The 45th Western Regional Meeting of the American Chemical Society November 6-8, 2015

Keisuke Ikehata and Michael Kleinman*, Program Chairs*

FRIDAY AFTERNOON

California State University, San Marcos
USU 2300D

Fire & Water

S. P. Thompson, *Organizer*
K. Ikehata, *Organizer, Presiding*

1:30 1. Forest fire arson: Linking field investigative data to potential sources. **D.A. Birkholz**

2:00 2. Marijuana extraction labs: Assessing the explosion dangers. **D. Kirby**, L. Higgins, T. Burton

2:30 3. Experimental observation of large mass-independent isotopic anomalies from diffusion of H_2O. **G. Dominguez**

3:00 Intermission.

3:30 4. Self-healing corrosion resistant coatings: An enabling technology for the use of alternate waters for cooling. **G. Rajagopalan**

4:00 5. Standard heats of oxidation for characterized soils in the remediation of chemically-contaminated groundwater. **N. Moulton**, S.P. Mezyk

4:30 6. Synthesis and characterization of a graphene desalination membrane. **N. Pon**, J. Torres, X. Huang, R.B. Kaner

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SBSB 1102

Inorganic Nanomaterials

K. Ikehata, *Organizer*
M. T. Kleinman, *Organizer, Presiding*

1:30 7. Fine tuning the magnetic properties of cobalt ferrite thin films by controlling the nanoscale structure. **S. Robbennolt**, A. Buditama, H. Kang, P. Nordeen, G. Carman, S.H. Tolbert

2:00 8. Preparation of fluorescent magnetic nanomaterials. **L. Dong**

2:30 9. Using bulky terphenyl thiolates as capping ligands for gold thiolate nanoclusters. **N. Mendelson**

3:00 Intermission.

3:30 10. Computational studies of states of carboranedithiols on Au{111}. **O. Irving**, J. Thomas, A. Serino, D. Goronzy, E.J. Izal, J. Dadras, A. Alexandrova, P.S. Weiss, T. Base, H. Auluck

4:00 11. Synthesis and characterization of PtSn bimetallic nanoparticles: Comparison between two synthesis strategies. **R. Morales**

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Natural Products

K. Ikehata, M. T. Kleinman, *Organizers*
Z. Haque, S. P. Thompson, *Presiding*

1:30 12. The culture and chemistry of chocolate. **J.A. Trischman**

2:00 13. Efficacy of highly antioxidative aqueous extract of olive leave as cargo in nano-vesicular emulsion system. **Z. Haque**, A.C. Saddam, X. Zhang

2:30 14. Investigation of antioxidant behavior of catechins from green tea extracts. **Y. Zhou**, Y. Liu

3:00 Intermission.

3:30 15. Folding, unfolding, and misfolding of the RNA pseudoknot structural motif via massively parallel molecular dynamics. **K. Nguyen**

4:00 16. Peroxyl radical formation chemistry of tobacco-specific nitrosamines. **B. Daws**

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Organic Chemistry

Biological Chemistry and Novel Reactions

K. Ikehata, M. T. Kleinman, *Organizers*
S. P. Sun, *Presiding*

1:30 17. Synthesis, guest binding, and metal coordination of functionalized self-folding deep cavitands. **M. Mettry**, R.J. Hooley

2:00 18. Fluorescent cytidine analogues for the study of nucleic acids. **D.D. Burns**, R. Lee, B.W. Purse

2:30 19. Assigning the structure of sibongilene: A pseudolaric acid precursor. **T. Palazzo**, S. Mafu, B. Harrod, D.J. Tantillo, P. Zerbe

3:00 Intermission.

3:30 20. Nucleophile, radical trap, or both? The role of alkenes in the intramolecular reactions of oxime and oxime ether radical cations. **N. Armada**, P. De Lijser

4:00 21. *In situ* formation and reactions of benzylic diazo compounds. **R. Squitieri**, K.N. Lamb, G. Shearn-Nance, C. Soldi, J. Hein, J.T. Shaw

4:30 22. A modular approach to crowded benzoquinolines. **D.J. Dibble**, A. Mazaheripour, D.E. Laidlaw, R. Lopez, M. Umerani, Y. Park, A.A. Gorodetsky

FRIDAY EVENING

California State University, San Marcos
USU 2300A&B

WRM Poster Session

K. Ikehata, M. T. Kleinman, *Organizers*

6:00 - 8:00

23. Observations during prolonged sample exposure with 5N sodium hydroxide on the stability of memantine HCl internal standard in samples. S. Ghosh, C. Weng, **A. Ng**

24. Synthesis of homopropargyl alcohols via three-component coupling of allenyl carbenoids, acyclic organozirconium species, and aldehydes/ketones. **J. Stec**, A.R. Henderson, R.J. Whitby

25. Progressive new methods towards the total synthesis of azaspirene and its analogs: Promising new cancer treatments. **T. Montgomery**, M.J. Kelly, M.B. Bergdahl

26. Synthesis and characterization of hematite nanoparticles for mercury capture. **J. Jung**, S. Liguori, J. Wilcox

27. 3-D interconnected mesoporous tantalum nitride as a novel water splitting photocatalyst. **H. Kang**, S.H. Tolbert

28. Metathesis: The versatile problem solver. **J.H. Phillips**

29. Monitoring atmospheric ammonia through passive diffusion collection on California State Polytechnic University Pomona campus. **L. Aranda**, M. Torres, Y. Liu

30. Preparation of γ-aminoalcohols with pendant quinolyl moiety by reduction of ketoimines with sodium borohydride. **K.J. Goosherst**, D.B. Green, J.M. Fritsch

31. Copolymerization of L-lactide and ε-caprolactone by bis-ligated magnesium complexes binary catalyst systems. **R.M. Slattery**, J.M. Fritsch

32. Nanocrystalline magnesium as an anode material for lithium-ion battery applications. **T.C. Lin**, E. Detsi, J.B. Cook, S.H. Tolbert

33. Stress-induced lift-off silicon foil using epoxy. **H. Chang**

34. The study of spectroscopic and electrochemical properties of substituted anthraquinone an undergraduate laboratory setting. M.M. Allard, **J.D. Rojas**, **R.M. Morales**

35. New cellular delivery vehicles: Polymyxin B and guanidinopolymyxin B. **K. Hamill**, L.C. McCoy, Y. Tor

36. High performance liquid chromatographic determination of four biological aminothiols after microwave-enhanced derivatization with SBD-F. **M.B. Blayney**, S.E. Helm, D.B. Green

37. Highly stereoselective synthesis of lagunamide A: Unprecedented potential for anti-malarial and anti-cancer bioactivity. **B. Banasik**, L. Wang, **A.S. Kanner**, **N. Kohnen**, M.B. Bergdahl

38. Online spectra database for undergraduate organic chemistry laboratories. **J. Charonnat**, K. Hazen, N. Paronian

39. Monobocylation of diamines in continuous flow. **A. Ku**, A.C. Evans

40. Towards continuous flow syntheses of levomilnacipran. **M. Nguyen**, C. Ayoub, A.C. Evans, J. Feng

41. Enzyme degassing for RAFT polymerization in continuous flow. **S. Matsuda**, A.C. Evans

42. Thermally controlled multivalent interactions between biomimetic polymer NPs and target biomacromolecules. **A.C. Weisman**, K.J. Shea, K. Yoshimatsu

43. A β-hairpin peptide derived from transthyretin 106-121 that forms square hydrophobic channels. **S. Yoo**, N. Truex, A. Kreutzer, J.S. Nowick

44. X-ray crystallographic structures of amyloid oligomers: A dodecamer of $A\beta_{17-36}$ that forms an annular pore. **A. Kreutzer**, I.L. Hamza, J.S. Nowick

45. How do undergraduate students conceptualize acid-base chemistry? Development, validation, and utilization of a learning progression-based measure. **W. Romine**, A. Todd, T. Clark

46. Formation and stability of silver nanoparticles formed by the reduction of silver ions by humic acid. **R. Leslie**, D. Pullman

47. NMR characterization of ionicity and transport properties for a series of diethylmethylamine based protic ionic liquids. **F. Thompson**

48. Application of α,β-dipeptides in organocatalysis under solvent-free conditions. **C.G. Ortiz**

49. Synthesis of imidazolium chiral ionic liquids derived from (*S*)-prolinamine and their application in asymmetric Michael reaction. **A. Zuniga**

50. Alkylation of acids, alcohols, and phenols using *N*-(1)-adamantyl-*O*-isopropyl-4-nitrobenzenesulfonimidate. **H. Truong**

51. Gaining structural insights into folding of the carboxyl-terminal domain of GIV using circular dichroism spectroscopy. **A. Maddox**

52. Structural elucidation of the nano-bio interface: Histidine on fumed silica nanoparticles. **H. Swanson**

53. Novel thermochromic compounds as sensors for high strain experiments. **J. Sanz**, J.R. de Alaniz

54. Aryl di-*n*-butyl phosphates and derivatives as selective inhibitors of butyrylcholinesterase: Compounds with potential for the treatment of Alzheimer's disease. **T. Tran**

55. Binding properties of curcumin with DNA: Influence of the water network in the DNA minor groove. **A. El-Magboub**

56. In-class and online student performance in a pharmacy problem-based learning class. **A. El-Magboub**

57. Synthesis of bivalent organothiophosphate compounds and their inhibition of butyrylcholinesterase for potential treatment of Alzheimer's disease. **A. Tahira**

58. Synthesis of nanoparticle polymer and testing affinity with IgG. **R. Dalal**

59. Effects of tetra-alkyl bisphosphates on BuChE activity using HEPES as a function of pH. **K. Villarreal**

60. A unique approach to identify solid tumor selective compounds using a combination of two *in vitro* cancer cell screenings. **L. Liu**

61. Progress toward the synthesis of gelsedilam. **C.M. Saunders**, F.D. Fernandes, J.T. Shaw

62. New α-helix mimetics targeting the E6 protein in the human papillomavirus. **E. Armenta**

63. Investigation of LEF-1 flexibility vs. DNA binding activity. **A. Pientka**

64. An efficient domino amination-oxidation reaction for the copper-catalyzed synthesis of anilines. **C. Thomas**

65. PLGA film formulations for sustained release of a water-soluble drug. **A. Tumabayeva**

66. Identification, characterization, and modification of fatty acid alkyl esterases found in *Staphylococcus aureus*. **B. Saylor**, J.J. Love

67. Development of redox mediators for lithium-sulfur batteries. **A. Scheuermann**

68. X-ray single crystal analysis of *n*-type organometallic dopants for organic semiconductors. **E. Jucov**

69. Targeting bacterial antioxidant defense to improve antibiotic treatment efficacy of stationary phase *E. coli*. **J. Wang**

70. Sensitive nonlinear multi-photon laser wave-mixing detection methods for environmental and biomedical applications. **M. Murphy**

71. Synthesis and *in vitro* evaluation of asymmetric 1,5-diheteroarylpenta-1,4-dien-3-ones as anti-prostate cancer agents. **X. Zhang**

72. Assessment of UCH-L3 substrate selectivity using engineered ubiquitin fusions with varying linker lengths. **P. Suon**, J.J. Love

73. Anti-mycobacterial drug discovery using extract UA 774 from the surface of *Ulva californica* . **J. Guzman**, J.A. Trischman

74. Analytical method for reliable H_2O-ice production for astrochemical experiments. **M. Park**

75. Effect of hydrophobicity and charge in the oligomerization of amyloidogenic peptides and the design of a pH-switchable oligomer. **Y. Wang**, J.S. Nowick

76. Using protein design to engineer the Cif epoxide hydrolase for neutralization of mycotoxins. **M. Acevedo**, P. Suon, J.J. Love

77. Isotopic fractionation as a result of sublimation of water-ice. **E. Christensen**, M. Park

78. Identification of anti-mycobacterial compounds from the extract of a marine bacterial isolate (UA446) taken from the surface of *Ulva californica*. **T. Fallert**, J.A. Trischman

79. Optimization of a designed protein-protein interface. **B. Maniaci**, J.J. Love

80. Synthesis of small molecules for potential hepatitis C virus translation inhibition. **W. Frauman**

81. New small molecule α-helix mimetics targeting protein-protein interactions of the human papillomavirus. **E. Kroneberger**

82. Synthesizing redox probes to increase the capabilities of biosensors. **H. Effarah**

83. Chapters in novel antibiotics: Isolating a natural product of marine bacteria challenged with *Mycobacterium marinum*. **A. Bulthuis**, J.A. Trischman

84. 3-*O*-alkyl-2,3-dehydrosilibinins: Synthesis and antiproliferative activity towards prostate cancer cells. **S. Zhang**

85. Regulation of vascular mitochondrial plasticity: Role of cellular crosstalk. **C. Sauceda**

86. Ball milling as an approach to molecular encapsulation. **S. Journey**, B.W. Purse

87. Investigation and review of surrogate parameters to evaluate oxidation of trace organic contaminants during ozonation of wastewater effluents. **R. Tackaert**

88. Mixed quantum and classical simulation of the hydrated electron: Temperature dependence in resonance Raman spectra, excited states relaxation, and whether the electron resides in a cavity. **C. Zhou**

89. Formation and stability of silver nanoparticles formed by the reduction of silver ions by humic acid. **R. Leslie**

90. Oxidative cyclization reactions of benzaldehyde oximes with built-in heteroaromatic nucleophiles. **A.A. Alshreimi**

91. Antimycobacterial ceramides produced by a marine surface bacterium. J.A. Trischman, **G. Allognon**, A. Bulthuis

92. Catalytic anhydride-Mannich reactions of *N*-sulfonyl imines. **S.W. Laws**, M.J. Di Maso, J.T. Shaw

93. Structural study of isotopically modified antifreeze glycoproteins (AFGPs) using high-resolution nuclear magnetic resonance (NMR) spectroscopy. **C. Her**, S. Vazquez, S. Maitra, K.V. Krishnan

94. Development of molecular photoswitches as MRI contrast agents. **A. Faulkner**, E.I. Balmond, B.K. Tautges, B.M. Hodur, J.T. Shaw, A. Louie

95. First semester general chemistry undergraduates' ability to distinguish variables in the experimental design of a stoichiometry activity in structured and guided inquiry modes. **E. Hoong**

96. Fabrication of wafer-scale, low resistance, single carbon nanotube devices. **A. Rajapakse**, P.G. Collins

97. Conformational equilibrium dynamics of β-methyl-amino-L-alanine (BMAA) and its carbamate adducts using NMR spectroscopy. **A. Alonzo**

98. Analysis of mercury concentration in three common cigarette brands sold in the United States as a viable source of human exposure. **S. Freitag**, S. Aloisio

99. A lanthanum(III)-catalyzed multi-component reaction for the synthesis of substituted malonamides with interesting photophysical properties. **J. Jennings**, C.P. Bhatt, A.K. Franz

100. Effect of the overlap between the vertical ionization energies and the adiabatic ionization energies of DNA nucleobases. **H. Kwon**, K.G. Bacani, V. Andrianarijaona

SATURDAY MORNING

California State University, San Marcos
USU 2300C

Analytical Chemistry

K. Ikehata, M. T. Kleinman, *Organizers*
R. D. Lai, *Presiding*

8:30 101. Development of separation and detection method for chemotherapeutic drugs. **K. Ng**

9:00 102. Sensitive detection of nicotine and its metabolites by laser wave-mixing spectroscopy for second- and third-hand smoke studies. **Z. Munshi**, J.S. Pradel, W.G. Tong

9:30 103. Development of an analytical method for quantifying chemical tracers associated with livestock activities. **D. Ricci**, J. Miller-Schulze

10:00 Intermission.

10:30 104. Development of paper- and thread-based microfluidic assays for point-of-care (POC) diagnostic devices. **F.A. Gomez**, L. Estala, M. Arrastia, A. Avoundjian, A. Gonzalez, C. Gallibu, C. Gallibu

11:00 105. Sensor for the detection of petroleum analytes in air and aqueous environments. **S.T. Hobson**

11:30 106. Applications of nuclear magnetic resonance spectroscopy in nanomaterials characterization. **C. Guo**, J.L. Yarger

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SBSB 1105

Biochemical Technology

K. Ikehata, M. T. Kleinman, *Organizers*
K. M. Hamadani, *Presiding*

8:30 107. Purification and characterization of the *Drosophila melanogaster* (Dm) IκKβ/IκKγ complex. **W. Rogers**, T. McDowell, T. Huxford

9:00 108. Structural study of prolonged NF-κB responses regulated by IκBβ. **T.T. Nguyen**, T. Huxford

9:30 109. Biophysical characterization of reflectin isoforms from squid and cuttlefish. **L. Phan**, W.G. Walkup, D.D. Ordinario, Y. van Dyke, A.A. Gorodetsky

10:00 Intermission.

10:30 110. An *in-vitro* sample generation strategy for single-molecule spectroscopy. **K.M. Hamadani**, S. Marqusee, P. Wu, J. Cate

11:00 111. Using QM/MM to guide the engineering of an artificial haloperoxidase. **G. Anderson**, R. Gomatam, R.N. Behera

11:30 112. Design of self-assembling RNA nanotriangles from crystal structures. **M.A. Boerneke**, S. Dibrov, T. Hermann

California State University, San Marcos
USU 2300D

Chemical Education

Laboratory Approaches

K. Ikehata, M. T. Kleinman, *Organizers*
R. L. Deming, *Presiding*

8:30 113. A simple experiment to introduce nanophytotoxicity to first-year undergraduate students. S. Ross, M. Owen, B. Pedersen, G. Liu, **W.J. Miller**

9:00 114. Microwave-assisted esterification: A discovery-based microscale laboratory experiment. M. Reilly, R.P. King, A.J. Wagner, **S.M. King**

9:30 115. Optimizing the learning experience in the general chemistry laboratory. **S. Abbas**

10:00 Intermission.

10:30 116. Trying to elucidate the spectroscopic and electrochemical properties of substituted anthraquinones using undergraduate research students using a joint experimental and computational chemistry approach. **M.M. Allard**

11:00 117. Qualitative analysis in the general chemistry II laboratory: How much is too much? **S. Abbas**

11:30 118. Electronic lab notebooks in the organic chemistry laboratory: Optimization of hardware and software parameters. **K. Albizati**

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SBSB 1107

Colloids and Surface Chemistry

K. Ikehata, M. T. Kleinman, *Organizers*
B. Chou, *Presiding*

8:30 119. Proton conduction in a cephalopod structural protein. **D.D. Ordinario**, L. Phan, E. Karshalev, J. Jocson, A.A. Gorodetsky

9:00 120. Protein-based protonic transistors. **D.D. Ordinario**, L. Phan, J. Jocson, T.N. Nguyen, A.A. Gorodetsky

9:30 121. Polymer hydrogel nanoparticles used as artificial heat shock proteins for immunoglobulin G. **B. Chou**, R. Dalal, K.J. Shea

10:00 Intermission.

10:30 122. Box effects in nonliving and living polymerization of slow or nondiffusing monomers confined to a 2D surface. **A. Benedicto**

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Environmental Chemistry

Ecology, Analysis, and Wastewater

K. Ikehata, *Organizer, Presiding*
G. Rajagopalan, *Presiding*

8:30 123. Possible factors in seagrass decline. **E.L. Johnson**, S. Wyllie-Echeverria, R.A. Lyons

9:00 124. Co-digestion of high strength wastes: Need for a holistic approach. **G. Rajagopalan**

9:30 125. Radiocarbon dating of wastewater: Effect on fossil carbon emission quantification. **L.Y. Tseng**, A.K. Robinson, X. Xu, J. Southon, D. Rosso

10:00 Intermission.

10:30 126. A novel isolation and separation scheme for the characterization of dissolved organic matter in landfill leachate. **B. Cottrell**, M. Pinto, S. Bolyard, D.P. Soulsby, W.J. Cooper, D. Reinhart

11:00 127. Detecting neonicotinoid pesticides with QCM detectors in a gas chromatograph. **W.K. Tolley**

11:30 128. Enzymatic treatment of dye wastewater using fungal laccases and peroxidases: An overview. **K. Ikehata**

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SBSB 1109

Medicinal Chemistry

K. Ikehata, M. T. Kleinman, *Organizers*
D. Van Vranken, *Presiding*

8:30 129. Discovery of potent and kinase-selective p21-activated kinase 1 (PAK1) inhibitors. **W. Lee**

9:00 130. Potent synergy between small molecules and fluconazole against *Candida albicans*. **D. Van Vranken**, H. Liu, U. Ilandari Dewage, F. Wang, K.A. Scott, C. Shen, S. Lane

9:30 131. Wnt mimetics as anti-cancer drugs: Design and synthesis of drugs that reduce β-catenin and attenuate cell proliferation. **A. Jelowicki**

10:00 Intermission.

10:30 132. X-ray crystallographic structure of oligomers formed by a toxic β-hairpin derived from α-synuclein: Trimers and higher-order oligomers. **P. Salveson**

11:00 133. X-ray crystallographic structures of amyloid oligomers: A toxic crosslinked trimer of β-hairpins derived from $A\beta_{17-36}$. **A. Kreutzer**, R.K. Spencer, S. Yoo, J.S. Nowick

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SBSB 1103

Organic Chemistry

Metal Catalysis

K. Ikehata, M. T. Kleinman, *Organizers*
S. Dey, *Presiding*

8:30 134. Mechanistic insights into photo-induced, copper-catalyzed alkylations of amines. **J. Ahn**, K. Hannoun, T. Ratani, S. Creutz, J.C. Peters, G.C. Fu

9:00 135. Methodology and mechanistic studies of catalytic asymmetric annulations to form silyl-spirooxindoles. **B. Armstrong**, B. Shupe, A.K. Franz

9:30 136. Counterion effects in the catalytic stereoselective synthesis of 2,3'-pyrrolidinyl spirooxindoles. **J.P. MacDonald**, B.H. Shupe, J. Schreiber, A.K. Franz

10:00 Intermission.

10:30 137. Condensation versus hydroamination for the one-step synthesis of α-tetrasubstituted amines. **C.H. Larsen**, C. Pierce, M. Nguyen, Z.L. Palchak, H. Yoo, D. Lussier

11:00 138. Nickel-catalyzed cross-electrophile coupling reactions of primary and secondary benzylic esters with aryl halides. **M. Konev**

11:30 139. Thermal- and metal-mediated cycloaromatization reactions of conjugated tri-π systems. **K.M. Veccharelli**, J.M. O Connor

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SBSB 2109

Organometallic Chemistry

K. Ikehata, *Organizer*
M. T. Kleinman, *Organizer, Presiding*

8:30 140. Isolation of bis(copper) key intermediates in Cu-catalyzed azide-alkyne "click reaction". **D. Tolentino**, L. Jin, M. Melaimi, G. Bertrand

9:00 141. Highly encumbered group VI transition metal catalysts capable of exploiting minor polarization of alkynes to give high regioselectivity in hydrostannation. **K. Mandla**

9:30 142. Synthesis of a functionalized metal-ligand supramolecular complex for incorporation into polymers. **S.G. Martin**, K. Teppang, S. Journey, S. Moss, B.W. Purse

10:00 Intermission.

10:30 143. Organoferrous compounds as antitumor agents. **C. Hoong**

11:00 144. Insight into the mechanism and reactivity of ruthenium ROMP catalysts at the single-molecule and single-particle level. **Q. Easter**

11:30 145. Characterization of metal-ligand interactions in artificial metalloproteins using electron paramagnetic resonance spectroscopy. **M. Flores**, T.L. Olson, D. Wang, S. Edwardraja, S. Shinde, J.C. Williams, G. Ghirlanda, J. Allen

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SBSB 2111

Physical Chemistry

K. Ikehata, M. T. Kleinman, *Organizers*
P. W. Langhoff, *Presiding*

8:30 146. Quantum-mechanical definition of atoms and bonds in molecules. **P.W. Langhoff**, J.D. Mills, J. Boatz

9:00 147. Range-separated hybrids with correct scaling to the high-density limit. **B. Krull**, F. Furche, J. Yu

9:30 148. Cubic scaling random phase approximation for molecular systems. **G. Chen**

10:00 Intermission.

10:30 149. Reexamining the hydrated electron's first excited state lifetime through temperature-dependent femtosecond transient absorption. **E. Farr**

11:00 150. Visualization of electron-photon-plasmon coupling in single azulene molecules with the STM. **A. Yu**, S. Li, W. Ho

11:30 151. Probing intermolecular coupled vibration by STM inelastic electron tunneling spectroscopy. **Z. Han**, C. Xu, C. Chiang, G. Czap, D. Yuan, R. Wu, W. Ho

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SBSB 2140

Polymer Nanomaterials

K. Ikehata, M. T. Kleinman, *Organizers*
S. Zhang, *Presiding*

8:30 152. Synthesis of polybenzoquinolines as graphene nanoribbon precursors. **D.J. Dibble**, Y. Park, M. Umerani, A. Mazaheripour, A.A. Gorodetsky

9:00 153. Assembly of graphene oxide. **S. Zhang**

9:30 154. Aza-Diels–Alder route to polyquinolines. **D.J. Dibble**, M. Umerani, A. Mazaheripour, Y. Park, A.A. Gorodetsky

10:00 Intermission.

10:30 155. Molecular mechanisms of biomolecule binding at nanostructured interfaces. H. Swanson, C. Guo, S.K. Davidowski, **G.P. Holland**

11:00 156. Molecular dynamics simulations of stacked DNA base surrogates. C.B. Markegard, **A. Mazaheripour**, J. Jocson, A.G. Wardrip, A.M. Burke, M. Dickson, A.A. Gorodetsky, H. Nguyen

11:30 157. Infrared invisibility stickers inspired by cephalopods. **L. Phan**, D.D. Ordinario, E. Karshalev, W.G. Walkup, M.A. Shenk, A.A. Gorodetsky

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The Many Faces of CHAL

S. P. Thompson, *Organizer, Presiding*

8:30 158. Intellectual property considerations for small and mid-size chemical businesses. **S.P. Thompson**

9:00 159. Pay for delay settlements in pharmaceutical cases. **G.M. Halpenny**

9:30 160. Processing invention disclosures at a university technology transfer office. **R.C. Smith**

10:00 Intermission.

10:30 161. Review of recent federal circuit decisions relevant to what scientists need to know about patent filing and prosecution. **S.P. Thompson**

California State University, San Marcos
SBSB 1102

Theory and Experiment Working Together: From Synthetic Chemistry to Drug Design: Symposium in Honor of Kendall Houk

D. J. Tantillo, *Organizer, Presiding*

8:30 162. Hidden in plain site: Discovery of a widespread, yet highly sought-after enzyme function. **J.B. Siegel**

9:00 163. Catalytic enantioselective dihalogenation for the synthesis of polyhalogenated natural products. **N.Z. Burns**

9:30 164. Diverse origins of isotope effects revealed by experiment and theory. **D.J. O'Leary**

10:00 Intermission.

10:15 165. Origin of the selectivity difference between pyridine *N*-oxide and pyridine substrates for Rh(III)-catalyzed C-H functionalization. **S.R. Neufeldt**, G. Jimenez-Oses, J.R. Huckins, O.R. Thiel, K.N. Houk

10:45 166. Phosphines and phosphinocatalysis. **O. Kwon**

11:15 167. Automated reaction analysis and the power of data-rich reaction progress measurements. **J. Hein**

SATURDAY AFTERNOON

California State University, San Marcos
SBSB 1102

Theory and Experiment Working Together: From Synthetic Chemistry to Drug Design: Symposium in Honor of Kendall Houk

D. J. Tantillo, *Organizer, Presiding*

1:15 168. Interplay of theory and experiment in (I) the design of GK-GKRP inhibitors and (II) the origins of rate acceleration in heteroaryl-substituted S_NAr substrates. **M.D. Bartberger**

1:45 169. The interplay of experiment and computation in rearrangement reactions relevant to alkaloid synthesis. **C.D. Vanderwal**

2:15 170. Mediated electron transfer: An electrochemical approach. **R.D. Little**

2:45 Intermission.

3:00 171. Do aza-*ortho*-quinone-methide mediated transformations involve aza-*ortho*-quinone-methides? D.M. Walden, R.C. Johnston, A. Jaworski, M.T. Hovey, M.P. Meyer, K. Scheidt, **P. Cheong**

3:30 172. Adventures in aldehyde C-H bond activation. **V.M. Dong**

4:00 173. Computational studies of cation-π interactions and applications to neuroscience. **D.A. Dougherty**

4:30 174. My career in chemistry with Woodward, cycloadditions, and the interplay of computation and experiment. **K.N. Houk**

California State University, San Marcos
SBSB 1105

Biochemical Technology

K. Ikehata, M. T. Kleinman, *Organizers*
K. M. Hamadani, *Presiding*

1:30 175. Mechanical analysis of three coaxial electrospun synthetic biopolymers. **R. Anderson**

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Chemical Education

Classroom Innovations

K. Ikehata, M. T. Kleinman, *Organizers*
R. L. Deming, *Presiding*

1:30 176. College students' understandings of phase transitions: Semantic, experiential, and energy-related difficulties. **P.G. Jasien**

2:00 177. Three questions: What have students absorbed from lecture? **J.A. Parr**

2:30 178. Interdisciplinary and collaborative methods in chemical education. **L.H.G. Solomon**, D.L. Garin, M. McBane

3:00 Intermission.

3:30 179. Nine years and counting: S-STEM scholarships as a tool for success at CSUSB. **K.R. Cousins**

4:00 180. Contextualized chemistry: Bringing career relevance to your classroom. **J. Clarke**

4:30 181. Using technology to reach out to new generation for a fully online chemistry course. **K. Ng**

California State University, San Marcos
USU 2300C

Crystallography for the Next Generation

K. A. Kantardjieff, *Organizer*
B. Rupp, *Presiding*

1:30 182. Protein crystallography facilities at the Stanford Synchrotron Radiation Laboratory. **S. Russi**

2:00 183. X-ray crystallography and HIV-1 vaccine design. **R. Stanfield**

2:30 184. Protein molecular modeling for chemical biology. **A. Orry**

3:00 Intermission.

3:30 185. Elucidating chemical structure at beamline 11.3.1 at the advanced light source. **K.J. Gagnon**, G.Y. Morrison, J.R. Nasiatka, S.J. Teat

4:00 186. Targeted crystal growth of rare earth intermetallics with synergistic magnetic and electrical properties. **J. Chan**

4:30 Panel Discussion.

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SCI2 242

Environmental Chemistry

Advanced Oxidation

K. Ikehata, *Organizer, Presiding*
G. Rajagopalan, *Presiding*

1:30 187. Advanced oxidation applied to water reuse and drought mitigation. **D. Hokanson**

2:00 188. Chloramine reactivity in wastewater: Kinetics and mechanisms of chlorinated byproduct formation. J. Gleason, J. Castillo, **S.P. Mezyk**

2:30 189. Sulfate radical remediation of pharmaceutical contaminated wastewaters: Impact of dissolved organic matter. **T. Reutershan**, S. Mezyk

3:00 Intermission.

3:30 190. Investigating the impact of solution chemistry on advanced oxidative processes in reverse osmosis permeate treatment. **W. Li**, S.D. Patton, H. Liu

4:00 191. Treatment of groundwater contaminated with volatile and semi-volatile organics using ozone- and UV-based advanced oxidation processes. **L. Qu**, **Y. Li**, L. Wang, K. Ikehata

4:30 192. Chlorine radical and chloramine reactivity with wastewater constituent species in support of advanced oxidation processes. **K.D. Couch**, S.P. Mezyk

California State University, San Marcos
SBSB 2109

Inorganic Chemistry

K. Ikehata, M. T. Kleinman, *Organizers*
C. H. Larsen, *Presiding*

1:30 193. A one-step ligand synthesis and the systematic study of gold(III) complexes of substituted 2-(2'-pyridyl)quinolines. **M.D. Sterling**, L.E. Bishop, A.L. Rheingold, C.H. Larsen

2:00 194. Isolable variants of an iron nitridocarbonyl cluster $[Fe_4N(CO)_{12}]^n$ in two states of charge (n = 0, -1). **M.J. Drance**, J.S. Figueroa

2:30 195. $Co(CNAr^{Mes2})_4$, an isolobal analogue of $Co(CO)_4$, and its reactivity. **C. Chan**, J.S. Figueroa

3:00 Intermission.

3:30 196. A room temperature stable singlet phosphinidene. **D.A. Ruiz**, L. Liu, G. Bertrand

California State University, San Marcos
SBSB 1109

Medicinal Chemistry

K. Ikehata, M. T. Kleinman, *Organizers*
J. Gustafson, *Presiding*

1:30 197. Novel α-helix mimetics for inhibition of protein-protein interactions associated with human papillomavirus. **A. Orchard**

2:00 198. Docking studies illuminate a likely binding mode of noncanonical opioid peptides. **M.J. Ferracane**, J.V. Aldrich

2:30 199. Exploiting atropsiomerism to increase the target selectivity of promiscuous inhibitors. **J. Gustafson**

3:00 Intermission.

3:30 200. Potential early diagnosis of multiple sclerosis based on sensitive analysis of biomarkers using nonlinear laser methods. **A. Jackson**, W.G. Tong

4:00 201. Sensitive detection of colorectal cancer biomarker carcinoembryonic antigen by laser wave-mixing spectroscopy and capillary electrophoresis. **J.S. Pradel**, W.G. Tong

4:30 202. Nickel catalyzed stereospecific cross coupling: Novel approaches to optically enriched triarylmethanes. **L. Hanna**

California State University, San Marcos
SBSB 1103

Organic Chemistry

Polymers and Novel Materials

K. Ikehata, M. T. Kleinman, *Organizers*
T. Palazzo, *Presiding*

1:30 203. Disiloxanediols as anion-binding and hydrogen-bonding catalysts. **K. Diemoz**, S. Wilson, A.K. Franz

2:00 204. Metal-free cationic polymerization of styrene utilizing a boron-rich cluster photo-catalyst. **P. Chong**

2:30 205. Withdrawn.

3:00 Intermission.

3:30 206. Synthesis and electrochemical characterization of oligonucleotide-inspired organic nanowires. **A. Mazaheripour**, A.G. Wardrip, J. Jocson, N. Hüsken, A.M. Burke, A.A. Gorodetsky

4:00 207. Chemical compartmentalization for controlling reactivity in kinetically stable molecular capsules. **B.W. Purse**

4:30 208. Unlocking the genome of halogenated polycyclic aromatic hydrocarbons. **B. Schatschneider**

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SBSB 2111

Physical Chemistry

K. Ikehata, M. T. Kleinman, *Organizers*
S. G. Sayres, *Presiding*

1:30 209. Utilizing tabletop XUV spectroscopy to explore how electronic spin influences the alignment from strong-field multiple ionization. **S.G. Sayres**

2:00 210. Non-adiabatic molecular dynamics with spin-symmetry breaking for describing photochemistry of acetaldehyde. **J. Vincent**

2:30 211. Methods for qNMR: Spin counting in NMR coil volume. **M. Huang**, L. Chi, R.E. Gerald , K.H. Woelk

3:00 Intermission.

3:30 212. Moderated PEF from transitioning between the micro and macroscopic usage of Coulomb's law. **E.G. Zoebisch**

4:00 213. *Ab initio* kinetic model for parallel addition reactions of interesting radicals. **P. Winter**, A. Lopez, A.L. Cooksy

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SBSB 2140

Polymer Nanomaterials

K. Ikehata, M. T. Kleinman, *Organizers*
M. T. Fontana, *Presiding*

1:30 214. X-ray spectroscopic characterization of organic semiconductor nanowires. **A. Mazaheripour**, N. Hüsken, J. Jocson, G. Kladnik, A. Cossaro, L. Floreano, A. Verdini, A.G. Wardrip, A.M. Burke, K. Miller, A.V. Marsukar, I. Kymissis, D. Cvetko, A. Morgante, A.A. Gorodetsky

2:00 215. Structural disorder and organic solar cell performance: A drift-diffusion study. **B.Y. Finck**, B.J. Schwartz

2:30 216. Tuning the degree of intermixing in sequentially-processed polymer/fullerene photovoltaics: The role of swelling by solvent additives. **M.T. Fontana**, J.C. Aguirre, S. Hawks, G. Zhang, P. Yee, H. Kang, R. Huber, L. Schellas, Z. Fan, S.H. Tolbert, B.J. Schwartz

3:00 Intermission.

3:30 217. Tracking transplanted cells with paramagnetic fluorinated nanoemulsions. **A.A. Kislukhin**

4:00 218. Evaluation of the cellular biocompatibility of collagen- and synthetic polymer-coated gold nanoparticles. **O.T. Truica**, J. Rejman, N. Leopold

California State University, San Marcos
SBSB 1107

Process Organic Chemistry

K. Ikehata, M. T. Kleinman, *Organizers*
A. Evans, *Presiding*

1:30 219. Prebiotic flow synthesis of bioactive nucleoside precursors. **A. Evans**, J. Kading, J. Feng

2:00 220. Towards a continuous flow synthesis of levomilnacipran. **C. Ayoub**, M. Nguyen, A.C. Evans

2:30 221. Flow chemistry enabling safer and novel chemistry. **H. Graehl**, L. Kocsis, R.V. Jones

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Recent Advances in Base Metal Catalysis

E. Tollefson, *Organizer, Presiding*

1:30 222. Cyclopropane synthesis via stereospecific intramolecular reductive cross-electrophile couplings. **E. Tollefson**, L. Erickson, E.R. Jarvo

2:00 223. Still paying for Pd in your Pd-catalyzed reactions? Why? Use Fe nanoparticles containing naturally occurring ppm Pd, and get it for free! S. Handa, Y. Wang, F. Gallou, B.H. Lipshutz, **E.B. Landstrom**

2:30 224. Nickel-catalyzed activation of amides and simple esters. **L. Hie**, N.K. Garg, N.F. Fine Nathel, T. Shah, E. Baker, X. Hong, Y. Yang, P. Liu, K.N. Houk

3:00 Intermission.

3:30 225. Nickel-catalyzed asymmetric reductive cross-coupling between heteroaryl iodides and α-chloronitriles. **N.T. Kadunce**

4:00 Panel Discussion.

California State University, San Marcos
SBSB 1105

Energy and Fuel Chemistry

K. Ikehata, M. T. Kleinman, *Organizers*
S. P. Thompson, *Presiding*

2:00 226. Review of biofuels and biofuels-related technology patents and patent applications. **S.P. Thompson**

2:30 227. Mesoporous MoS_2 as a transition metal dichalcogenide exhibiting pseudocapacitive Li and Na-ion charge storage. **J.B. Cook**, H. Kim, Y. Yan, J. Ko, B. Dunn, S.H. Tolbert

3:00 Intermission.

3:30 228. Photochemical charge transfer observed in nanoscale hydrogen evolving photocatalysts using surface photovoltage spectroscopy. **J. Wang**

4:00 229. Numerical and experimental study of a reactive flow with a perovskite catalyst. **J. Arbelaez**, C. Nieto, W. Silva

California State University, San Marcos
USU 2300A&B

WRM Poster Session

K. Ikehata, M. T. Kleinman, *Organizers*

2:00 - 5:00

230. Effectiveness of socially-mediated and online learning tools in general chemistry. **K.A. Kaiser**

231. Development of specific, irreversible inhibitors for a receptor tyrosine kinase EphB3. **A. Kung**, C. Zhang

232. DFT calculations relating hydricities, pK_a, and redox potentials in coordination and organometallic iridium(III) complexes. **R. Adams**, A. Lopez, S. Bellows, T. Cundari

233. Alkylation of amino acids by anticancer drug, chlorambucil. **T. Wang**, **B. Brook**

234. A historical perspective of the STS (science-technology-society) movement and an application of STS teaching approach in the community college chemistry classroom. **G. Perkins**

235. Synthesis of alkanethiolate-capped platinum nanoparticle catalysts with enhanced activity using alkylthiosulfate ligand precursor. **K. San**, Y. Shon

236. C-H amination of tetrahydroisoquinoline. **K. Bay**, S. Han, B.M. Stoltz

237. Plant growth and soil chemistry: Standard solution models and measurement errors. P. Johnson, **L. Huang**

238. The effects of high leverage on the optimum product yield of oxazoline. P. Johnson, **L. Huang**

239. Get involved with the ACS Division of Chemical Education. **J.L. Sarquis**

240. Characterizing the Rubisco / Rubisco activase interaction via assembly studies. **A.J. Serban**

241. Novel peptidomimetic inhibitors for the West Nile virus NS2B-NS3 protease. **J. Truong**, B. Espinosa

242. Thin film crystallization. **K. Ulle**

243. Activity and selectivity of Pd nanoparticle catalysts for alkyne hydrogenation in water: Effects of graphene oxide supports and thiolate surface ligands. **V. Chen**, Y. Shon

244. TNA protects DNA and RNA from nuclease digestion under simulated physiological conditions. **M. Culbertson**, K.W. Temburnikar, S. Sau, J. Liao, S. Bala, J.C. Chaput

245. Antioxidant activity, total phenolics and total flavonoids content study of *Yucca whipplei* blossoms. C. Bwiza, M. Quach, A. Hidalgo, T. Yoon, D. Paez, J. Kalimba, J. Luong, D. McCarthy, M. Barth, **Y. Hu**

246. Dye-sensitized solar cell based on the natural dye extract from elderberry leaves. J. Kalimba, J. Luong, **Y. Hu**

247. Effects of steric hindrance near the metal surface of unsupported palladium nanoparticle catalysts for alkene isomerization. **P. Tieu**, Y. Shon

248. Elucidating molecular pathways of prostate field cancerization: Potential role of EGR-1 as a master regulator. **K. Gabriel**, M. Bisoffi

249. Computational study of butyrylcholinesterase inhibition by dialkyl phenyl phosphate derivatives. **S.G. McCoy**, W. Alvarado, A. Garcia, E.J. Sorin

250. Computational study of the addition of ammonia, methylamine, and dimethylamine to acetaldehyde catalyzed by a single water molecule: Energetics for carbinolamine formation. **J.E. Perez**, M.K. Louie, A. Sinha

251. β-hairpins: Molecular accessories for helical peptide expression. **M.E. Lokensgard**, J.J. Love

252. Sensitive detection of proteins and cancer markers by nonlinear laser wave-mixing detection and capillary electrophoresis. **M. Brown**, J.S. Pradel, S. Ramos, W.G. Tong

253. Triplet state dynamics in the visible light absorbing zinc chlorodipyrrin. **W. Thornbury**, S. Das, A. Bartynski, M.E. Thompson, S.E. Bradforth

254. A synthetic siderophore as a molecular shuttle. **A.A. Avanes**, J. Saboury, A. Davidian, C. Bezjian, B. Ulloa, M. Pinto, C.G. Gutierrez

255. Crystallization processes modeled by Monte-Carlo simulation of two-dimensional surface diffusion. **M. Salem**, M. Schmidt

256. A poster session demonstrating graduate student teaching assistants' competence in the design and implementation of a student-centered lesson plan. **M.A. Boerneke**, H. Dembinski, S. Brydges

257. Relationship between speech and gesture to support molecular-level explanations of macroscopic phenomena in the context of acid-base titration. **A. Lien**, B.L. Gonzalez

258. Synthesis of homochiral metal-organic frameworks using tetradentate ligands. **E. Nguyen**, X. Zhao, X. Bu

259. Photoelectrochemical characterization CuGaSe hotocathodes. **B. Bachman**, T.G. Deutsch, J. Young

260. Spectroelectrochemical characterization and solvent effect on the tautomerism of free-base corrole. **F. Kohl**, G.N. Calvillo, S. Klein, A. Loogman, S. Becerra, E.A. Aleman

261. Visualization of organic molecules: An analysis of students' visual-spatial ability at a large primarily undergraduate institution. **A. Garcia**, L. Perez

262. Novel synthesis of modified nucleic acids and nucleoside analogs for solid phase synthesis of ribonucleic guanidine (RNG). **A. Chavez**

263. Systematic structure modifications of imidazo[1,2-a]pyrimidines to reduce and predict aldehyde oxidase-mediated metabolism. **M.A. Ornelas**

264. Synthesis and investigation of soluble PyQuin gold(III) complexes. **E. Roman**, M.D. Sterling, C.H. Larsen

265. Real-time reaction kinetics by quantitative nuclear magnetic resonance spectroscopy. **J. Singh**, C. Her, K.V. Krishnan

266. Revolutionary view on third-hand smoke by NMR spectroscopy: A chemometric approach. **J. Vang**, K.V. Krishnan, A. Hasson

267. Thermodynamic and electrochemical studies of a $[Ni(bisphosphine)_2]^{2+}$ complex in water and organic solvents. **B.M. Ceballos**, J.Y. Yang, C. Tsay

268. Fragmentation studies of flubendiamide under various atmospheric conditions. **E. Rangel**

269. Novel biomarkers for HIV-1 disease progression. **T. Taylor**, A. Pandya, K. Borgmann, A. Ghorpade

270. Small molecule activation using transition metal-Si complexes. **A. Bartrom**, H. Harman

271. Carbon dioxide reduction to formate by a multi-functional, redox-active borane. **J. Taylor**, A. McSkimming, H. Harman

272. Automatic classification of surface-bound bacteria cell motion by image analysis and tracking algorithms. **S. Shen**

273. Reactions of a germylene and stannylene with water and methanol: Evidence of sigma-bond metathesis in the formation of {Sn(μ-OR)}2. **J. Erickson**