S. Mojarad**

10. Social media and ethics in the classroom: Reflection and analysis. **C. Sorensen-Unruh**

11. Out to Innovate™ 2019: NOGLSTP's career summit for LGBTQ+ students, faculty, and professionals in science, technology, engineering, and mathematics. **C.J. Bannochie**, B.L. Belmont

12. Chemists with disabilities, contributions to the profession. **C. Supalo**

TUESDAY MORNING – PROF

Herman Skolnik Award Symposium Honoring Dr. Kimito Funatsu

Sponsored by CINF, Cosponsored by PROF

Beyond the Bench: Non-Traditional Careers in Chemistry

Sponsored by CHAL, Cosponsored by PROF and YCC

2019 ACS International Award for Research in Agrochemicals: Advances in the Physiology & Biochemistry of Insect Control

Sponsored by AGRO, Cosponsored by AGFD, BIOL, MEDI and PROF

State of the Art: Diversity & Inclusion in Chemistry Education

Sponsored by CHED, Cosponsored by CEI and PROF

ACS-AGFD Young Scientist Award

Sponsored by AGFD, Cosponsored by PROF

TUESDAY AFTERNOON – PROF

Elucidating Reaction Mechanisms with Computational & Experimental Chemistry

Sponsored by CMA, Cosponsored by COMP and PROF

AGFD Award Symposium Honoring Dr. Fidel Toldra

Sponsored by AGFD, Cosponsored by PROF

SCC

SENIOR CHEMISTS COMMITTEE

TUESDAY MORNING – SCC

Gerry Meyer: The First 100 Years

Sponsored by SCHB, Cosponsored by BMGT, CHED, ENFL, HIST and SCC

TUESDAY AFTERNOON – SCC

Gerry Meyer: The First 100 Years

Sponsored by SCHB, Cosponsored by BMGT, CHED, ENFL, HIST and SCC

SCHB

DIVISION OF SMALL CHEMICAL BUSINESSES

J. Sabol, *Program Chair*

SUNDAY AFTERNOON – SCHB

Chemical Angel Network

Chemists Investing in Chemical Companies

Sponsored by BMGT, Cosponsored by PROF and SCHB

SUNDAY EVENING – SCHB

SECTION A

San Diego Convention Center

TBD

Chemical Business Poster Session

G. W. Ruger, *Organizer*

6:00 - 8:00

1. Innovation, entrepreneurship, and SCHB. **P.C. Lauro, G.W. Ruger, A. Kantak, D.J. Deutsch, M. Chorghade, J.E. Sabol, J.L. Maclachlan, R. Chorghade, J.L. Bryant, J. Crotty, C.A. Burton, N.A. Vaidya**
2. Chemical Angel Network chemical professionals investing in chemistry enabled businesses. **S.S. White, M. Vreeke, J.C. Giordan**
3. Marie Agan lab services: Playing up our strengths. **M.L. Agan**

MONDAY MORNING – SCHB

SECTION A

Hilton San Diego Bayfront

Indigo Ballroom H

Liquid Assets: The Business of Water

Cosponsored by ANYL, BMGT and I&EC

D. Mason, *Organizer*

V. V. Rajasekharan, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 4. State of the water industry: Bringing clarity to complex water industry issues. **B.S. Martin, D. Flancher**

- 8:30 5. Changing what's possible at the water-food-energy nexus. **C.A. Martin**
- 8:55 6. Role of water for industrial purposes. **C. McInnis**
- 9:20 7. Energy assessment at industrial and municipal wastewater treatment plants. **D. Ladner, M. Carbajales-Dale, E. Carraway, P. Litherland**
- 9:45 Intermission.
- 10:00 8. Legal perspective in water business. **K. Drake**
- 10:25 9. Decentralized wastewater treatment: Benefits and considerations for sustainable water and sanitation. **N. Mladenov**
- 10:50 10. Evolution of access sensor technologies, LLC and the on-target™ water test cards. **J. Hofstetter, T. Reilly, C. Henry**
- 11:15 11. Aqusens: AI-based lens-free platform for automated identification and characterization of micro-object/organisms in water. **M. Batalin, Z. Gorocs, A. Ozcan**

When Chemists Go to Washington: 45 Years of the ACS Public Policy Fellowships

Sponsored by PROF, Cosponsored by SCHB

MONDAY AFTERNOON – SCHB

SECTION A

Hilton San Diego Bayfront

Indigo Ballroom H

Holistic Approaches to Sustainability in Chemical Businesses

Cosponsored by CEI

A. Paradise, *Organizer*

J. Y. Tanir, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 12. Building a culture of sustainability through science. **A. Paradise**

1:30 13. Getting closer to holistic sustainability through the lens of green chemistry. **S.K. van Bergen**

1:55 14. DOZN™: Quantitative green chemistry evaluator. **E. Ponnusamy**

- 2:20 15. Green nanomaterials: Journey from lab to manufacturing. **S.V. Patwardhan**
- 2:45 Intermission.
- 3:05 16. IP strategies for green and sustainability technologies. **S.K. Cyr**, D. Weingarten
- 3:30 17. Driving to greener lab operations in a fast paced renewable chemicals business. **G. Goldsby**
- 3:55 18. Creating a sustainable chemical enterprise from corporate culture through to RD&D (research, development & deployment). **C.T. Hunt**
- 4:20 19. Reducing the environmental impact of plastic biotechnology devices: Improvements in design, manufacturing, and energy sourcing. **S. Weitze**

MONDAY EVENING – SCHB

SECTION A

San Diego Convention Center
TBD

Sci-Mix

G. W. Ruger, *Organizer*

8:00 - 10:00

- 2, 3, 11. See Previous Listings.
22. See Subsequent Listings.

TUESDAY MORNING – SCHB

SECTION A

Hilton San Diego Bayfront
Indigo Ballroom H

Academic Entrepreneurship

M. Chorghade, *Organizer, Presiding*

- 8:00 Introductory Remarks.
- 8:15 20. Analysis of university-based startup companies in the chemical space. **D.G. Mackanic**
- 8:40 21. Student-led projects as seeds of entrepreneurship and employability. **H. Miles**
- 9:05 22. Advancing innovation & entrepreneurship education for STEM students. **R.M. Kuffner**
- 9:30 Concluding Remarks.

SECTION A

Hilton San Diego Bayfront
Indigo Ballroom H

Gerry Meyer: The First 100 Years

Cosponsored by BMGT, CHED, ENFL, HIST and SCC
W. F. Carroll, *Organizer*
J. L. Liu, *Organizer, Presiding*

- 10:00 Introductory Remarks.
- 10:05 23. CO₂ utilization via carbon mineralization and enhanced extraction of alkaline metals and rare earth elements from unconventional resources. **A.A. Park**
- 10:30 24. Metal derivative reaction engineering: Gateway to novel energy conversion technology. **L. Fan**
- 10:55 25. Shape-selective synthesis of value-added chemicals from coal-derived polyaromatic hydrocarbons. **C. Song**
- 11:20 26. Ionic liquid processing of Wyoming coal for acid-free rare earth element extraction. **K.R. Di Bona**, G. Gurau, C. Hill, R.D. Rogers
- 11:45 Concluding Remarks.

TUESDAY AFTERNOON – SCHB

SECTION A

Hilton San Diego Bayfront
Indigo Ballroom H

Gerry Meyer: The First 100 Years

Cosponsored by BMGT, CHED, ENFL, HIST and SCC
J. L. Liu, *Organizer*
W. F. Carroll, *Organizer, Presiding*

- 1:15 Introductory Remarks.
- 1:20 27. Gerry Meyer: Legacy of the nineteenth-century pioneers to the territory of New Mexico. **M.Z. Hoffman**
- 1:40 28. Introducing centenarian Gerry Meyer. **J.V. Thomas**
- 2:00 29. Gerry Meyer joins an elite group, the Centennial Chemists Club (CCC): Report on its achievements. **N.D. Heindel**
- 2:20 30. Gerry Meyer: Professional, scientist, educator, leader, outstanding volunteer, mentor, and friend. **E.A. Nalley**
- 2:40 Intermission.
- 2:55 31. Gerry Meyer: American Institute of Chemists (AIC) giant. **D.M. Manuta**
- 3:15 32. Gerry Meyer at 100: The man, the regional myth, the legend. **J.L. Bryant**, D.R. Porterfield
- 3:35 33. Gerry Meyer and Sigma Xi. **J.E. Sabol**
- 3:55 Concluding Remarks.

SOCED

SOCIETY COMMITTEE ON EDUCATION

V. Goss, *Program Chair*

MONDAY MORNING – SOCED

SECTION A

Marriott Marquis San Diego Marina
Marina Ballroom Salon G

Ocean Science: Research Reflections at the Marina

Cosponsored by ENVR
V. Goss, *Organizer, Presiding*

- 10:15** 1. Ocean science: Research reflections at the marina. **P. Jensen, L. McCormick, A. Griffin**

MONDAY AFTERNOON – SOCED

SECTION A

Marriott Marquis San Diego Marina
Marina Ballroom Salon G

Eminent Scientist Lecture with Dr. Marya Lieberman

Cosponsored by ANYL
V. Goss, *Organizer, Presiding*

- 12:00** 2. What if you could identify street drugs with a paper test card?. **M. Lieberman**

TOXI

DIVISION OF CHEMICAL TOXICOLOGY

T. Spratt, *Program Chair*

SUNDAY MORNING –TOXI

SECTION A

Omni San Diego Hotel
Gallery 1

Translation Aspects of DNA Repair

S. Shuck, *Organizer, Presiding*

D. H. Tamae, *Presiding*

- 8:30 Introductory Remarks.
- 8:35 1. Electron flow through proteins. **H.B. Gray**
- 9:10 2. Competition between repair and oxidation of the endogenous DNA adduct, 3(2-deoxy- β -D-erythro-pentofuranosyl)pyrimido[1,2- β]purin-10(3H)-one (M_1dG). **L.J. Marnett**, P.J. Kingsley, O.R. Wauchope, M.M. Mitchener, A. Vemulapalii, P.P. Christov, C.J. Rizzo
- 9:45 3. Highways for repair of heterochromatic DNA breaks. **I. Chiolo**
- 10:20 Intermission .
- 10:35 4. Hyperglycemia induced DNA damage and inhibition of DNA repair: Potential mechanistic link between diabetes and increased cancer risk. **J.S. Termini**
- 11:10 5. SUMO2 conjugation of PCNA facilitates chromatin remodeling to resolve transcription-replication conflicts. **Y. Liu**

SUNDAY AFTERNOON –TOXI

SECTION A

Omni San Diego Hotel
Gallery 1

Founder's Award Symposium: The Role of Carbonyl Metabolism in Health & Disease

T. M. Penning, *Organizer, Presiding*

- 1:00 Award Presentation.
- 1:10 Introductory Remarks.
- 1:25 6. Histone modification by bifunctional electrophiles derived from lipid and carbohydrate metabolism. **L.J. Marnett**, J.J. Galligan, P.J. Kingsley, J.A. Wepy

- 2:05 7. Interactions of aldehydic bifunctional electrophiles and high mobility group box-1 with RAGE. **I.A. Blair**, K.P. Gillespie, R.K. Sanku, L. Weng, C. Mesaros
- 2:45 Intermission.
- 3:00 8. Aldehyde dehydrogenases: From metabolic and alcohol-related diseases to cancer stem cells. **V. Vasilou**, D.C. Thompson
- 3:40 9. Aldo-keto reductases and NRF2. **J.D. Hayes**
- 4:20 10. Role of human aldo-keto reductases (AKRs) in hormonal & chemical carcinogenesis. **T.M. Penning**

MONDAY MORNING –TOXI

SECTION A

Omni San Diego Hotel
Gallery 1

Student & Post-Doctoral Scholar Symposium

TOXI Young Investigators

E. G. Prestwich, U. Sarkar, *Organizers, Presiding*

- 8:00 11. Epigenetic changes in alveolar type II lung cells of A/J mice following exposure to cigarette smoke and LPS. **J. Fernandez**, Q. Han, A. Rajczewski, C. Seiler, A. Lee, N.Y. Tretyakova
- 8:20 12. Oxidation of RNA at naturally occurring modifications. **I. Sappy**, A. Akrimah, **M. Bedi**, A.C. Bryant-Friedrich
- 8:40 13. DNA glycosylase NEIL1 demonstrates lesion specificity from RNA editing. **E.R. Lotsof**, J. Yeo, B.M. Anderson-Steele, S.S. David
- 9:00 14. Sequencing for 8-oxo-7,8-dihydroguanine in a mammalian genome before and after oxidative stress. **J. Zhu**, A.M. Fleming, C.J. Burrows
- 9:20 15. Embryonic exposure to 2, 2', 3, 5', 6 polychlorinated biphenyls (PCB-95) alters GABAergic and antioxidant transcriptome in zebrafish. **P. Ranasinghe**, C.M. Lee
- 9:40 16. Nrf2 signaling increases bioactivation of the mutagenic air pollutant 3-nitrobenzanthrone. **J.R. Murray**, L. de la Vega, J.D. Hayes, T.M. Penning
- 10:00 Intermission.

- 10:15** **17.** Interstrand cross-links at strand breaks derived from abasic sites in duplex DNA. **K. Housh**, Z. Yang, K.M. Johnson, K.S. Gates
- 10:35** **18.** Replicative bypass and mutagenic properties of alkylphosphotriester lesions in *Escherichia coli*. **J. Wu**, Y. Wang, J. Yuan
- 10:55** **19.** Development of an ultra performance liquid chromatography-mass spectrometry (UPLC-MS) assay for the quantification of cisplatin-Induced DNA intra- and interstrand cross-links. **A. Groehler**, J. Sornkom, O. Schärer
- 11:15** **20.** High-resolution/accurate-mass DNA adductomics to identify adducts formed by the hypoxia-activated alkylating agent, CP-506 and its metabolites. **M. Solivio**, J. Gilissen, A. Stornetta, P.W. Villalta, A. Heyerick, S. Deschoemaeker, S. Balbo
- 11:35** **21.** Identification of a new *N'*-nitrosonoronicotene (NNN)-specific DNA adduct *N*⁶-((5-(3-pyridyl) tetrahydrofuran-2-yl)-2'-deoxyadenosine in rat liver. **Y. Li**, A.T. Zarth, E.S. Carlson, P. Upadhyaya, S.S. Hecht

Advances in Exposure Modeling for Human Health Assessments

Sponsored by AGRO, Cosponsored by TOXI

MONDAY AFTERNOON –TOXI

SECTION A Omni San Diego Hotel Gallery 1

Current Approaches to Discovery Phase Safety Assessment in the Industry

P. F. Guengerich, N. A. Meanwell, *Organizers, Presiding*

- 2:00** Introductory Remarks.
- 2:05** **22.** Strategies for early safety assessment of potential drug candidates at Amgen and lessons learned. **M. Fielden**
- 2:35** **23.** Early safety assessment strategies for drug discovery at Celgene and lessons learned. **J.R. Piccotti**
- 3:05** **24.** Strategies towards the design of safer compounds at Takeda and lessons learned. **R. Naven**, Y. Dragan
- 3:35** **25.** Reactive metabolism strategy applied to drug safety assessment: Focus on risk prevention. **K.J. Coe**, V. Shah, K. Wang, T. Koudriakova

- 4:05** **26.** Strategies for early safety assessment of potential drug candidates at Bristol-Myers Squibb: Preclinical evaluation of hepatobiliary toxicity. **M. Gill**, L. Sivaraman, B. Murphy, P. Cheng, K. Chadwick, M. Graziano, L. Lehman-McKeeman
- 4:35** **27.** Integrated platform, utilizing transcriptomic profiling and metabolite identification studies, to derisk drug bioactivation-mediated liver injury. **K. Mitra**, J.J. Monroe, W. Kang, K. Tanis, J. Lebron, F. Sistare

Advances in Exposure Modeling for Human Health Assessments

Sponsored by AGRO, Cosponsored by TOXI

TUESDAY MORNING –TOXI

SECTION A Omni San Diego Hotel Gallery 1

Emerging Topics in Chemical Toxicology

T. Spratt, *Organizer, Presiding*

- 8:00** Introductory Remarks.
- 8:05** **28.** Delivering web-based access to data and algorithms to support computational toxicology: US EPA CompTox Chemicals Dashboard. **A.J. Williams**, C. Grulke, A. Richard, R. Judson, G. Patlewicz, I. Shah, J. Wambaugh, K. Paul-Friedman, J. Dunne, J. Edwards
- 8:40** **29.** DARPA's microphysiological systems (MPS) program. **B. Ringeisen**
- 9:15** **30.** Dare to repair: From DNA chemistry to cancer. **S.S. David**
- 9:50** Intermission.
- 10:05** **31.** E-cigarette aerosols for *in vitro* and *in vivo* toxicology studies: Key considerations. **I. Stepanov**, V. Jain, A. Alcheva
- 10:40** **32.** Developing DNA repair pathway specific genotoxic signatures. **J. Li**, N. Dey, **R. Sobol**

Biostimulants in Agriculture: Chemistry & Regulatory Aspects

Sponsored by AGRO, Cosponsored by BIOL, MEDI and TOXI

SECTION A

Omni San Diego Hotel
Gallery 1Chemical Research in Toxicology Young
Investigator Award SymposiumS. J. Sturla, *Organizer*S. Balbo, *Presiding*

- 2:00 Award Presentation.
- 2:05 33. Annotating the small-molecule exposome by subtraction. **G. Patti**
- 2:40 34. *E.coli*-produced genotoxin colibactin: DNA adduct identification using untargeted adductomics and *in vivo* detection using high resolution mass spectrometry. **P.W. Villalta**, M.R. Wilson, Y. Jiang, A. Stornetta, P. Boudreau, A. Carra, C.A. Brennan, E. Chun, L. Ngo, L. Samson, B. Engelward, W.S. Garrett, E.P. Balskus, S. Balbo
- 3:15 Intermission.
- 3:30 35. Integrative experimental modelling reveals novel genome-scale mutation fingerprints of carcinogens. **J. Zavadil**
- 4:05 36. High resolution mass spectrometry-based approaches for the investigation of chemical carcinogenesis. **S. Balbo**, R.P. Dator, A. Stornetta, V. Guidolin, L.A. Maertens, P.W. Villalta

SECTION A

Omni San Diego Hotel
Gallery 1

Keynote Lecture

Embracing Translation in Toxicology: A National
Toxicology Program StrategyT. Spratt, *Organizer, Presiding*

- 5:00 Introductory Remarks.
- 5:05 37. Embracing translation in toxicology: National toxicology program strategy. **B. Berridge**

Biostimulants in Agriculture: Chemistry &
Regulatory Aspects

Sponsored by AGRO, Cosponsored by BIOL, MEDI and TOXI

SECTION A

San Diego Convention Center
TBD

TOXI Poster Session

Mechanisms of Cellular Responses to Exogenous
and Endogenous ToxinsT. Spratt, *Organizer, Presiding*

7:00 - 9:00

38. Combined *in vitro* assays for eye irritation assessment. **N. Bhowmik**, M. Guo, T. Moore, P. Leung
39. Kinetics of formation and removal of DNA adducts in mice exposed to tobacco and meat carcinogens by UPLC-mass spectrometry. **B. Yun**, R. Bonala, F. Johnson, T. Rosenquist, A.P. Grollman, R. Turesky
40. Mass spectrometric quantitation of apurinic/aprimidinic sites in tissues of rats treated with 4-(methylnitrosamino)-1-(3-pyridyl)-1-butanone and *N'*-nitrosornicotine. **J. Guo**, H. Chen, R.J. Turesky, S.S. Hecht
41. Mutagenicity of the C8-adenine adduct derived from the environmental carcinogen 6-nitrochrysene in *Escherichia coli* and human cells. **B.V. Powell**, A.K. Basu
42. Rad4/XPC initial binding discriminates repair-resistant lesions from efficiently-repaired ones in global genomic nucleotide excision repair. **H. Mu**, J. Min, Y. Zhang, N.E. Geacintov, S. Broyde
43. Elucidating the roles of estrogens in the development and prognosis of malignant pleural mesothelioma. **G. Zhang**, L. Duan, T.M. Penning
44. Facile synthesis of DNA duplexes containing a chemically-defined, derivatizable, covalent cross-link. **K. Housh**, K.S. Gates
45. Iterative approach for the development of a CNS-active oxime reactivator for nerve agent exposure. **M. Malfatti**, B. Bennion, H. Enright, N. Be, S. Hok, C.L. Cadieux, T. Carpenter, V. Lao, E. Kuhn, M.W. McNerney, F.C. Lightstone, T. Nguyen, C.A. Valdez
46. Probing the thermostability and DNA loading efficiency of beta sliding clamp variants with perturbed dimer interfaces. **M.L. Liriano**, B. Koleva, P.J. Beuning
47. Application of a read-across approach to address data gaps in human health screening level risk assessments and the chemicals management plan. **P. Cebrowski**

- 48.** Endogenous microbial generation of acrolein: Strategies to assess the effects of intestinal acrolein formation. **K. Hurley**, A. Ramirez-Garcia, S. Diedrich, J. Zhang, C. Lacroix, E. Slack, C. Schwab, S.J. Sturla
- 49.** Effect of sequence context on 1, *N*⁶-ethenoadenine repair by the AlkB family DNA repair enzymes. **R. Qi**, K. Bian, Q. Tang, F. Chen, D. Li
- 50.** Is food type important for *in vitro* post ingestion bioaccessibility models of polychlorinated biphenyls sorbed to soil. **J. Starr**, W. Li, S.E. Graham, H. Shen, F. Waldron
- 51.** Translesion synthesis past DNA-peptide crosslinks is dependent on local DNA sequence context. **J. Thomforde**, S. Ji, S. Naldiga, S. Pujari, A.K. Basu, N.Y. Tretyakova
- 52.** Replication studies of chemically stable analogs of *N*7-methylguanine and *N*3-methyladenine in *Escherichia coli* cells. **J. Yuan**, Y. Wang
- 53.** Probing interactions between *E. coli* DNA polymerase III and single-stranded DNA binding protein to gain insights into polymerase management. **J. Mclsaac**, M. Ondrechen, P.J. Beuning
- 54.** Quantitation of carboxyethylguanine adducts in leukocyte DNA from smokers and nonsmokers using LC-NSI-HRMS/MS. **G. Cheng**, S. Balbo, P.W. Villalta, S.S. Hecht
- 55.** Withdrawn
- 56.** Replication studies of purine 5',8-cyclonucleosides in cells. **Y. Wang**, H. Du, Y. Wang
- 57.** DNA base sequence effects on 4-aminobiphenyl lesion-induced mutational spectra. **Y. Chen**, K. Bian, X. Zhou, S. Howarth, Q. Mylie, D. Li
- 58.** Human translesion synthesis DNA polymerases function in transcriptional bypass and repair of *N*²-alkyl-2'-deoxyguanosine lesions. **Y. Tan**
- 59.** Evaluation of tobacco smoke and diet as sources of exposure to two heterocyclic aromatic amines for the U.S. population: NHANES 2013-2014. **L. Zhang**, L. Wang, Y. Li, Y. Xia, B. Xia, C. Sosnoff, B.N. Pine, B. deCastro, B. Blount
- 60.** Multi-omics characterization of an inflammatory bowel disease mouse model. **Q. Han**, T.J. Kono, C.G. Knutson, C. Seiler, N.Y. Tretyakova
- 61.** Heavy metal toxicants deposition and destruction in pulmonary surfactant layer: Classical density functional prediction. **H. Liu**, Y. Liu, Y. Shang, H. Liu
- 62.** Investigation of kinase inhibitor hepatotoxicity with induced pluripotent stem cell-derived hepatocytes. **A.S. Bunev**
- 63.** Reactive oxygen species-activated DNA damage agents to selectively targeting cancer by oxidative-cyclizing. **H. Zhu**, J. Liu, M. Wunderlich, M. Edward
- 64.** Unhooking of DNA-DNA interstrand cross-links by the base excision repair glycosylase NEIL3. **X. Guo**, K. Housh, T. Haldar, M. Imani Nejad, K.S. Gates
- 65.** Oxidative stress and mitochondrial dysfunction in tail of zebrafish induced by persistent organic pollutant. **E. Ko**, **S. Lee**, M. Choi, S. Shin
- 66.** Studying the assembly of nucleotide excision repair complexes by biochemical and crosslinking mass spectrometry approaches. **A. Groehler**, B. Kim, H. Kim, J.E. Yeo, O. Schärer
- 67.** DNA probe-based screening strategy for selectivity engineering of 8-oxoguanine glycosylase. **J. Sun**, N.M. Antczak, S.J. Sturla
- 68.** Mapping the interactions of UmuD and the beta clamp loader in *E. coli*. D. Murison, **R. Dilworth**, P.J. Beuning
- 69.** Amplification and sequencing of 5'-aldehyde lesions resulting from DNA oxidation. **J. Wu**, S.J. Sturla
- 70.** MG-adducts as biomarkers of metabolic disease. **C.A. Hernandez**
- 71.** Investigating the metabolic and biological effects of glyoxalase 1 inhibition and knockdown in cancer cell lines. **B. Cordova**, **S. Ahmad**, N. Gardon, S. Shuck, L. Reque, L. Chan, A. Matavousian, J. Mason, S. Kenney, J. Anderson, L. Soetyono, J.S. Termini, **D.H. Tamae**
- 72.** Structural insights into aflatoxin B₁ (AFB₁)-associated mutational spectrum. **R. Tomar**, A. Patra, M. Egli, M.P. Stone
- 73.** Environmental polycyclic aromatic hydrocarbons and risk of lung cancer in never smokers. **C. Mesaros**, T.M. Penning
- 74.** Independent synthesis and fate of DNA lesions generated from oxidative damage at the C-5' of thymidine. **C.A. Dim**, M. Bedi, A.C. Bryant-Friedrich
- 75.** Withdrawn
- 76.** Chemical metabolism and toxicological relevance of microbial glycerol dehydratase from human gut microbiota. J. Zhang, K. Hurley, A.J. Ramirez, C. Lacroix, C. Schwab, **S.J. Sturla**
- 77.** Investigating base excision repair using "designer" chromatin. **J. Sczepanski**, D. Banerjee, C. Deckard
- 78.** Medical countermeasures for the individual service member to maintain combat effectiveness and prevent or reduce injury from the battlefield. **S.N. Olatunji**

- 79.** Multiple deuterated phenanthrene metabolites as probes for the metabolism of carcinogenic PAHs in humans: Phenotyping, genotyping and potential application in human health risk assessment. **K. Luo**, J.B. Hochalter, V. Paiano, J. Wang, C. Sipe, S. Carmella, S.E. Murphy, D. Hatsukami, J. Jensen, N. Fujioka, S. Lam, L. Bergstrom, D. Midthun, S. Hecht
- 80.** Base-resolution analysis of thymine glycol (Tg) in DNA by polymerase-aided differential coding. **F. Tang**, B. Yuan, Y. Wang
- 81.** Biological effects of the cooked meat carcinogen PhIP in human prostate cancer. **M. Bellamri**, C. Brown, P. Murugan, C. Weight, R. Turesky
- 82.** Evaluating the value of primary human cells for the prediction of *in vivo* toxicity in early drug discovery. **T. Takai**, R. Naven
- 83.** Estrogenic activity of polycyclic aromatic hydrocarbon metabolites in human endometrial cells. **I. Lee**, C. Mesaros, T.M. Penning
- 84.** Investigating the role of cysteine oxidation by environmentally induced oxidative stress on the DNA glycosylase MUTYH. **C. Khuu**, N. Nunez, S.S. David
- 85.** Underestimation of toxin levels in the aerosol of electronic cigarettes. **S. Vreeke**, R.M. Strongin
- 86.** DNA damage as a toxicity mechanism of NMC ($\text{Li}_x\text{Ni}_{1/3}\text{Mn}_{1/3}\text{Co}_{1/3}\text{O}_2$) nanomaterial to bacteria *Shewanella oneidensis* MR-1 and *Bacillus subtilis*. **V. Guidolin**, T.A. Qiu, T. Pho, P.W. Villalta, C.L. Haynes, V. Feng, S. Balbo
- 87.** Reactive oxygen species (ROS)-dependent release of an anticancer drug from a targeting peptide. **G. Premnauth**, E.J. Merino
- 88.** Translesion synthesis of tandem DNA lesions containing 2-deoxyribonolactone 5' to thymine glycol in human cells. **S. Naldiga**, H. Huang, M.M. Greenberg, A.K. Basu
- 89.** Evaluation of postnatal Chlorpyrifos administration in rat pups. **M. Bourgeois**, R. Harbison, J. Driver, J. Ross
- 90.** Expression of the catalytic domain of DNA polymerase zeta from dictyostelium discoideum. **S.K. Mauldin**
- 91.** Synthesis and study of RNA oxidative damage product, 3'-deoxy-3',4'-didehydrouridine-5'-aldehyde. **A. Akrimah**, M. Bedi, A.C. Bryant-Friedrich
- 92.** Unregulated Mitochondrial function exposed in Persistent organic pollutants Mixture. **E. Ko**, M. Choi, S. Shin

WEDNESDAY MORNING –TOXI

SECTION A
Omni San Diego Hotel
Gallery 1

Epigenetic Response to Endogenous & Exogenous Toxins

N. Y. Tretyakova, Y. Wang, *Organizers, Presiding*

- 8:00** Introductory Remarks .
- 8:05** **93.** Epigenetic regulation via oxidized forms of Me C and inflammation-mediated epigenetic deregulation. **N.Y. Tretyakova**, C. Seiler, J. Fernandez, Q. Han
- 8:40** **94.** Reversible histone glycation drives disease-associated changes in chromatin architecture. **Y. David**
- 9:15** **95.** Base modifications in DNA non-canonical structures regulate transcription. **A.M. Fleming**, C.J. Burrows
- 9:50** Intermission.
- 10:05** **96.** Transcription-coupled recognition of DNA lesions and endogenous epigenetic modifications. **D. Wang**
- 10:40** **97.** Targeted quantitative proteomic approaches toward understanding epitranscriptomic regulations. T. Qi, M. Huang, Y. Sun, W. Miao, Y. Wang

Biostimulants in Agriculture: Chemistry & Regulatory Aspects

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WEDNESDAY AFTERNOON –TOXI

SECTION A
Omni San Diego Hotel
Gallery 1

Topics in Chemical Toxicology

P. J. Beuning, L. Zhao, *Organizers, Presiding*

- 1:00** **98.** Magic of the chemosynthetic livers which is the best porphyrin. **M. Chorghade**
- 1:20** **99.** Genome-wide CRISPR screening to identify modulators of formaldehyde toxicity in erythroid cells. **C. Vulpe**, Y. Zhao, A. Tagmount, L. Zhang
- 1:40** **100.** Higher advanced oxidative modifications in hemoglobin of oral cancer patients as measured by nanoflow liquid chromatography tandem mass spectrometry. **H.C. Chen**, Y. Lin, C. Wu, T. Lin, D. Wu

- 2:00 101.** Competitive binding of human DNA glycosylase hNEIL1 and DNA damage-sensing factor XPC-RAD23B to oxidatively generated guanine lesions. **V. Shafirovich**, M. Kolbanovskiy, N.E. Geacintov
- 2:20 102.** Probing chemical biology of DNA damage using NMR. **M.P. Stone**, S.N. Bamberger, A.H. Kellum, C.K. Malik, T.L. Johnson-Salyard, M.V. Voehler, C.J. Rizzo, R.S. Lloyd
- 2:40 103.** Molecular modeling of genotoxic azo dyes, Sudan I and Sudan II, and their metabolites. **R.J. Bienstock**, L. Perera, M.A. Pasquinelli
- 3:00** Intermission.
- 3:20 104.** Comprehensive toxicity information of every chemical for better R&D decisions. **N. Vaidya**
- 3:40 105.** Emission of respirable particles from fused deposition modeling 3D printers. **P. Byrley**, B. George, K.R. Rogers, W.K. Boyes
- 4:00 106.** Glutamine drives glutathione synthesis and contributes to radiation sensitivity of A549 and H460 lung cancer cell lines. **G. Boysen**, A. Jamshidi-Parsian, E. Siegel, R.J. Griffin
- 4:20 107.** Carbon dioxide enhances the pulmonary tumorigenic activity of the tobacco specific nitrosamine, 4-(methylnitrosamino)-1-(3-pyridyl)-1-butanone (NNK). **L.A. Peterson**, D.E. Seabloom, W.E. Smith, K.R. Vevang, M.K. Oram, M.G. O'Sullivan, L. Zhang, S. Hecht, S. Balbo, T.S. Wiedmann
- 4:40 108.** Oxidative decarboxylation of 2-oxoacids by hydroperoxides can be used to lower peroxide values in citrus oils. **M.J. Calandra**, Y. Wang

WCC

WOMEN CHEMISTS COMMITTEE

R. Cole, *Program Chair*

SUNDAY MORNING – WCC

SECTION A

Hilton San Diego Bayfront
Indigo 204 A/B

Merck Research Award Symposium

A. E. Weber, *Organizer, Presiding*

D. Strong, *Presiding*

- 8:25** Introductory Remarks.
- 8:30** 1. 2'3'-cGAMP is an immunotransmitter produced by cancer cells and regulated by ENPP1. **J. Carozza**, V. Böhnert, K. Shaw, K. Nyugen, G. Skariah, J. Brown, M. Rafat, R. von Eyben, E. Graves, J. Glenn, M. Smith, L. Li
- 8:50** 2. Synthesis of a carolacton tool compound enables identification of a unique biofilm target in *Streptococcus mutans*. **A.E. Solinski**, A. Scharnow, A.J. Fraboni, W.M. Wuest
- 9:10** 3. Chemical modification of carbon nanotubes for gene delivery into intact plants. **G.S. Demirer**, N. Goh, M. Landry
- 9:30** 4. Monomeric property transfer predicts oligomeric nonaqueous solubility. **S.G. Robinson**, Y. Yan, K. Hendriks, M.S. Sanford, M.S. Sigman
- 9:50** 5. Ratiometric imaging of pH with dicobalt PARACEST MRI probes. **A.E. Thorarinsdottir**, K. Du, S.M. Tatro, J.H. Collins, D. Harris
- 10:10** Intermission.
- 10:20** 6. Resource sparing approaches to accelerate drug discovery. **H. Mitchell**
- 11:00** 7. Development of flavin-dependent biocatalytic methods and applications in total synthesis. **S.A. Dockrey**, A.R. Narayan
- 11:20** 8. Activation of diverse carbon–heteroatom and carbon–carbon bonds via palladium(II)-catalyzed β -X elimination. **V.T. Tran**, J.A. Gurak, K.S. Yang, K.M. Engle
- 11:40** 9. Enabling new methods for the formation of C–C bonds through metallaphotoredox catalysis. **T.Q. Chen**, C. Le, T. Liang, P. Zhang, D.W. MacMillan
- 12:00** Concluding Remarks.

MONDAY MORNING – WCC

2019 ACS Catalysis Lectureship for the Advancement of Catalytic Science: Symposium in Honor of Maria Flytzani-Stephanopoulos & Charles Sykes

Sponsored by CATL, Cosponsored by WCC

Rising Stars: Women in Medicinal Chemistry

Sponsored by MEDI, Cosponsored by WCC

Surfaces & Interfaces in the Environment: Symposium in Honor of Vicki Grassian Catalysis, Surfaces & Minerals

Sponsored by COLL, Cosponsored by ENVR and WCC

Women Make COMP

Sponsored by COMP, Cosponsored by PROF and WCC

MONDAY AFTERNOON – WCC

2019 ACS Catalysis Lectureship for the Advancement of Catalytic Science: Symposium in Honor of Maria Flytzani-Stephanopoulos & Charles Sykes

Sponsored by CATL, Cosponsored by WCC

Women Make COMP

Sponsored by COMP, Cosponsored by PROF and WCC

Surfaces & Interfaces in the Environment: Symposium in Honor of Vicki Grassian

Aqueous Surfaces to Ocean & Organic-Surface Interactions

Sponsored by COLL, Cosponsored by ENVR and WCC

Journal of Polymer Science Innovation Award: Symposium in Honor of Patricia Dankers

Sponsored by PMSE, Cosponsored by WCC

TUESDAY MORNING – WCC

Accelerating Scientific Breakthroughs at the Energy-Water Nexus in Engineered & Natural Environment

Sponsored by ENFL, Cosponsored by WCC

Remarkable Women in Organic Chemistry

Sponsored by ORGN, Cosponsored by WCC

TUESDAY AFTERNOON – WCC

SECTION A

Hilton San Diego Bayfront
Indigo 206

Eli Lilly: Supporting Women in Chemistry

M. Jeffries-El, *Organizer, Presiding*

S. R. Hare, *Presiding*

- 1:45** Introductory Remarks.
- 1:50** **10.** Efforts toward complex small molecule scaffolds from biorenewable resources. **J.A. Dabrowski**
- 2:10** **11.** Nickel-catalyzed cross-electrophile coupling reactions of sulfonamides for diastereoselective cyclopropane synthesis. **E. Lucas**
- 2:30** **12.** Glycosylated cluster nanomolecules with multivalent binding capabilities. **E.A. Qian**, Y. Han, M. Messina, H.D. Maynard, P. Kral, A.M. Spokoyny
- 2:50** **13.** Quantification of eicosanoids and metabolites in human disease. **G.L. Milne**
- 3:10** Intermission.
- 3:20** **14.** Research and teaching: Catalyst for staying engaged in a lifetime of chemistry. **J. Alexander**
- 3:40** **15.** 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**
- 4:00** **16.** Withdrawn
- 4:20** **17.** Transitioning from a chemist to an innovator and an entrepreneur. **S.H. Rachakonda**
- 4:40** Concluding Remarks.

Remarkable Women in Organic Chemistry

Sponsored by ORGN, Cosponsored by WCC

WEDNESDAY MORNING – WCC

Surfaces & Interfaces in the Environment: Symposium in Honor of Vicki Grassian

Organic-Surface interactions & Organic Aerosols

Sponsored by COLL, Cosponsored by ENVR and WCC

WEDNESDAY AFTERNOON – WCC

Surfaces & Interfaces in the Environment: Symposium in Honor of Vicki Grassian

Nano in the Environment & Plenary Lecture

Sponsored by COLL, Cosponsored by ENVR and WCC

YCC

YOUNGER CHEMISTS COMMITTEE

D. Williams and M. Brann, *Program Chairs*

SUNDAY AFTERNOON – YCC

Hilton San Diego Bayfront
Sapphire Ballroom MN

Our Element(s): Younger Chemists from Around the World

Cosponsored by IAC
C. Dunne, J. J. O'Neil, P. Wangtrakuldee, *Organizers*
G. I. Onyenanu, *Presiding*

- 2:00** Introductory Remarks.
2:05 **1.** Our element(s): Younger chemists from around the world. **C. Dunne**
2:35 **2.** "Caesium". **N.A. LaFranzo**
3:05 **3.** "Nickel". **L. Ferrins**
3:35 **4.** "Helium". **E. McConnell**
4:05 Closing Remarks.

MONDAY MORNING – YCC

SECTION A
Hilton San Diego Bayfront
Sapphire Ballroom MN

Getting your First Industrial Job

Cosponsored by PROF
T. K. Shah, *Organizer, Presiding*

- 10:00** Introductory Remarks.
10:05 **5.** Panel discussion and networking. **T.K. Shah**
11:35 Closing Remarks.

Chemistry of Aged Beer & Spirits

Sponsored by AGFD, Cosponsored by YCC

TUESDAY MORNING – YCC

Hilton San Diego Bayfront
Indigo 206

Going with the Flow of Water: Career Paths & Journeys

Going with the flow of water: career paths and journeys

Cosponsored by CEI
D. E. Williams, *Organizer*
M. Brann, *Organizer, Presiding*

- 10:00** Introductory Remarks.
10:05 **6.** Panel discussion and networking. **J. Schmitt, M. Brann**
11:35 Concluding Remarks.

Beyond the Bench: Non-Traditional Careers in Chemistry

Sponsored by CHAL, Cosponsored by PROF and YCC