

## Draft Final Program

### INOR

#### DIVISION OF INORGANIC CHEMISTRY

S. Koch and N. Radu, *Program Chairs*

#### SUNDAY MORNING

Section B

#### Frontiers in C-H Activation and Functionalization

T. Gunnoe, *Organizer*

S. Golisz, *Organizer, Presiding*

#### 8:30 Introductory Remarks.

**8:40 1.** Cp\*Ir complexes in catalytic alkane hydroxylation. **R. Crabtree**, O. Eisenstein, D. Balcells, M. Zhou, N. Schley

**9:10 2.** Emergence of predictable selectivity for aliphatic C—H oxidations. **M. C. White**

**9:40 3.** Overcoming the oxidant problem: Implementing strategies for aerobic oxidation of C-H bonds. **S. S. Stahl**

**10:10** Intermission.

**10:25 4.** Mechanistic aspects of homogeneously-catalyzed hydrocarbon oxidation with platinum and palladium complexes. **J. E. Bercaw**

**10:55 5.** Functionalization of M<sup>II</sup>-C(sp<sup>2</sup>, sp<sup>3</sup>) bonds under environmentally benign conditions (M = Pd, Pt). **A. N. Vedernikov**, W. N. Oloo, D. Wang

**11:25 6.** Oxidative dehydrosulfurization and selective bond activation by "roll-over" cyclometalated Pt<sup>II</sup> complexes: Theory and experiment in concert. **H. Schwarz**, B. Butschke

Section C

#### Materials Chemistry for Solar Energy Capture

J. Papanikolas, J. Pietryga, *Organizers*

R. Lopez, *Presiding*

#### 8:30 Introductory Remarks.

**8:40 7.** Design of supramolecular complexes for solar energy capture and utilization via hydrogen production from water. T. A. White, J. Knoll, J. Wang, K. Quinn, R. Zhou, R. Shaw, S. M. Arachchige, **K. J. Brewer**

**9:20 8.** Development of molecular electrocatalysts for hydrogen production and carbon dioxide reduction. **D. DuBois**

**10:00 9.** Oxidizing water and reducing CO<sub>2</sub>. **T. J. Meyer**

**10:40** Intermission.

**11:00 10.** Progress and problems in visible light water splitting. Y. Zhao, E. A. Hernandez-Pagan, N. M. Vargas-Barbosa, S. Lee, W. Youngblood, E. S. Smotkin, **T. E. Mallouk**, A. L. Moore, T. A. Moore, D. Gust

**11:40 11.** Electrochemical proton-coupled electron transfer. **S. Hammes-Schiffer**

Section E

#### Chemistry of Materials

C. Lugmair, *Organizer*

J. Schneider, *Presiding*

**8:30 12.** Gadolinium doped europium sulfide nanostructures. **W. L. Boncher**, S. L. Stoll

**8:50 13.** Survival stories of catalytic nanoscale gold: Clusters in gas phase, protected by ligands and supported by oxides. **H. Häkkinen**

**9:10 14.** Electrochemical reduction of MnO<sub>2</sub> nanowires to produce hierarchical nanomaterials with superior supercapacitor properties. **J. W. Duay**, S. Sherrill, Z. Gui, J. Hu, S. Lee

**9:30 15.** Chemical synthesis of Au-based L<sub>12</sub>-type intermetallic nanoparticles. **J. F. Bondi**, R. E. Schaak

**9:50 16.** Nanoplates vs. microspheres: Synthesis and surface chemistry of Bi<sub>2</sub>WO<sub>6</sub> crystals for improved photocatalytic activity. **A. K. Mann**, S. E. Skrabalak

**10:10 17.** Synthesis of oxide nanobowls for size- and shape-selective photooxidation. **C. P. Canlas**, N. Ray, J. Lu, S. Lee, R. Winans, P. Stair, J. Elam, J. M. Notestein

**10:30** Intermission.

**10:40 18.** Synthesis, characterization, electrospinning of novel tin amide alkoxides for lithium-ion battery application. **T. Q. Doan**, T. J. Boyle, L. M. Otley, S. M. Hoppe, T. M. Alam

**11:00 19.** Heterometallic beta-diketonates: Volatile precursors for the synthesis of materials. **E. V. Dikarev**

**11:20 20.** Metal-organic frameworks as materials for capturing carbon dioxide from flue gas. **T. M. McDonald**, J. R. Long

**11:40 21.** Expedient growth of crystalline metal-organic frameworks thin films. **M. Li**, M. Dincă

**12:00 22.** Synthesis, characterization and functional properties of CNT-hybrid materials. **J. J. Schneider**

Section F

#### Nanoscience

##### General Studies

S. Wong, *Organizer*

A. Greytak, D. Nikles, *Presiding*

**8:30 23.** Simultaneous determination of the adsorption constant and the photoinduced electron transfer rate for a CdS quantum dot-viologen complex with transient absorption spectroscopy. **A. J. Morris-Cohen**, M. T. Frederick, L. C. Cass, E. A. Weiss

**8:50 24.** Fabrication and thermo-mechanical characterization of jute fiber reinforced polypropylene clay based nanocomposite. **K. Dey**, R. Khan

**9:10 25.** Application of nanoporous organosilicates to detection of nitroenergetic compounds and volatile hydrocarbon solvents. **B. J. Melde**, B. J. Johnson, S. A. Trammell

**9:30 26.** Bandgap engineering of InP nanocrystal quantum dots through shell thickness and composition. **A. M. Dennis**, A. Piryatinski, J. A. Hollingsworth

**9:50 27.** Challenging the trade-offs in synthesis and application of core/shell nanocrystal fluorophores. **A. B. Greytak**

**10:20** Intermission.

**10:40 28.** Synthesis of AlMn nanoparticles. L. Zhang, G. B. Thompson, **D. E. Nikles**

**11:10 29.** Green chemistry by nanocatalysis. **V. POLSHETTIWAR**

**11:30 30.** Stepwise construction of high-order colloidal nanoparticle heterostructures. **M. R. Buck**, J. F. Bondi, R. E. Schaak

**11:50 31.** Toward controlling the stoichiometry of Cu<sub>2</sub>ZnSnSe<sub>4</sub> through a solution-based synthesis method. **L. M. Wally**, S. C. Riha, A. L. Prieto

Section A

#### Organometallic Chemistry

##### Applications to Organic Transformations

N. Radu, *Organizer*

R. Froese, *Presiding*

**9:00 32.** Zinc(II) mediated desymmetrization of (multi)salen ligands: Access to versatile reagents. **A. W. Kleij**, J. Benet-Buchholz, E. Martin, M. Martínez-Belmonte, E. Escudero-Adán

**9:20 33.** Oxidation of alcohols by palladium nanoparticles supported on siliceous mesocellular foam. E. Johnston, **O. Verho**, M. Kärkäs, J. Bäckvall

**9:40 34.** Asymmetric catalysis of the polarized Nazarov reaction. **T. Vaidya**, G. F. Manbeck, A. J. Frontier, R. Eisenberg

**10:00 35.** Synthesis, characterization, and reactivity of group 6 W(IV) terminal imido and oxo complexes supported by the monocyclopentadienyl amidinate ligand set. **B. L. Yonke**, P. P. Fontaine, P. Y. Zavalij, L. R. Sita

**10:20** Intermission.

**10:30 36.** Catalytic hydrocarbons bond activation and nitriles [3+2] cyclization with ethyl diazoacetate using a Ag(I) pyridyl-pyrrolide trimer. **J. A. Flores**, K. Pal, B. Pinter, J. Karty, M. Pink, D. J. Mindiola, K. G. Caulton

**10:50 37.** Ruthenium-catalyzed hydrogenation and hydrogenolysis of furan derivatives. **A. Shankaralinge gowda**, F. T. Ladipo

**11:10 38.** Insights into the mechanism of the Pt-catalyzed hydrosilylation of isopropenyl compounds. **S. Putzien**, O. Nuyken, F. E. Kuehn

Section D

#### Lanthanide and Actinide Chemistry

N. Radu, *Organizer*

E. Schelter, *Presiding*

**9:00 39.** Synthesis and reactivity of 1,4-diaza-1,3-butadiene complexes of group 3 metals. **H. Kaneko**, H. Nagae, H. Tsurugi, K. Mashima

**9:20 40.** Mechanistic implications of ion pairing in uranyl-peroxide clusters growth. **P. Miró**, B. Vlaisavljevich, P. C. Burns, L. Gagliardi, C. J. Cramer

**9:40 41.** Actinide separations under acidic conditions. **D. T. Hobbs**, T. C. Shehe

**10:00 42.** High temperature UC<sub>2</sub> phase: A rotational solid. **X. Wen**, R. L. Martin

**10:20 43.** Exploring the chemistry of transuranic elements in ionic liquids. **K. M. Long**, G. S. Goff, W. H. Runde

**10:40 44.** From antiferromagnetic PrCo<sub>2</sub>P<sub>2</sub> to ferromagnetic Pr<sub>0.8</sub>Eu<sub>0.2</sub>Co<sub>2</sub>P<sub>2</sub> via chemical compression. K. Kovnir, W. M. Reiff, A. P. Menushenkov, A. A. Yaroslavtsev, R. V. Chernikov, **M. Shatruk**

**11:00 45.** Simple isolation of a series of non-classical cerium(IV) compounds. **E. J. Schelter**

#### Empowering Tomorrow's Science Super Heroes

Sponsored by PRES, Cosponsored by ANYL, BMGT, CHED, CINP, COMSCI, FUEL, GEOC, HIST, I&EC, INOR, MEDI, PHYS, PROF, and YCC  
**SUNDAY AFTERNOON**

Section B

#### Frontiers in C-H Activation and Functionalization

S. Golisz, T. Gunnoe, *Organizers*

R. Periana, *Presiding*

**1:30 46.** Hydrofluoroarylation of alkyne by Ni catalyst: Reaction mechanism from a DFT approach. **O. Eisenstein**, J. Guihaumé, R. N. Perutz

**2:00 47.** Ground and transition-states of metal-ligand complexes that activate hydrocarbon C-H bonds. **D. H. Ess**

**2:30 48.** Mechanisms for catalytic activation and functionalization of alkanes by metal-oxo sites. **W. A. Goddard**, M. Cheng, L. Liu, R. Nielsen, J. Mueller

**3:00** Intermission.

**3:15 49.** Theoretical insights into the partial oxidation of methane over supported metal clusters. **M. Neurock**, C. Buda, Y. Chin, E. Iglesia

**3:45 50.** Electrochemical and photoelectrochemical hydrocarbon oxidation by metal oxo complexes: Mechanism and interfaces. **T. J. Meyer**  
**4:15 51.** Strategies for catalytic C-H bond activation from biological analogy. **J. T. Groves**

Section A

### **Fifty Years of Inorganic Chemistry: A Celebration of Past, Present, and Future**

#### **Bonding, Spectroscopy, and Magnetism**

R. Eisenberg, *Organizer, Presiding*

**1:30** Introductory Remarks.

**1:40 52.** Inorganic chemistry – the field and the journal: Personal experiences and recent results. **R. H. Holm**

**2:05 53.** Geometric and electronic structure contributions to Cu/O<sub>2</sub> reactivity. **E. I. Solomon**

**2:30 54.** 50 years of inorganic chemistry: From inspirations to innovations. **K. N. Raymond**

**2:55 55.** Foray into Wernerian and non-Wernerian coordination chemistry over the years. **K. R. Dunbar**

**3:20** Intermission.

**3:35 56.** Fifty years of metal oxos. **H. Gray**

**4:00 57.** Dioxygen activation by nickel complexes: Synthesis, structure and reactivity. **C. G. Riordan**

**4:25 58.** Multiple-site proton-coupled electron transfer: Principles and applications to dioxygen production and reduction. **J. M. Mayer, S. M. Barnett, V. W. Manner, J. J. Warren, C. T. Carver, T. A. Tronic, B. D. Matson, R. Hayoun, J. N. Schrauben, K. I. Goldberg**

**4:50 59.** (Reverse) evolution of organometallic chemistry: Roles for fundamental Fe(CO)<sub>3-n</sub>(CN) and Fe(NO)<sub>2</sub> units in biology. **M. Y. Darensbourg**

Section C

#### **Materials Chemistry for Solar Energy Capture**

J. Pietryga, J. Papanikolas, *Organizers*  
Y. Kanai, *Presiding*

**1:30 60.** Modifying interfaces for efficient solar energy conversion. **S. Bent**

**2:10 61.** Multiple exciton generation and collection in a model photovoltaic system. **B. A. Parkinson**

**2:50 62.** n-Butylamine capped CdSe quantum dot sensitized solar cells. **N. Fuke, P. Szymanski, A. Y. Kuposov, V. W. Manner, L. B. Hoch, M. Sykora**

**3:30** Intermission.

**3:50 63.** Exciton dissociation at nanostructured donor-acceptor interfaces. **G. Rumbles, N. Kopidakis,**

A. Ferguson, D. Coffey, J. Holt, J. Blackburn

**4:30 64.** Hybrid photovoltaics based on electrochemical polymerization of PEDOT on patterned, catalyst free nanopillars. G. Mariani, Y. Wang, P. Wong, R. B. Laghumavarapu, R. B. Kaner, **D. L. Huffaker**

**5:10 65.** Gas phase plasma synthesis of group IV nanocrystals and applications in photovoltaics. **U. Kortshagen**

Section D

#### **Young Investigator Symposium**

F. Gabbai, *Organizer, Presiding*

**1:30** Introductory Remarks.

**1:35 66.** Oxygen evolution mediated by a cobalt-based thin-film electrocatalyst. **Y. Surendranath, D. G. Nocera**

**1:55** Introductory Remarks.

**2:00 67.** Tuning the shape of semiconductor nanowires for advanced photovoltaics. **J. Zhu, Y. Cui**

**2:20** Introductory Remarks.

**2:25 68.** Magnetic bistability in mononuclear iron(II) pyrrolide complexes and cyano-bridged chain compounds. **T. D. Harris, D. E. Freedman, W. H. Harman, M. V. Bennett, C. Coulon, H. Fong, A. Chang, J. D. Rinehart, A. Ozarowski, M. T. Sougrati, F. Grandjean, G. J. Long, R. Clerac, C. J. Chang, J. R. Long**

**2:45** Introductory Remarks.

**2:50 69.** Postsynthetic modification of metal-organic frameworks. **K. K. Tanabe, S. M. Cohen**

**3:10** Intermission.

**3:20** Introductory Remarks.

**3:25 70.** Reactivity of ( $\alpha$ -diimine)Pd<sup>+</sup> species with vinyl ethers. **C. Chen, S. Luo, R. Jordan**

**3:45** Introductory Remarks.

**3:50 71.** Unique and unmatched coordination chemistry of boron-rich ligands. **A. M. Spokoiny, C. A. Mirkin**

**4:10** Introductory Remarks.

**4:15 72.** Metal-directed protein self-assembly. **E. N. Salgado, F. Tezcan**

**4:35** Introductory Remarks.

**4:40 73.** Multicomponent supramolecular chemistry: Dynamics, self-assembly, and functionality of multicomponent supramolecular systems. **Y. Zheng, P. J. Stang**

Section E

#### **Inorganic Spectroscopy**

S. Ronco, *Organizer*

T. Jackson, *Presiding*

**1:30 74.** Spectroscopic and computational studies of high-valent manganese centers: Insights into ground and excited state electronic structure. **T. A. Jackson, D. F. Leto, G. Wijeratne, K. Bane**

**1:50 75.** Spectroscopic study of Cu(CN)<sub>2</sub>- nanoclusters doped in different alkali halides in comparison with pure KCu(CN)<sub>2</sub> and NaCu(CN)<sub>2</sub> single crystals. **X. Li, Z. Pan, D. A. Welch, R. D. Pike, H. H. Patterson**

**2:10 76.** Computing the <sup>7</sup>Li NMR spectra of hydrated Li<sup>+</sup> clusters using ab initio and molecular dynamic simulations. **T. M. Alam, S. B. Rempe, D. Hart**

**2:30 77.** NMR diffusion measurements in the recognition of ion pairing. **P. S. Pregosin**

**2:50 78.** Time-resolved imaging and sensing using highly luminescent transition metal complexes. **J. Williams, L. Murphy**

**3:10** Intermission.

**3:20 79.** Raman scattering as a probe into the local symmetry of extended solids. **R. Andrews, P. Woodward**

**3:40 80.** Site-selective probing of the oleic acid chemical bond on a cobalt nanoparticle interface. **M. M. van Schooneveld, T. Schmitt, F. M. de Groot**

**4:00 81.** Effects of strong donor/acceptor electronic mixing in ruthenium(II) poly-pyridyl complexes manifested in their spectroscopic and electrochemical properties and supported by computational methods. **M. M. Allard, J. F. Endicott**

**4:20 82.** Synthesis, characterization, and reactivity of uranium  $\alpha$ -diimine complexes. **S. J. Kraft, P. E. Fanwick, S. C. Bart**

**4:40 83.** Intrinsic dual emission in colloidal Mn<sup>2+</sup>-doped nanocrystals: Synthesis, spectroscopy, and thermometry. **D. R. Gamelin, V. A. Vlaskin, N. Janssen, E. J. McLaurin, R. Beaulac, J. van Rijssel**

Section F

#### **Nanoscience**

##### **Complex Nanostructures**

S. Wong, *Organizer*

A. Harper-Leatherman, E. Menke, *Presiding*

**1:30 84.** 1D nanostructures by endo and exotemplating of polymer fibers. **J. J. Schneider**

**1:50 85.** Effect of oxygen-containing functional groups on specific capacitance of carbon nanotube electrochemical capacitors. **A. I. Aria, M. Guittet, M. Gharib**

**2:10 86.** Colloidal synthesis of narrow bandgap semiconductor nanosheets. **D. D. Vaughn II, R. E. Schaak**

**2:30 87.** Self-limited plasmonic nanowelding. **E. C. Garnett, J. J. Cha, W. Cai, S. T. Connor, F. Mahmood, Y. Cui, M. L. Brongersma, M. D. McGehee**

**2:50 88.** Core-shell nanowire electrodeposition for advanced

photovoltaics. **E. Menke, S. Ghosh, J. Hujdic**

**3:20** Intermission.

**3:40 89.** Progress towards encapsulation of alcohol dehydrogenase in nanostructured aerogel architectures. **A. S. Harper-Leatherman**

**4:10 90.** Aqueous room-temperature synthesis of bulk-immiscible late transition metal alloys. **E. R. Essinger-Hileman, D. DeCicco, J. F. Bondi, R. E. Schaak**

**4:30 91.** Self-assembly of uniform polyhedral silver nanocrystals into densest packings and exotic superlattices. **J. Henzie, P. Yang**

**4:50 92.** Ultrahigh density intercalation of metal atoms in Bi<sub>2</sub>Se<sub>3</sub> nanoribbons. **K. J. Koski, J. J. Cha, C. Wessells, Y. Cui**

**5:10 93.** Surface modification of inorganic molecular sieves for mixed matrix membrane (MMM) fabrication. **M. E. Lydon, C. Jones, S. Nair**

#### **Celebration of the 100th Anniversary of Marie Curie's Nobel Prize in Chemistry**

Sponsored by NUCL, Cosponsored by INOR, PROF, and WCC

##### **Gibbs Medal Centennial**

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##### **Recycling Carbon: Catalyzed Conversion of Non-food Biomass to Fuels and Chemicals**

##### **Symposium in Memory of Dr. Victor Lin**

Sponsored by I&EC, Cosponsored by CATL and INOR

##### **Resource-efficient Chemistry: Energy, Electrochemistry and Environment**

##### **Strengthening Links to Research in Germany**

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##### **Science on the Hollywood Screen**

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**SUNDAY EVENING**

Section A

#### **Materials Chemistry for Solar Energy Capture**

J. Papanikolas, J. Pietryga, *Organizers*

**6:00 - 8:00**

**94.** High surface area columnar metal oxide photoanodes using pulsed laser deposition. **R. Ghosh, M. K. Brennaman, T. J. Meyer, R. Lopez**

**95.** Multiple pathways for electrocatalytic reduction of carbon dioxide by polypyridyl ruthenium complexes. **Z. Chen, T. J. Meyer**

96. Efficient light-harvesting in microscale metal-organic frameworks by energy migration and interfacial electron transfer quenching. **C. A. Kent**, D. Liu, J. M. Papanikolas, T. J. Meyer, W. Lin

97. Development of iridium pincer catalysts for water oxidation. **L. Pranger**, M. Brookhart, J. Templeton

98. Zinc-alloyed iron pyrite nanocrystals for photovoltaics. **D. Molk**, Y. Yang

99. TiO<sub>2</sub> surface anchoring polyfluorene-based ionic transition metal complex polymers as light-harvesting assemblies. **E. Puodziukynaitė**, R. M. Walczak, L. Wang, Y. Sun, R. L. House, K. S. Schanze, J. M. Papanikolas, J. R. Reynolds

100. Germanium nanoparticles for solar energy conversion. **E. Muthuswamy**, S. M. Kauzlarich

101. Electrochemical water oxidation with carbon-grafted molecular catalysts. **K. E. deKrafft**, Z. Xie, C. Wang, X. Su, B. J. Hinds, W. Lin

102. Dye sensitization of n- and p-type gallium phosphide photoelectrodes. **D. Choi**, B. A. Parkison

103. Investigation of the photoelectrochemical properties of BaBiO<sub>3</sub> single crystals. **C. Jiang**, B. A. Parkinson

104. Energy transfer in ruthenium and osmium functionalized coiled-coil peptides. **S. Bettis**, D. Wilger, C. Materese, M. Minakova, G. Papoian, J. M. Papanikolas, M. L. Waters

105. Facile synthesis of 3D photonic crystal fluorinated tin oxide (FTO) electrodes for photovoltaic devices. **Z. Yang**, T. Xu

106. Technologically relevant nanomaterials for thermal energy storage in concentrated solar power plants. **S. Pradhan**, C. J. Curtis, D. Blake, G. Glatzmaier

107. Bi-Sb alloy nanoparticles for efficient thermal energy storage. **J. Wang**, G. Glatzmaier, D. Blake, C. J. Curtis

108. Mixed morphology of tio<sub>2</sub> nanotube and tio<sub>2</sub> nanoparticles for dye sensitized solar cells. **J. CHOI**, S. Park, T. Park

109. Effect of a cobalt-based oxygen evolution catalyst on the stability and the selectivity of photo-oxidation reactions of a WO<sub>3</sub> photoanode. **J. A. Seabold**, K. Choi

110. Cost effective surface treatments to enhance electron transfer in CZTS nanoparticle thin films. **A. Wolfe**, S. Riha, A. Prieto

111. Formation of nanocrystal films for photovoltaic applications. **W. B. Heuer**, A. R. Smith, S. Baril, J. E. Boercker, J. G. Tischler, E. E. Foos, W. Yoon

112. Development of black Ru(II) complexes as chromophores for

photoredox reactions. **R. H. Schmehl**, J. Gu

113. Interfacial photophysical dynamics for ruthenium polypyridine derivatized chromophore-catalyst assembly sensitized TiO<sub>2</sub>. **W. Song**, C. Glasson, J. Concepcion, M. Brennaman, T. J. Meyer

114. Facile synthesis of TiO<sub>2</sub> films for dye sensitized solar cells using atmospheric pressure dielectric barrier discharge jet. **H. Seo**, C. Elliott

115. Free standing metal-oxide semiconductor as dye-sensitized solar cells electrolyte spacer and its electrochemical analysis. **J. Lim**, Y. Jo, H. Pak, M. Kang, Y. Jun

116. Toward more efficient polycrystalline thin film CdTe photovoltaic devices: Spectroscopic analysis for material characterization and photovoltaic device metrology. **D. Kuciauskas**

117. Designed growth of photovoltaic nanowire arrays on patterned substrates. **M. Nath**, S. Patil

118. Solution routes to thin film FeS<sub>2</sub> pyrite for photovoltaics. **H. A. Platt**, P. A. Hersh, A. Miedaner, C. J. Curtis, M. F. van Hest, D. S. Ginley

119. Layer-by-layer assembly of light harvesting arrays for molecular based solar cells. **P. H. Dinolfo**, P. K. Palomaki, A. Krawicz

120. TiO<sub>2</sub> nanotube films via pulsed laser deposition for dye sensitized solar cells. **S. D. Perera**, K. J. Balkus

121. Semiconductor contact effects in high-performance, air-stable, inverted organic solar cells. **E. C. Garnett**, M. L. Brongersma, Y. Cui, M. D. McGehee

122. Solar irradiation energy control of polymer nanocomposites. **J. Kang**, I. A. Marshall, M. N. Torrico, C. R. Taylor, J. Kim, G. Sauti, L. J. Gibbons, C. Park, S. E. Lowther, P. T. Lillehei, R. G. Bryant

Section B

### Organometallic Chemistry Applications to Organic Transformations

N. Radu, *Organizer*

6:00 - 8:00

123. Oxidation of alcohols by palladium nanoparticles supported on siliceous mesocellular foam. **E. Johnston**, O. Verho, M. Kärkäs

124. Characteristics and reactivity of  $\eta^2$  polyaromatic hydrocarbon complexes. **L. Strausberg**, M. Li, W. D. Harman, W. H. Myers

125. Development of a highly active multidentate alkyne metathesis catalyst resisting alkyne polymerization. **K. Jyothish**, W. Zhang

126. Rum, scotch, tequila, and vodka: Green solvents in the Suzuki reaction with a novel, phosphine-free palladium

catalyst. **N. Fisher**, S. Hurst, G. S. Nichol, K. Cluff

Section C

### Lanthanide and Actinide Chemistry

N. Radu, *Organizer*

6:00 - 8:00

127. Slowly tumbling Eu<sup>III</sup> complexes as contrast agents for magnetic resonance imaging. **J. Garcia**, M. J. Allen

128. Quantification of C-H quenching in near-IR luminescent lanthanoid cryptates. **C. Bischof**, J. Wahsner, J. Scholten, S. Trosien, M. Seitz

129. Solution behavior of DOTP analogs and their lanthanide(III) complexes. **R. Sevcik**, **J. Vanek**, **P. Lubal**, Z. Kotkova, P. Hermann, J. Kotek

130. Development of ligand supports for lanthanide-based scintillators. **K. V. Vasudevan**, J. C. Gordon, R. E. Muenchausen, N. A. Smith, B. L. Scott

131. Employing high anisotropy and strong exchange-coupling in f-element single-molecule magnets. **J. D. Rinehart**, K. R. Meihaus, M. Fang, W. J. Evans, S. A. Kozimor, B. M. Bartlett, J. R. Long

132. Controlling itinerant magnetism of RCo<sub>2</sub>P<sub>2</sub> phases (R = rare earth) via iso- and aliovalent substitutions into the rare-earth sublattice. **C. M. Thompson**, K. Kovnir, M. Shatrak

133. Conjugation of DOTA to ester amide dendrimer for increased T<sub>1</sub> and T<sub>2</sub> MRI relaxivity. **H. M. Kieler-Ferguson**, P. J. Klemm, J. M. Fréchet

134. On the existence of erbium hexaboride nanowires. **Z. Gernhart**, R. M. Jacobberger, J. R. Brewer, C. Cheung

Section D

### Inorganic Spectroscopy

S. Ronco, *Organizer*

6:00 - 8:00

135. X-band rapid-scan EPR. **D. G. Mitchell**, M. Tseitlin, R. W. Quine, V. M. Meyer, G. R. Eaton, S. S. Eaton

136. Relaxation times of isotopically-substituted nitroxide radicals in aqueous solution. **J. R. Biller**, S. S. Eaton, G. R. Eaton, G. M. Rosen

137. Quantitative analysis of the "dithiolate folding effect" in Cp<sub>2</sub>M(dithiolene) systems. **D. F. Kavanagh**, D. L. Lichtenberger, N. J. Wiebelhaus, J. H. Enemark

138. Spectroscopic and kinetic investigation of a peroxomanganese(III) complex supported by an aminopyridyl pentadentate ligand and its conversion to a dinuclear manganese(III,IV) complex. **D. F. Leto**, V. W. Day, T. A. Jackson

139. Remarkable luminescence properties of a series of N-heterocyclic

carbene (NHC) complexes. **S. Chitikuri**, A. Powell, A. Cowley, **M. rawashdeh-Omary**

Section E

### Environmental Aspects of Inorganic Chemistry

S. Koch, *Organizer*

6:00 - 8:00

140. Comparative studies of natural adsorbent and synthetic coagulant in wastewater treatment. **M. E. CHUKWUEDO**, E. O. JATTO

141. Phosphate remediation using iron oxyhydroxide in aqueous systems. **A. Apblett**, **T. Reed**

142. Innovative method for heavy metal ions detection using highly luminescent phosphorescent di-platinum (II) octaphosphite complex. **O. El-bjeirami**, M. Chehbouni, N. T. Satumtira, M. A. Omary

Section F

### Chemistry of Materials

C. Lugmair, *Organizer*

6:00 - 8:00

143. Hierarchical assembly sea urchin-like double-shelled titania hollow microspheres. **L. Tan**, G. Wang, M. Yang

144. Crystal structures of Mn and Co dichloride monohydrate and deuteration effect on magnetism. **G. C. DeFotis**, S. Pagola, K. T. Trowell, K. C. Havas, Z. D. Reed, D. G. Chan

145. Magnetism of cobalt dibromide dihydrate and monohydrate. **G. C. DeFotis**, A. S. Hampton, C. L. DeSanto, C. M. Davis

146. Preparation of porous manganese oxide nanomaterials by one-pot synthetic sol-gel method. **M. Davis**, C. Gümeç, C. Kiel, L. Hope-Weeks

147. Functionalized nanostructured materials: In search of novel systems against bone tumors. **S. Gómez-Ruiz**, S. Sánchez-Muñoz, D. Pérez-Quintanilla, S. Morante-Zarcelo, I. Sierra, S. Prashar, R. Paschke, G. N. Kaluderović

148. Solvothermal preparation of nanocrystalline SnS<sub>2</sub> via hot-injection and thermal decomposition methods. **C. L. Exstrom**, S. A. Darveau, T. E. Webber, M. A. Ingersoll, C. Neville, R. J. Soukup, N. J. Ianno, S. Amitabha

149. Optical properties of amine-substituted difluoroboron  $\beta$ -diketonates. **A. D. Chien**, T. Liu, N. D. Nguyen, G. Zhang, C. L. Fraser

150. Facile one-step method for synthesizing colloidal gold nanocrystals. **K. McCann**, Y. Yang

151. Thermal conduction analysis of layered functionally graded materials. **O. A. Olatunji-Ojo**, S. K. Boetcher, T. R. Cundari

- 152.** Reduced low dimensional rare earth compounds. **C. Chen**<sup>1</sup>, & R. Hughbanks<sup>1</sup>
- 153.** Synthesis, structure, and properties of the rare-earth zintl compounds:  $\text{Eu}_{10}\text{Mn}_6\text{Sb}_{13-x}\text{As}_x$ . **N. Kazem**, J. Grebenkemper, C. Uvarov, S. M. Kauzlarich
- 154.** Selective and reversible adsorption of a guest species by a metal-organic framework held together by intermolecular [I-] interactions. **D. Baird**, J. Brandes, P. Fanwick
- 155.** Hydroxyapatite biomineralization through structural DNA templates. **S. Ngoun**, H. Butts, V. Baratham, **A. E. Gerdon**
- 156.** Colloidal synthesis of air stable and highly crystalline germanium nanoparticles. **D. D. Vaughn II**, J. F. Bondi, R. E. Schaak
- 157.** Modifying  $\text{Mg}_2\text{Si}$  for enhanced thermoelectric properties. **O. Janka**, T. Yi, S. M. Kauzlarich
- 158.** Lithium salts with fractal patterns synthesized by template assisted route. **G. Wang**, L. Tan, M. Yang
- 159.** Magnetism and transport properties of Te doped  $\text{Yb}_{14}\text{MnSb}_{11}$ . **T. Yi**, C. Uvarov, P. Klavins, S. Bux, J. Fleurial, F. Makhmudov, M. Abdusalyamova, S. Kauzlarich
- 160.** Nanopopping effect of residual silicas on reversible lithium storage over highly ordered mesoporous  $\text{SnO}_2$  materials. **J. Shon**, H. Kim, S. Kong, S. Hwang, G. Park, C. Pak, J. Kim
- 161.** Spin exchange interactions in  $(\text{C}_2\text{N}_2\text{H}_{10})[\text{Fe}(\text{HPO}_3)\text{F}_3]$  determined by electronic structure calculations. **H. Koo**
- 162.** Development of a large-pore periodic mesoporous tungsten oxide with a face centered cubic structure for carbon capture. **B. A. Kokoszka**, C. Liu, N. K. Finamore, K. Landskron, D. T. Moore
- 163.** Electrical field driven ion sweeping for carbon dioxide capture applications using ionic liquid and solid electrolytes. **C. Liu**, N. K. Finamore, B. Kokoszka, D. T. Moore, K. Landskron
- 164.** Electric field swing adsorption (EFSA) for carbon capture applications. **N. K. Finamore**, C. Liu, B. A. Kokoszka, K. Landskron, D. T. Moore
- 165.** Synthesis and structure of  $(\text{La}_x\text{Ce}_{1-x})_2\text{Pt}_2\text{Ga}_{8+6x}$ ,  $x=1/3$ . **H. Hong**, P. Holton, R. T. Macaluso
- 166.** Investigation of the metal center redox properties in metal organic frameworks. **J. L. Harding**, M. M. Reynolds
- 167.** Study of mechanical and thermo-mechanical properties of epoxy based nanocomposites with different types of clays. **k. P. Bastola**, L. R. Ojha, s. lageshethy, K. D. Ausman
- 168.** Determination of sodium dithionite and quantification of its decomposition products using ion-exchange chromatography. **T. James**, A. Apblett, N. Materer
- MONDAY MORNING** Section A
- Fifty Years of Inorganic Chemistry: A Celebration of Past, Present, and Future**
- Energy, Photochemistry, and Sensing**
- R. Eisenberg, *Organizer*  
A. Balch, *Presiding*
- 8:30** Introductory Remarks.
- 8:40 169.** Following the electrons to solar fuels. **T. J. Meyer**
- 9:05 170.** Reductive side of water splitting and the light driven generation of hydrogen from water: New developments, strategies, and results. **R. Eisenberg**
- 9:30 171.** Luminescent biomolecular and cellular probes derived from cyclometalated iridium(III) polypyridine complexes. **K. K. Lo**
- 9:55 172.** From the WGS to copolymers from cyclic ethers: Chemistry of carbon dioxide. **D. J. Darensbourg**
- 10:20** Intermission.
- 10:35 173.** Characterization of intermediates involved in water oxidation and  $\text{CO}_2$  reduction. **E. Fujita**, J. T. Muckerman, D. E. Polyansky, R. Zong, R. P. Thummel
- 11:00 174.** Versatile metal-ligand chromophoric building blocks: From design to assembly and functions. **V. Yam**
- 11:25 175.** Photochemical upconversion derived from inorganic sensitizers. **F. N. Castellano**
- 11:50 176.** Mastering photosynthesis with inorganic chemistry. **D. G. Nocera** Section B
- Frontiers in C-H Activation and Functionalization**
- S. Golisz, T. Gunnoe, *Organizers*  
J. Groves, *Presiding*
- 8:30 177.** Development of transition metal-mediated reactions relevant to catalysts for selective C-H functionalization. **T. Gunnoe**, J. R. Webb, M. J. Pouy, J. R. Andreatta, T. M. Figg, B. M. Prince, T. R. Cundari, J. T. Groves
- 9:00 178.** Activation of the C-H bond of alkanes by surface metal hydrides: From alkanes metathesis to non oxidative methane coupling. **j. m. basset**, j. m. basset
- 9:30 179.** Dehydrogenation and related reactions of alkanes catalyzed by pincer-iridium complexes. **A. S. Goldman**, K. Krogh-Jespersen, M. Brookhart
- 10:00** Intermission.
- 10:15 180.** Modulating catalyst reactivity with acidic and basic solvents. **R. A. Periana**, B. Hashiguchi, S. Bischof
- 10:45 181.** Single-step liquid fuels via zeolite-supported hybrid Fischer-Tropsch catalysts. C. L. Kibby, K. Jothimurugesan, T. Das, H. Lacheen, **R. Saxton**
- 11:15 182.** Selective, catalytic functionalizations of aryl and alkyl C-H bonds. **J. F. Hartwig** Section C
- Materials Chemistry for Solar Energy Capture**
- J. Pietryga, J. Papanikolas, *Organizers*  
M. Beard, *Presiding*
- 8:30 183.** Mapping the kinetics of charge transfer processes responsible for the photocatalytic activity of semiconductor-Pt catalyst. **P. V. Kamat**, C. Harris
- 9:10 184.** Photocatalytic water oxidation at the GaN (10 $\bar{1}$ 0) – water interface. **J. T. Muckerman**, X. Shen, Y. A. Small, J. Wang, L. Li, P. B. Allen, M. V. Fernandez-Serra, M. S. Hybertsen
- 9:50 185.** Semiconducting materials for photoelectrochemical water-splitting. **J. A. Turner**
- 10:30** Intermission.
- 10:50 186.** High surface area vertically aligned metal oxide nanostructures for dye-sensitized photoanodes by pulsed laser deposition. **R. Lopez**, R. Ghosh, M. K. Brennaman, K. G. Hanson, T. J. Meyer
- 11:30 187.** First principles investigations of condensed phase dynamics and nanostructured materials for solar energy conversion. **Y. Kanai** Section D
- Inorganic Catalysts**
- S. Koch, *Organizer*  
X. Zhao, *Presiding*
- 8:30 188.** Oxygen reduction at a single cobalt center: Electronic tuning and secondary coordination sphere effects. **R. K. McGuire**, D. K. Dogutan, D. G. Nocera
- 8:50 189.** Water oxidation mechanisms of Ru–Hbpp, cis-(bpy)<sub>2</sub>Ru(OH)<sub>2</sub> and Ru(DAMP)(bpy) catalysts. **M. Z. Ertem**, P. Miró, T. K. Todorova, A. Llobet, L. Gagliardi, C. J. Cramer
- 9:10 190.** Water addition reactions in model monomeric Ru 2,2'-bipyridine complexes involving "Covalent Hydration" of bipyridine ligand: Thermodynamic favorability and spectroscopic signatures as a function of metal oxidation and overall spin states. **A. Ozkanlar**, J. L. Cape, J. K. Hurst, A. E. Clark
- 9:30 191.** Adding proton channels to a hydrogen oxidation catalyst. **S. Lense**, Y. Cheng, W. Shaw
- 9:50 192.** Electrochemical reduction of  $\text{CO}_2$  by rhenium catalysts of the type  $\text{Re}(\text{bipy})(\text{CO})_3\text{Cl}$ . **J. M. Smieja**, E. E. Benson, F. Mariskal, C. P. Kubiak
- 10:10** Intermission.
- 10:20 193.** Effects of structural variation in  $[\text{Ni}(\text{P}_2\text{N}_2)_2](\text{BF}_4)_2$  type proton reduction electrocatalysts. **U. J. Kilgore**, M. P. Stewart, M. L. Helm, J. A. Roberts, D. H. Pool, R. M. Bullock, D. L. DuBois
- 10:40 194.** Understanding the importance of the hydrogenase scaffold to catalysis using homogenous mimics. **M. L. Reback**, A. Jain, S. Lense, Y. Cheng, D. DuBois, T. Squier, W. Shaw
- 11:00 195.** Electrochemical oxygen reduction by iron tetraphenylporphyrins bearing pendant proton relays. **C. T. Carver**, J. M. Mayer, B. Matson
- 11:20 196.** Water oxidation by mononuclear ruthenium complexes with TPA-based ligands. **X. Zhao**, J. Ivie, W. Singh, B. Radaram, R. Grudzien, J. Reibenspies, C. Webster Section E
- Chemistry of Materials**
- C. Lugmair, *Organizer*  
B. Leonard, *Presiding*
- 8:30 197.** Synthesis of multimetallic carbide nanomaterials for fuel cell applications. **B. M. Leonard**
- 8:50 198.** Sputtered PtRu catalysts for direct methanol fuel cells. **A. A. Dameron**, T. S. Olson, S. T. Christensen, J. E. Leisch, K. E. Hurst, S. Pylypenko, J. B. Bult, A. R. Corpuz, D. S. Ginley, R. P. O'Hayre, T. Gennett, H. N. Dinh
- 9:10 199.** Nontoxic chemical route to  $\text{Cu}_2\text{ZnSn}(\text{S}, \text{Se})_4$  thin film solar cells using molecular precursors. **W. Ki**, H. W. Hillhouse
- 9:30 200.** Q-CdSe sensitized  $\text{TiO}_2$  inverse opals and disordered films for amplifying solar energy conversion by slow light effects. S. Bayram, M. El Makkaoui, **L. Halaoui**
- 9:50 201.** Rapid one-step method to synthesize  $\text{TiO}_2$  nanoparticle clusters for dye sensitized solar cells. **H. Seo**, D. J. Pulsipher, E. R. Fisher, C. Elliott
- 10:10 202.** Electrochromic performances of NiO enhanced by ozone: A fundamental understanding of the coloration mechanism. **F. LiN**, G. Chen, D. T. Gillaspie, A. C. Dillon, R. M. Richards
- 10:30 203.** Towards molecular magnetic tunnel junctions: A platform for molecular spintronics. **P. Truitt**, J. Tee, N. Abdullah, M. Chisholm, E. Johnston-Halperin
- 10:50** Intermission.
- 11:00 204.** In situ doping of magnesium nanoparticles to improve hydrogen

storage kinetics. **N. Forseth**, T. Arthur, N. Norberg, A. Prieto

**11:20 205.** Phase purity and solid solubility limit of manganese in AgInSe<sub>2</sub> chalcopyrites. **J. D. Lucas**, B. Karuppannan, J. Yao, J. A. Aitken

**11:40 206.** Electrodeposition of Cu<sub>2</sub>Sb onto high surface area foams. **R. Bayer**, J. Mosby, A. Prieto

**12:00 207.** Solid state metathesis route to fine crystallites of Mn- and MnFe-based room temperature magnetocaloric materials and control of critical properties by microstructuring. **S. Kwon**, H. Kim, K. Ahn, S. Lee, K. Lee, T. Numazawa

**12:20 208.** Study of the effect of experimental variables on the formation of core-shell particles. **J. Tirano**, H. Zea

Section F

## Nanoscience Applications

S. Wong, *Organizer*

A. Apblett, S. Hunyadi Murph, *Presiding*

**8:30 209.** Atomically precise synthesis of ultra-small Cu cluster catalysts with high colloidal stability. **S. Biswas**, C. Kumar

**8:50 210.** Exploring shapes, sizes and faceting of nanoscale metal particles for applications in fuel cell catalysis. **G. J. Leong**, **R. M. Richards**, **H. N. Dinh**

**9:10 211.** Functionalized magnetic nanoparticles as a support for magnetically separable hydrogenation catalysts. **L. M. Bronstein**, S. H. Gage, Z. B. Shifrina, N. V. Kuchkina, B. D. Stein, M. S. Bryan, P. E. Sokol, L. Z. Nikoshvili, V. G. Matveeva, E. M. Sulman

**9:30 212.** Multifunctional nanostructure design by the combination of atomic layer deposition and electrochemical deposition for electrical energy storage. **S. A. Sherrill**, J. Duay, Z. Gui, P. Banerjee, G. W. Rubloff, S. Lee

**9:50 213.** Low temperature precursors for nanocrystalline sorbents for arsenic. **A. Apblett**, T. Reed, A. Bagabas

**10:20** Intermission.

**10:40 214.** Advanced nanocomposite materials with energy related applications. **S. Hunyadi Murph**

**11:10 215.** Computational photochemistry for clean energy. **M. A. Zwijnenburg**

**11:30 216.** Encapsulation of nanocrystal arrays with semiconductor matrices for low-temperature processing of all-inorganic solar cells. **M. Zamkov**, T. O'conner, M. Imboden, E. Khon, D. Roth, E. Kinder, P. Moroz

**11:50 217.** Development of a wet chemical nanoprecursor route towards CuAlO<sub>2</sub> thin films for optoelectronic applications. **P. D. Thanh**, T. V. Thu, D. Mott, S. Maenosono

**12:10 218.** Synthesis and characterization of FeS<sub>2</sub> nanocrystals for use in photovoltaic devices. **S. J. Fredrick**, A. L. Prieto

## Celebration of the 100th Anniversary of Marie Curie's Nobel Prize in Chemistry

Sponsored by NUCL, Cosponsored by INOR, PROF, and WCC

## Recycling Carbon: Catalyzed Conversion of Non-food Biomass to Fuels and Chemicals

### Lignocellulose/Cellulose to Sugars and Derivatives

Sponsored by I&EC, Cosponsored by CATL and INOR

## MONDAY AFTERNOON

Section A

## Fifty Years of Inorganic Chemistry: A Celebration of Past, Present, and Future

### Bioinorganic Chemistry and Metals in Biology

R. Eisenberg, *Organizer*

V. Pecoraro, *Presiding*

**1:30** Introductory Remarks.

**1:40 219.** Utilizing the secondary coordination sphere to control metal-mediated transformations. **A. Borovik**

**2:05 220.** Inorganic chemistry to detect and treat cancer. **S. J. Lippard**

**2:30 221.** Biomimetic chemistry for the next fifty years: De novo design of zinc and copper proteins. **V. L. Pecoraro**, M. Zastrow, M. Tegoni, A. F. Peacock, J. Stuckey, F. Yu

**2:55 222.** Metal complexes and metalloproteins in DNA-mediated charge transport. **J. K. Barton**

**3:20** Intermission.

**3:35 223.** Design of prochelators that bind cellular metal ions in response to diverse stimuli. **K. J. Franz**

**4:00 224.** Synthetic inorganic chemistry for understanding metalloenzyme intermediates. **W. B. Tolman**

**4:25 225.** CO release chemistry of metal enolate and flavonolate complexes. **L. M. Berreau**

**4:50 226.** Analysis of second-sphere interactions in cytochromes using paramagnetic NMR. **K. L. Bren**

**5:15 227.** Molecular imaging approaches to studying the inorganic chemistry of the cell. **C. J. Chang**

Section B

## Frontiers in C-H Activation and Functionalization

T. Gunnoe, S. Golisz, *Organizers*

W. Goddard, *Presiding*

**1:30 228.** Catalytic alkane sulfochlorination. **P. Nickias**, K. Hirsekorn, W. Tenn

**2:00 229.** Factors controlling metal-carbon bond energies. **W. D. Jones**, M. E. Evans, T. Li

**2:30 230.** Industrial perspective on selective oxidation of alkylaromatic hydrocarbons to carboxylic acids. **V. Adamian**

**3:00** Intermission.

**3:15 231.** Catalytic C-H activation and functionalization with Cp\*Ir complexes. **E. A. Ison**

**3:45 232.** Functionalization of hydrocarbons mediated by tungsten alkyl allyl complexes. **P. Legzdins**

**4:15 233.** Exploratory and mechanistic investigations of carbon-hydrogen bond activation reactions and their applications to catalysis and organic synthesis. **R. G. Bergman**

**4:45** Concluding Remarks.

Section C

## Materials Chemistry for Solar Energy Capture

J. Pietryga, J. Papanikolas, *Organizers*  
J. Luther, *Presiding*

**1:30 234.** Third generation solar cells for PV and solar fuels based on quantum dots and quantum dot arrays. **A. J. Nozik**, M. C. Beard, J. M. Luther, J. C. Johnson, O. E. Tavi, A. G. Midgett, M. C. Hanna, B. K. Hughes

**2:10 235.** Optimizing the external quantum efficiency in nanoparticle-based solar cells. **S. A. Carter**, G. Zhai, C. France, A. Breeze

**2:50 236.** Solution-processed inorganic photovoltaics from semiconductor nanocrystals and molecular inks. **M. Law**

**3:30** Intermission.

**3:50 237.** Unconventional gap state of trapped exciton in lead sulfide quantum dots. **X. Jiang**, J. E. Lewis, E. Lafalce

**4:30 238.** Synthesis and optical properties of highly luminescent CuInS<sub>2</sub> based core/shell nanocrystals. **L. Li**, A. P. Pandey, J. M. Pietryga, V. I. Klimov

Section D

## Electrochemistry

B. Donovan-Merkert, *Organizer*

S. Maldonado, *Presiding*

**1:30 239.** "Charging" lithium ion batteries with a new cathode material of cobalt oxyfluoride (CoOF) nanostructures. **J. E. Cloud**, T. S. Yoder, Y. Yang

**1:50 240.** Synthesis and characterization of iron oxyfluoride nanostructures for lithium ion batteries. **T. S. Yoder**, J. E. Cloud, Y. Yang

**2:10 241.** Assessing the performance of single-component water reduction catalysts using coupled photochemical and electrochemical techniques. **J. I. Goldsmith**

**2:30 242.** Oxygen evolution mediated by a nickel-borate thin-film electrocatalyst. **D. Bediako**, D. G. Nocera

**2:50 243.** Ni-Al based oxide films for electrochromic devices. **F. LiN**, A. Norman, G. Chen, D. T. Gillaspie, A. C. Dillon, R. M. Richards

**3:10 244.** Fabrication of nanoporous platinum thin film by dealloying process and their electrochemical properties for highly efficient catalytic applications. **H. Jung**, D. Kim, H. Chun, J. Byun, Y. Jung

**3:30 245.** Synthesis of monodisperse Sn nanoparticles and their performance as negative electrodes in Li batteries. **L. Xu**, A. Dong, C. Kim, T. M. Mattox, D. J. Milliron, J. Cabana

**3:50** Intermission.

**4:00 246.** Single-step aqueous electropolymerization of separators for Li-ion rechargeable batteries. **D. J. Bates**, T. S. Arthur, M. Rawls, A. L. Prieto

**4:20 247.** Electrochemistry of nickel-based molecular electrocatalysts for hydrogen production in acidic ionic liquids. **D. H. Pool**, M. P. Stewart, J. A. Roberts, O. J. Molly, U. J. Kilgore, W. J. Shaw, R. M. Bullock, D. L. DuBois

**4:40 248.** Investigations into the effect of transition metal adsorbates on photocatalytic water oxidation at well-defined TiO<sub>2</sub> (110) surfaces. **G. E. Alliger**, A. G. Stack, G. M. Brown

**5:00 249.** Thin metal nanotubes synthesized by electrochemical deposition in AAO templates. **S. Kim**, S. Cho, T. M. Nguyen, S. Lee

**5:20 250.** SERS strategy for in situ and real time measurement of the structural and surface chemical properties of electrodeposited semiconductor thin films. **S. MALDONADO**

Section E

## Lanthanide and Actinide Chemistry

N. Radu, *Organizer*

S. Bart, *Presiding*

**1:30 251.** Efficient visible luminescence from nine-coordinate lanthanide complexes containing bis(pyrazolyl)pyridine and β-diketonate ligands. **J. M. Stanley**, B. J. Holliday

**1:50 252.** Effects of subtle changes in cyclopentadienyl substituents on actinide metallocene reactivity. **N. A. Siladke**, W. J. Evans, J. W. Ziller

**2:10 253.** DFT study of Cp<sub>2</sub>Th and Cp<sub>2</sub>U catalysts for hydrodenitrogenation (HDN) and hydrodesulfurization (HDS). **A. W. Pierpont**, R. L. Martin, E. R. Batista, J. L. Kiplinger, N. E. Travia

**2:30 254.** Reactivity of CX<sub>2</sub> (X=O,S) with organometallic f-element complexes: A theoretical approach. **L. Castro**, L. Maron

**2:50 255.** Synthesis and characterization of trivalent uranium alkyl complexes. **E. M. Matson**, P. E. Fanwick, S. C. Bart

**3:10** Intermission.

**3:20 256.** Generation of uranium(IV) bis(imido) intermediates in the synthesis U(V) and U(VI) bis(imido) complexes. **J. M. Boncella**, R. E. Jilek, L. P. Spencer, B. L. Scott

**3:40 257.** Syntheses and magnetic properties of paramagnetic uranium (IV) phosphine complexes. **B. S. Newell**, M. P. Shores

**4:00 258.** New frontiers in actinide imido chemistry: Preparation and reactivity of uranium(IV) imido dihalides. **R. E. Jilek**, J. M. Boncella

**4:20 259.** Organometallic reactions mediated by low-valent uranium with redox-active ligands. **S. C. Bart**, S. J. Kraft, B. A. Schaefer, P. E. Fanwick

**4:40 260.** On the nature of actinide- and lanthanide-metal bonds in heterobimetallic compounds. **B.**

**Vlaisavljevich**, P. Miró, C. J. Cramer, I. Infante, S. T. Liddle, L. Gagliardi

Section F

## Nanoscience

### Zero-dimensional Nanoparticles

S. Wong, *Organizer*

D. Gamelin, W. Gladfelter, *Presiding*

**1:30 261.** Multi-timescale map of radiative and nonradiative decay pathways for excitons in CdSe quantum dots. **K. E. Knowles**, E. A. McArthur, E. A. Weiss

**1:50 262.** Electronic structure determination by electrochemical and photophysical methods in semiconductor nanocrystal quantum dots. **Y. Ghosh**, A. Dennis, A. Steinbruck, J. A. Hollingsworth

**2:10 263.** Tailoring the photophysics of colloiddally grown germanium nanocrystals via size control and doping. **N. R. Neale**, D. A. Ruddy, J. C. Johnson

**2:30 264.** Photochemically reduced TiO<sub>2</sub> nanoparticles as proton-coupled electron transfer reagents. **J. N. Schrauben**, J. M. Mayer

**2:50 265.** Electron transfer rate and yield dependence on ZnO nanocrystal size and excited state reduction potential of porphyrin dyes. **A. J. Bierbaum**, A. S. Huss, R. Chitta, D. J. Ceckanowicz, K. R. Mann, D. A. Blank, **W. L. Gladfelter**

**3:20** Intermission.

**3:40 266.** Spins in colloidal ZnO nanocrystals. **D. R. Gamelin**, S. T. Ochsenein, N. Janssen, A. W. Cohn

**4:10 267.** Dependence of energy transfer on the overlap integral parameter between quantum dots and various Cr complexes. **P. T. Burks**, A. D. Ostrowski, P. S. Wagenknecht, A. A. Mikhailovsky, P. C. Ford

**4:30 268.** Identification of tri-alkyl acyloxy phosphonium as a key intermediate in the synthesis of CdSe nanocrystals. **H. Liu**, R. G. Rodriguez

**4:50 269.** Fast and reproducible synthesis, purification and characterization of semiconductor quantum dots. **Q. Song**, J. Bass, X. Ai, J. Yamanaga, S. Chakrabarty, A. Bagabas, P. Rice, T. Topuria, C. J. Scott, G. Young, R. Miller

**5:10 270.** Facile one-pot synthesis of iron arsenide nanoparticles: Toward sacrificial templates for [111] superconducting nanostructures. **M. Nath**, P. Sood

### Celebration of the 100th Anniversary of Marie Curie's Nobel Prize in Chemistry

Sponsored by NUCL, Cosponsored by INOR, PROF, and WCC

#### Gibbs Medal Centennial

Sponsored by HIST, Cosponsored by COLL, COMSCI, I&EC, INOR, ORGN, PETR, and PHYS

### Recycling Carbon: Catalyzed Conversion of Non-food Biomass to Fuels and Chemicals

#### Chemicals and Fuels from Biological and Enzymatically Catalyzed Routes

Sponsored by I&EC, Cosponsored by CATL and INOR

#### Undergraduate Poster Session

#### Inorganic Chemistry

Sponsored by CHED, Cosponsored by INOR and SOCED

#### MONDAY EVENING

Section A

#### Sci-Mix

S. Koch, N. Radu, *Organizers*

**8:00 - 10:00**

**95, 96, 97, 98, 100, 108, 109, 115, 118, 123, 128, 131, 132, 134, 136, 142, 148, 151, 152, 156, 157, 161, 166.** See previous listings.

**393, 399, 407, 409, 410, 413, 416, 418, 420, 424, 427, 429, 430, 432, 435, 436, 439, 442, 443, 446, 452, 453, 454, 456, 459, 460, 463, 466, 587, 591, 592, 593, 596, 599, 600, 612, 616, 618, 622, 623, 629, 630, 635, 639, 647, 650.** See subsequent listings.

#### TUESDAY MORNING

Section A

### Fifty Years of Inorganic Chemistry: A Celebration of Past, Present, and Future

#### Main Group Chemistry, Catalysis, and Bond Activation

R. Eisenberg, *Organizer*

E. Solomon, *Presiding*

**8:30** Introductory Remarks.

**8:40 271.** Carbenes for the activation of small molecules and the stabilization of

unusual phosphorus and boron species.

**G. BERTRAND**

**9:05 272.** Coordination chemistry of a trigonal binucleating cryptand ligand including superoxide disproportionation reactivity. **G. E. Alliger**, N. Lopez, R. McGuire, D. G. Nocera, **C. C. Cummins**

**9:30 273.** Forty nine years of noble gas chemistry. **K. Seppelt**

**9:55 274.** Reactions of heavier main group compounds with small molecules. **P. P. Power**

**10:20** Intermission.

**10:35 275.** Evolving inorganic chemistry of N-heterocyclic carbenes. **G. H. Robinson**

**11:00 276.** Inorganic crystalline nanocontainers: Properties and applications. **L. De Cola**, M. Mauro, C. Strassert, N. Darmavan

**11:25 277.** Small molecule reactivity with polynuclear reaction sites. **T. Betley**

Section B

### ExxonMobil Solid State Chemistry Faculty Fellow Award

#### Symposium in Honor of Amy L. Prieto

Cosponsored by WCC

K. Choi, *Organizer, Presiding*

**8:30** Introductory Remarks.

**8:40 278.** Electrodeposition as a synthetic tool for solid-state energy storage materials. **D. J. Bates**, D. C. Johnson, J. M. Mosby, M. T. Rawls, **A. L. Prieto**

**9:10 279.** Lamellar assembly of cadmium selenide nanoclusters into quantum belts. **W. E. Buhro**, Y. Liu

**9:40 280.** Mining where we know there is gold: Revisiting the tungsten and molybdenum bronzes. **L. F. Schneemeyer**

**10:10** Intermission.

**10:40 281.** Synthesis of Si nanoparticles for combine fluorescence MRI detection. **S. M. Kauzlarich**

**11:10 282.** Crystal growth of complex oxides: Effective strategies for the discovery of new phases. **H. zur Loye**

**11:40 283.** Transparent films of quantum dot gels: Mechanism and kinetics of assembly. **L. Perera**, I. R. Pala, **S. L. Brock**

Section C

### Towards Earth Abundant Solar Photocatalysis

#### Water Splitting/Carbon Dioxide Reduction

A. Rappe, *Organizer*

M. Shores, N. Damrauer, *Organizers, Presiding*

**8:30 284.** Towards earth abundant solar photocatalysis: Overview. **A. K. Rappe**, N. H. Damrauer, M. P. Shores

**8:45 285.** Bioinspired catalysts: Spinel composite electrodes for water oxidation and CO<sub>2</sub> reduction. **G. C. Gardner**, D. M. Robinson, C. C. Cady, Y. C. Go, P. Lobaccaro, Z. C. Maron, A. V. Biradar, M. C. Greenblatt, **G. Dismukes**, T. C. Asefa

**9:15 286.** Guiding principles for the catalytic reduction of CO<sub>2</sub> from theory. **C. B. Musgrave**, C. Lim, R. Bianco, P. J. Hay, J. T. Hynes

**9:45 287.** Ditopic molecular platforms for the conversion of carbon dioxide to energy rich species. **J. Rosenthal**

**10:05 288.** Charge transfer between bulk and quantized lead-salt semiconductors. **K. E. Knowles**, A. Rasmussen, M. McPhail, M. Malicki, T. Seideman, **E. A. Weiss**

**10:35** Intermission.

**10:50 289.** Molecular nickel diphosphine electrocatalysts for hydrogen oxidation and production: The function of proton relays in the secondary coordination sphere. **J. Yang**, S. E. Smith, M. O'Hagan, U. J. Kilgore, M. Rakowski DuBois, R. Bullock, D. L. DuBois

**11:10 290.** Nanoparticulate Ni colloids as catalysts for photochemically induced reduction of water to hydrogen. **K. Lebkowsky**, B. Shan, **R. H. Schmehl**

**11:30 291.** Activation of hematite nanorod arrays for photoelectrochemical water splitting. **R. Morrish**, C. Wolden

**11:50 292.** Integrating light absorbers and catalysts: Nanocrystal-enzyme complexes. **M. B. Beernink**, K. A. Brown, P. W. King, **G. Dukovic**

**12:20 293.** Chemical energy conversion in biology: Recent theoretical results on the active sites of nitrogenase and photosystem II. **F. Neese**, D. Pantazis, W. Ames, V. Krewald, M. Romelt, P. Ettenhuber, S. DeBeer

Section D

### Inorganic Catalysts

S. Koch, *Organizer*

D. Tyler, *Presiding*

**8:30 294.** Final frontier of nitrile hydration catalysis: Investigation of the activity of organometallic catalysts towards cyanohydrins. **S. M. Knapp**, D. R. Tyler

**8:50 295.** Evidence for iron nanoparticles catalyzing the asymmetric transfer hydrogenation of ketones. **J. F. Sonnenberg**, R. H. Morris, N. Coombs, P. A. Dube

**9:10 296.** Kinetic and mechanistic studies of supported-nanoparticle heterogeneous catalyst formation in contact with solution. **J. E. Mondloch**, R. G. Finke

**9:30 297.** Is it single-metal homogeneous or polymetallic heterogeneous catalysis? Further

investigation of the catalytically active species in benzene hydrogenation beginning with  $[\text{RhCp}^*\text{Cl}_2]_2$  via operando-XAFS, kinetic and poisoning studies. **E. Bayram**, J. C. Linehan, R. G. Finke, J. Fulton, J. A. Roberts, T. D. Smurthwaite, S. Ozkar, N. K. Szymczak  
**9:50** Intermission.

**10:00 298.** Aluminum-based classical and frustrated Lewis pairs in polymer synthesis. **Y. Zhang**, G. M. Miyake, E. Y. Chen

**10:20 299.** Atomically-controlled ultra-small gold catalysts. **S. Katla**, C. Kumar

**10:40 300.** Oxygen vacancy defects in ceria nanotubes. **C. Cheung**, N. J. Lawrence, J. R. Brewer, L. Wang, T. Wu, J. Wells-Kingsbury, G. Wang, Y. Soo, W. Mei

**11:00 301.** Intercalation of well-dispersed nanoparticles into the walls of mesoporous silica as a highly active and robust catalyst. **X. Wang**, L. Chen, J. Hu, R. Richards

**11:20 302.** Targeted synthesis and characterization of nanostructured B, Al, & Ga heterogeneous catalysts. **J. G. Abbott**, C. E. Barnes

Section E

## Bioinorganic Chemistry

S. Koch, *Organizer*  
C. Verani, *Presiding*

**8:30 303.** Fine-tuning redox potential by altering the secondary coordination sphere of the cupredoxin azurin. **N. M. Marshall**, Y. Lu

**8:50 304.** Investigating the reactivity and substrate specificity of the oxyferrous and ferric states of dehaloperoxidase B from *Amphitrite ornata*. **J. D'Antonio**, R. A. Ghiladi

**9:10 305.** Electron transfer in molybdenum enzymes: Sulfite oxidase (SO) and mitochondrial amidoxime reducing components (mARC). **A. Rajapakshe**, M. J. Cornelison, D. Reichman, R. Mendel, F. Bittner, J. H. Enemark

**9:30 306.** Investigations into the mechanism of chiral inversion of a Ni-tripeptide mimic of Ni-SOD. **A. M. Glass**, M. E. Krause, J. S. Laurence, T. A. Jackson

**9:50 307.**  $[\text{FeFe}]$  Hydrogenase H-cluster: Computational study of analogs to discern catalytic determinants of the natural cluster. **C. H. Chang**

**10:10 308.** Gel formulation containing mixed surfactant and lipids associating with carboplatin. **K. A. Woll**, E. J. Schuchardt, C. R. Willis, C. D. Ortengren, N. Hendricks, M. Johnson, E. Gaidamuskas, B. Baruah, A. G. Sostarec, D. R. Worley, D. W. Osborne, D. C. Crans

**10:30 309.** Tris(pyrazolyl)borate vs. tris(triazolyl)borate complexes of copper for modeling copper nitrite

reductase: The extra nitrogens create significant electronic and structural differences. **E. T. Papish**, M. Kumar, N. A. Dixon, A. C. Merkle, N. Lehnert, M. Zeller

**10:50** Intermission.

**11:00 310.** Metal complexes for selective inhibition of the 26S Proteasome in tumorous cells. **C. N. Verani**

**11:20 311.** Dirhodium metallopeptides as protein ligands. **A. N. Zaykov**

**11:40 312.** Kinetics of ground-state electron transfer through DNA. **A. L. Eckermann**, D. J. Feld, A. M. Scott, W. R. Michael, T. J. Meade

**12:00 313.** Development of redox-active ruthenium complexes for hypoxia selective cancer chemotherapy. **F. M. MacDonnell**, T. Janaratne, A. Yadav, A. Kenneth, C. A. Griffith, Y. Chen, A. Krishnan

**12:20 314.** Ferrocenyl amides as potential anticancer agents: Synthesis, characterization and interaction with lipid membrane interfaces. **A. A. Altaf**, A. Badshah, F. Javaid, M. N. Tahir, D. C. Crans

Section F

## Organometallic Chemistry Catalysis

N. Radu, *Organizer*  
G. Felton, *Presiding*

**8:30 315.** Catalysis of hydrogen-transfer reactions: Quantum-chemical models and insight. **T. Privalov**

**8:50 316.** Incorporation of peptides in the outer coordination sphere of Ni-based  $\text{H}_2$  production electrocatalysts. **A. Jain**, M. Reback, J. C. Linehan, D. L. Dubois, W. J. Shaw

**9:10 317.** Auto-tandem catalysis by water soluble  $\text{Cp}^*\text{Ir(III)}$  complexes: Hydrolysis of benzylic ethers and aerobic oxidation of benzylic alcohols. **D. A. Barrios**, E. A. Ison, R. A. Ghiladi

**9:30 318.** Hydrogenation of  $\text{CO}_2$  to MeOH by tandem homogeneous catalysis. **C. A. Huff**, M. S. Sanford

**9:50 319.** Synthesis and reactivity of neutral  $\kappa^2\text{-P,C}$  platinum chelates ( $\text{P-C}$ ) $\text{Pt(Me)(L)}$  ( $\text{L} = \text{PhCN}, \text{C}_2\text{H}_4$ ). **T. Sibray**, J. J. Adams, R. Dash, N. Arulsamy, D. M. Roddick

**10:10 320.** Self-assembled octanuclear metallosalens: The role of the second coordination sphere and catalytic applications. **A. W. Kleij**, R. M. Haak, J. Benet-Buchholz, E. C. Escudero-Adán, E. Martin, A. Decortes

**10:30** Intermission.  
**10:40 321.** Molybdenum olefin metathesis catalysts containing a 2,6-dimesitylphenylimido ligand. **L. C. Gerber**, R. R. Schrock

**11:00 322.** One-pot synthesis of  $\text{Mo}^0$  and  $\text{W}^0$  complexes possessing monodentate and multidentate

phosphine ligands. **Y. Ning**, A. A. Sarjeant, C. L. Stern, T. H. Peterson, S. T. Nguyen

**11:20 323.** Functionalization of rhenium-carbon bonds by a Baeyer-Villager type oxidation. **S. M. Bischof**, M. Cheng, R. J. Nielsen, T. B. Gunnoe, W. A. Goddard, R. A. Periana

**11:40 324.** Mechanistic aspects of selectivity in the hydroformylation of olefins catalyzed by rhodium bisdiazaphos complexes. **R. D. Froese**, C. R. Landis, A. L. Watkins

**12:00 325.** Electrocatalytic hydrogen production from organometallic compounds. E. S. Donovan, S. E. Froberg, B. A. Povirk, **G. A. Felton**

## Celebration of the 100th Anniversary of Marie Curie's Nobel Prize in Chemistry

Sponsored by NUCL, Cosponsored by INOR, PROF, and WCC

## Chemistry by Design: Building at the Molecular Level

Sponsored by CHED, Cosponsored by GEOC, INOR, MEDI, ORGN, PHYS, and YCC

## Reaction Mechanisms in Environmental Organic Chemistry

Sponsored by ENVR, Cosponsored by GEOC and INOR

## Recycling Carbon: Catalyzed Conversion of Non-food Biomass to Fuels and Chemicals

## Chemicals and Fuels from Homogenous Catalysis

Sponsored by I&EC, Cosponsored by CATL and INOR

## TUESDAY AFTERNOON

Section A

## Fifty Years of Inorganic Chemistry: A Celebration of Past, Present, and Future

## Solids, Structures, and Supramolecular Assemblies

R. Eisenberg, *Organizer*  
K. Poeppelmeier, *Presiding*

**1:30** Introductory Remarks.

**1:40 326.** Challenges of structure determinations then and now. **J. A. Ibers**

**2:05 327.** Exploring the materials beyond: An endless frontier for inorganic chemistry. **O. M. Yaghi**

**2:30 328.** Metals and fullerenes: Recent studies of exo- and endo-hedral structures. **A. L. Balch**

**2:55 329.** Emergent self-assembly of molecular spheres. **M. Fujita**

**3:20** Intermission.

**3:35 330.** Inorganic chemistry, our flaghead. **J. D. Corbett**

**4:00 331.** Concept of Zintl applied to new materials discovery. **S. M. Kauzlarich**

**4:25 332.** Polymorphism and local structure of crystalline and amorphous

Zinc-Indium-Tin oxide (ZITO). **K. R. Poeppelmeier**  
**4:50 333.** Adventures in crystal growth: The search for highly correlated materials. **J. Y. Chan**

Section C

## Towards Earth Abundant Solar Photocatalysis Solar Capture and Photovoltaics

N. Damrauer, *Organizer*  
M. Shores, A. Rappe, *Organizers*, *Presiding*

**1:30 334.** Scalability in solar energy conversion: The incorporation of earth-abundant materials in dye-sensitized solar cells. **J. K. McCusker**

**2:00 335.**  $\text{Fe(II)}$ -polypyridine complexes as photosensitizers in molecular assemblies for solar energy conversion. **E. Jakubikova**

**2:30 336.** Design of  $\text{Cu(I)}$  polypyridyl dyes for use in dye-sensitized solar cells. **L. Ashbrook**, C. Elliott

**2:50 337.** Multistep, photoinduced charge separation in a  $\text{Cu(I)}$  bis-phenanthroline based donor-chromophore-acceptor triad. **M. S. Lazorski**, C. Elliott

**3:10** Intermission.

**3:20 338.** Nanocrystalline thin film  $\text{Cu}_2\text{ZnSnS}_4$  photocathodes. **B. A. Parkinson**, S. Riha, A. Prieto

**3:40 339.** On the localization/delocalization dilemma in the electronic structure of d- and f-element oxides. **R. L. Martin**

**4:10 340.** Multiple excitons per single absorbed photon in organic materials. **J. Johnson**, A. Akdag, J. Michl, A. Nozik

**4:30 341.** Aqueous dye-sensitized hole injection into p-type phosphides from organic chromophores: An alternative design for highly efficient dye-sensitized photoelectrochemical cells. **S. Maldonado**

**4:50 342.** Earth abundant, non-toxic nanoparticle inks for photovoltaics. S. J. Fredrick, S. C. Riha, A. Wolfe, B. A. Parkinson, **A. L. Prieto**

Section E

## Coordination Chemistry Characterization and Applications

D. Crans, *Organizer*  
M. Mehn, N. Patmore, *Presiding*

**1:30 343.** Mixed valence in a hydrogen bonded dimolybdenum "dimer of dimers". L. McNeill, **N. J. Patmore**

**1:50 344.** Investigating effects of ancillary hydrogen bonding on anion-dependent spin-state switching. **S. R. Fiedler**, Z. Ni, M. P. Shores

**2:10 345.** Ligand field strength of alkylated vs. non-alkylated bisimidazoles as relevant to spin crossover in  $\text{Fe(II)}$  complexes. H. Phan, M. Chen, P. Chakraborty, Y. Calm, K.

Kovnir, L. Keniley, M. Meisel, A. Hauser, C. Achim, **M. Shatruk**

**2:30 346.** Strong magnetic interactions in metal complexes of bis-pyridyl substituted verdazyl radicals. **D. J. Brook**, C. Richardson

**2:50 347.** Structural and magnetic properties of binuclear and mononuclear compounds derived from 1,4,8-triazacycloundecane. **F. Chavez**, A. Banerjee, A. Tolla, S. Stjepanovic, W. Brennessel, R. Loloee, J. Costes, J. Tuchagues

**3:10 348.** Polyoxometalate-based single-molecule magnets. **X. Fang**

**3:30 349.** Reversible structural modulation and associated magnetic properties in a Co citrate cubane single molecule magnet. **L. R. Falvello**, J. Campo, E. Forcén-Vázquez, I. Mayoral, F. Palacio, C. Sáenz de Pipaón, M. Tomás

**3:50** Intermission.

**3:55 350.** Synthetic models of the water oxidation complex (WOC) of Photosystem II. **S. Mukherjee**, J. Stull, J. Yano, R. D. Britt, V. K. Yachandra, K. A. Abboud, G. Christou

**4:15 351.** Developing new iron and manganese oxidation catalysts. **M. P. Mehn**

**4:35 352.** Divergent oxidation of hexanuclear manganese and cobalt complexes. **A. R. Fout**, T. A. Betley

**4:55 353.** Controlled loadings of 1,10-phenanthroline on mesoporous silica: Metal complexation, spectroscopic characterization, and oxidative catalysis. **B. J. Smith**, T. P. Stack

**5:15 354.** Interaction of pyridine and 4-hydroxypyridine-2,6-dicarboxylic acids with heavy metal ions in aqueous solutions. **E. Norkus**, I. Stalnionienė, D. C. Crans

Section F

### Organometallic Chemistry Catalysis

N. Radu, *Organizer*  
E. Papish, *Presiding*

**1:30 355.** Catalytic hydrogenation of polar double bonds with ruthenium complexes of N and C donor ligands. **E. T. Papish**, M. Kumar, I. Nieto, J. DePasquale, M. Zeller

**1:50 356.** Catalytic C-H bond functionalization from high-spin iron imido complexes. **T. Betley**

**2:10 357.** Development of Pd- and Pt-catalysts for site-selective C-H functionalization. **A. J. Hickman**, M. S. Sanford

**2:30 358.** Copper and silver as homogeneous catalysts for carbene insertion into C-H and C=C bonds. J. A. Flores, N. Komine, K. Pal, C. Chen, M. Pink, B. Pinter, D. J. Mindiola, **K. G. Caulton**

**2:50 359.** Effects of aryl substituents on the kinetics and thermodynamics of C-H bond activation by a pincer-ligated iridium complex. **D. A. Laviska**, D. Y. Wang, K. Krogh-Jespersen, A. S. Goldman

**3:10 360.** Development of well-defined copper(I) catalysts for the addition of O-H and N-H bonds across alkyne bonds. **T. Gunnoe**, T. R. Cundari, S. A. Delp, J. Uddin, M. J. Pouy, V. M. Ramdeen, N. A. Cochrane, M. Sabat

**3:30** Intermission.

**3:40 361.** Reactivity of late transition metal hydrocarbyl complexes with oxygen delivery reagents. **J. R. Webb**, M. Sabat, T. R. Cundari, B. Prince, T. Gunnoe

**4:00 362.** Acceptor pincer chemistry of group 8 metals: Catalytic alkane dehydrogenation by (<sup>CF<sub>3</sub></sup>PCP)Ru(cod)H and (<sup>CF<sub>3</sub></sup>PCP)Os(cod)H. **B. C. Gruver**, J. J. Adams, S. J. Warner, N. Arulsamy, D. M. Roddick

**4:20 363.** Towards catalytic alkane oxidation via O<sub>2</sub> insertion into platinum methyl bonds. **G. Britovsek**, R. Taylor, A. Petersen

**4:40 364.** Carbon dioxide reduction catalyzed by mono and dinuclear ruthenium complexes. **P. Miró**, M. Z. Ertem, N. Planas, A. Llobet, L. Gagliardi, C. J. Cramer

**5:00 365.** Terminal and bridging palladium and nickel allyls for the activation of carbon dioxide. **N. Hazari**, J. Wu, D. P. Hruszkewycz, T. J. Schmeier

Section G

### Coordination Chemistry Synthesis

D. Crans, *Organizer*  
J. Kirby, M. Shatruk, *Presiding*

**1:30 366.** Redox reactions of aluminum(III). T. W. Myers, N. Kazem, M. Shanmugam, **L. A. Berben**

**1:50 367.** Multifunctional luminescent ruthenium complexes as supramolecular photo-redoxactive building blocks. **M. Jäger**, M. Schulze, U. S. Schubert

**2:10 368.** Oligomeric and dendritic phthalocyanines: High dielectric constant materials for solar cells. **G. Mezei**

**2:30 369.** Cleavage of the N-N bond in dinitrogen using a β-diketiminato supported iron(II) complex. **M. M. Rodriguez**, C. C. Scarborough, E. Bill, W. W. Brennessel, P. L. Holland

**2:50 370.** Reversible reduction of oxygen to peroxide facilitated by molecular recognition. **N. Lopez**, R. McGuire, G. E. Alliger, D. G. Nocera, C. C. Cummins

**3:10 371.** Dioxygen activation by trispyrazolylborate nickel(I) complexes. **W. L. Green**, E. R. Sirianni, C. G. Riordan

**3:30** Intermission.

**3:40 372.** Further attempts to decipher the counterion effect on the redox properties of bridged monovacant heteropolytungstates. **J. F. Kirby**

**4:00 373.** Synthesis and characterization of tripodal Schiff base complexes of first row transition metals. **A. M. McDaniel**, E. A. Hill, M. P. Shores

**4:20 374.** Iridium (I) hydrides supported by the encumbering phosphine P(CH<sub>2</sub><sup>1</sup>Ad)(i-Pr)<sub>2</sub> and its phosphite analog P(O<sup>1</sup>Ad)(i-Pr)<sub>2</sub>. **M. D. Millard**, J. S. Figueroa

**4:40 375.** Reactivity of first-row transition metal complexes supported by the wide bite-angle diphosphine <sup>iPr</sup>DPDBFphos. **E. E. Marlier**, S. J. Tereniak, C. C. Lu

**5:00 376.** Cyclodiphosphazanes with functionalities: Synthesis, reactivity and transition metal chemistry. **M. S. Balakrishna**, J. T. Magee, A. Nag

Section B

### Inorganic Nanoscience Award: Symposium in Honor of Catherine J. Murphy

Cosponsored by WCC  
R. Richards, *Organizer, Presiding*

**2:00 377.** Plasmonic nanoparticles inside cells: Light-induced molecular release. **N. J. Halas**

**2:30 378.** Biodegradable nanoparticles based on silicon and iron oxide for in-vitro and in-vivo applications. **M. J. Sailor**

**3:00 379.** Gold and silver nanoparticles(NP) for potential environmental and energy conversion applications. **M. A. El-Sayed**

**3:30** Intermission.

**3:40 380.** Plasmon-mediated syntheses of silver nanostructures. **C. Mirkin**

**4:10 381.** Controlling protein-ligand kinetics using 3D plasmonic materials. **T. W. Odom**

**4:40 382.** Development of a tetrapod-based fluorescent strain sensor for biological imaging. **A. Alivisatos**, C. Choi

Section D

### Environmental Aspects of Inorganic Chemistry

S. Koch, *Organizer*  
D. Crans, *Presiding*

**2:00 383.** Reduced nitrogen complexes: A series of *trans*-intermediates on the path to ammonia. **C. G. Balesdent**, J. L. Crossland, D. R. Tyler

**2:20 384.** Influence of As(V) on the oxidation of Fe(II) by dissolved oxygen. **W. Jung**, B. Jeon

**2:40 385.** Fluorescein-based fluorescent and colorimetric chemosensors for metals in aqueous media. **F. A. Abebe**, E. Sinn

**3:00 386.** MgO-TiO<sub>2</sub> mixed oxide nanoparticles: Comparison of flame vs. aerogel synthesis methods: Characterization and photocatalytic activities. **K. M. Shrestha**, K. J. Klubunde, C. M. Sorensen

**3:20 387.** Nanostructured metal oxides for cleaving glycerophospholipids. **A. Corpuz**, L. Chen, C. Cadigan, G. Atiaga, B. Ho, I. Narkeviciute, M. Posewitz, R. M. Richards

**3:40 388.** Uranium uptake from natural water sources using supported tungstic acid. **C. K. Perkins**, A. W. Apblett

**4:00 389.** Adsorption of phosphate via an iron coordination polymer. **D. Corter**

### Chemistry by Design: Building at the Molecular Level

Sponsored by CHED, Cosponsored by GEOC, INOR, MEDI, ORGN, PHYS, and YCC

**Reaction Mechanisms in  
Environmental Organic Chemistry**  
Sponsored by ENVR, Cosponsored by GEOC and INOR

**Recycling Carbon: Catalyzed  
Conversion of Non-food Biomass to  
Fuels and Chemicals**

**Chemicals and Fuels from  
Heterogeneous Catalysis**  
Sponsored by I&EC, Cosponsored by CATL and INOR

### TUESDAY EVENING

Section A

### Fifty Years of Inorganic Chemistry: A Celebration of Past, Present, and Future

R. Eisenberg, *Organizer*

**6:00 - 8:00**

**390.** Alkali metals in ethylenediamine: A computational study of optical absorption spectra and NMR parameters. **E. Zurek**

**391.** Insulated copper(I) wires: Structural polymorphs and photoluminescence. O. Hietsoi, C. Dubceac, A. S. Filatov, **M. A. Petrukhina**

**392.** First *endo*-complex of corannulene. S. N. Spisak, A. V. Zabula, A. S. Filatov, A. Y. Rogachev, **M. A. Petrukhina**

**393.** Highlights in inorganic chemistry from the 250 years that preceded the publication of *Inorganic Chemistry*. **S. A. Koch**

Section B

### Organometallic Chemistry Catalysis

N. Radu, *Organizer*

**6:00 - 8:00**

**394.** Cp\*Ir complexes in catalytic alkane hydroxylation. **M. Zhou**, R. H.

Crabtree, O. Eisenstein, D. Balcells, N. D. Schley

**395.** Catalytic transfer dehydrogenation methods for the synthesis of polyfunctionalized (hetero)aromatic molecules. **D. Pun**, S. Stahl

**396.** Light-driven water oxidation – catalyzed by a ruthenium complex containing a bioinspired ligand. **M. D. Kärkäs**, E. V. Johnston, E. A. Karlsson, B. Lee, T. Åkermark, M. Shariatgorji, L. Ilag, & Hansson, J. Bäckvall, B. Åkermark

**397.** Photochemical water oxidation: Inspired by nature. E. A. Karlsson, B. Lee, T. Åkermark, E. V. Johnston, **M. D. Kärkäs**, J. Sun, & Hansson, J. Bäckvall, B. Åkermark

**398.** Hydrogenation of unactivated alkenes using low-coordinate cobalt catalysts. **A. Kavara**, W. W. Brennessell, P. Holland

**399.** Designing Pd- and Pt-catalysts for C-H activation by H/D exchange. **A. J. Hickman**, M. S. Sanford

**400.** C-H bond functionalization of arenes using  $(Cp^*IrCl_2)_2$ . **K. L. Engelman**, Y. Feng, E. A. Ison

**401.** Synthesis of oxorhenium(V) diamido pyridine complexes and their role in oxygen atom transfer catalysis. **C. P. Lilly**, E. A. Ison

**402.** Catalytic C-H bond activation of benzene with  $Cp^*Ir$  complexes. **M. Lehman**, E. A. Ison

**403.** Experimental and theoretical comparisons of iridium(III) and rhodium(III) metalloporphyrins as carbenoid transfer catalysts. **B. J. Anding**, J. Brgoch, A. Ellern, G. J. Miller, L. K. Woo

**404.** Ethylene dimerization by  $(PP)PtMe(C_2H_4)^+$  (PP = chelating diphosphine) complexes. **B. M. Schmidt**, J. J. Adams, D. M. Roddick

**405.** Synthesis of a new class of chiral tridentate 1,3-bis(4,5-dihydrooxazol-2-ylimino)isoindoline-based pincer ligands. **L. Bernier**, J. L. Cryder, C. Moore, A. Rheingold, **C. J. Daley**

**407.** Electrocatalytic  $CO_2$  reduction using modified electrodes. **S. Elias**, J. Quinson, G. J. Britovsek\*, A. R. Kucernak\*

**408.** Zinc and copper complexes of  $\beta$ -diketiminate ligands: Synthesis, characterization, and catalytic applications. **S. Abbina**, G. Du

Section C

## Nanoscience Synthesis

S. Wong, *Organizer, Presiding*  
**6:00 - 8:00**

**409.** Synthesis of ligand-stabilized CoNi nanoparticles with tunable sizes and compositions. **K. E. Marusak**, A. C. Johnston-Peck, J. B. Tracy

**410.** Silver nanoparticles stabilized by sterically-bulky ligands. **K. A. Kozek**, A. C. Johnston-Peck, J. Wang, J. B. Tracy

**411.** Fabrication of free-standing, 3D metal microstructures via laser-induced aggregation. **D. W. Bemis**, R. A. Farrer

**412.** Production of multi-architected nanomaterials by simple electroreduction of manganese oxide nanorods. **J. W. Duay**, J. Hu, Z. Gui, S. Sherrill, S. Lee

**413.** Bioreduced metal nano-platelets and particles: Size, shape and optical properties. **S. K. St. Angelo**, E. L. Hartz, K. A. Cohen

**414.** Alloying and doping in colloidal Group IV nanocrystals. **D. A. Ruddy**, N. R. Neale

**415.** Nanoparticles synthesis and assembly under magnetic fields. **C. Chen**, Q. Chen

**416.** Bi-Sn eutectic nanoparticles: Large super cooling and size dependent phase stability. **J. Wang**, G. Glatzmaier, D. Blake, **C. J. Curtis**

**417.** New bis( $\beta$ -diketones) and their Cu molecular squares. **J. K. Cherutoi**, J. D. Sandifer, R. L. Fogarty, F. R. Fronczek, A. W. Maverick

**418.** Multifunctional organosilicon  $\beta$ -ketoenamides and their transition metal complexes. **Y. Marcos**, F. Armstrong, J. Edwards, F. R. Fronczek, A. W. Maverick

Section D

## Nanoscience Applications

S. Wong, *Organizer, Presiding*  
**6:00 - 8:00**

**419.** Electrical properties of electrospun carbon nanofibers. **N. E. Hedin**, V. Sobolev, L. Zhang, Z. Zhu, H. Fong, E. Handberg, G. Serfling

**420.** Synthesis and characterization of perfectly-ordered plasmonic nanorod arrays. **Y. Zhang**, B. Ashall, G. Doyle, D. Zerulla, G. U. Lee

**421.** Fabrication of mesoporous cobalt doped zinc oxide nanomaterials with capacitance activity: Factors affecting formation and surface morphology. M. Davis, **C. Gümeçi**, B. Black, C. Korzeniewski, L. Hope-Weeks

**422.** Surface-enhanced Raman scattering of hot spots formed between gold nanostructures and the gold film. **Y. Chang**, S. Wu, W. Hsu

**423.** Converting poly(ethylene terephthalate) waste into carbon microspheres in a supercritical  $CO_2$  system. **C. Chen**, L. Wei, Q. Chen

**424.** Development of fluorescent iron doped silicon nanoparticles for application in magnetic resonance imaging. **M. P. Singh**, S. M. Kaulzarich, A. Y. Louie

**425.** Use of polyhedral oligomeric silsesquioxanes to enhance thermomechanical and barrier properties of epoxy resin. **L. R. Ojha**, K. P. Bastola, K. D. Ausman

**426.** Highly ordered nanochannel arrays for large areas using chemical etching-assisted anodization. **S. Lee**, S. Lee

**427.** Nanoneedles and core-shell carbon nanotubes encapsulating FeSe nanowires. **S. C. Patil**, M. Nath

**428.** Fabrication of IR-reflecting multilayer structure based on metal-doped  $TiO_2$  and  $SiO_2$  films. **S. Kim**, M. S. Suh, J. W. Cho

Section E

## Inorganic Catalysts

S. Koch, *Organizer*  
**6:00 - 8:00**

**429.** Formation and reactivity of a porphyrin iridium hydride in water: Acid dissociation constants and equilibrium thermodynamics relevant to Ir-H and Ir-C bond dissociation energetics. **S. Bhagan**, B. B. Wayland

**430.**  $SnO_2$  nanoparticles embedded  $TiO_2$  nanofibers as highly efficient photocatalyst for degradation of Rhodamine B. **S. Hwang**, J. Jang

**431.** Modification of platinum-phosphinito nitrile hydration catalysts for enhanced hydration rates. **S. M. Knapp**, D. R. Tyler

**432.** Quantum chemical characterization of the mechanism of an iron-based water oxidation catalyst. **M. Z. Ertem**, L. Gagliardi, C. J. Cramer

**433.** Characterization of K-Fe-MOR and Fe-K-MOR catalysts prepared by wet ion-exchange method for simultaneous reduction of  $N_2O$  and  $NO$ . **K. Kang**, M. Seo, E. Park

**434.** Preparation of electrocatalysts for the reduction of  $CO_2$  to  $CO$ . **B. J. Boro**, A. M. Appel, B. R. Galan, J. C. Linehan, D. L. DuBois

**435.** Fluorinated phthalocyanines for electronic materials and green catalyst. **Y. Zhang**, A. Loas, H. Patel, S. Gorun

**436.** Use of interdigitated array electrodes to investigate the mechanism of hydrogen production with nickel bis-diphosphine complex electrocatalysts. **F. Liu**, D. Dubois, M. R. Dubois, J. Roberts, M. Bullock, **Y. Li**, B. A. Parkinson

**437.** Incorporation of hydrogen bonding functionalities in the second coordination sphere of metal complexes for the catalytic activation of water. **W. Hoffert**, **J. Yang**

**438.** Investigation of nano-crystalline metal nitrides as non-precious metal catalysts for the oxygen reduction reaction in fuel cells. **C. Caskey**, R. Richards

**439.** Supported MnOx oxidation catalysts from triazacyclononane coordination compounds and hybrid

surfaces. **J. M. Notestein**, A. Korinda, N. Schoenfeldt, Z. Ni, R. Meyer

**440.** Hydrogenation of carbon dioxide to formate using ruthenium bis(diphosphino) complexes: Investigation of ligands containing proton relays. **B. R. Galan**, J. C. Linehan, A. M. Appel, M. C. Rakowski-DuBois, D. L. DuBois

**441.** Molybdenum dinitrogen compounds supported by chelating diphosphine ligands containing proton relays and their proclivity towards reduction of the bound dinitrogen. **A. N. Groves**, C. J. Weiss, M. T. Mock, R. J. Rousseau, D. L. DuBois, R. M. Bullock

**442.** Surface-grafted cobaloximes as hydrogen catalysts in aqueous solution. **C. Eubanks**, D. Wheeler, M. Hamburger

**443.** Iron complex of a tridentate amido ligand for activation of carbon-chlorine bond. **Y. Gartia**, P. Ramidi, S. Pulla, A. Ghosh

**444.** Influence of electron withdrawing and electron releasing groups of Co (III)-diamide diamine complexes on cyclic carbonate synthesis. **P. Ramidi**, **S. Pulla**, Y. Gartia, A. Ghosh

**445.** Synthesis of oxazolidinones under mild reaction conditions from 2-aminoalcohols and diethyl carbonate using recyclable 1,3-dichlorodistannoxanes. **S. Pulla**, P. Ramidi, A. Ghosh, P. Munshi

**446.** Phospholipase activity of cerium(IV) complexes at lysosomal pH. **D. E. Williams**, K. B. Grant

**447.** Synthesis of  $C_3$ - and  $C_1$ -symmetric tripodal triphosphines as potential ligands for Cu(I)-catalyzed asymmetric P-C bond formation. **M. F. Cain**, R. P. Hughes, D. S. Glueck, J. A. Golen, A. L. Rheingold

Section F

## Electrochemistry

B. Donovan-Merkert, *Organizer*  
**6:00 - 8:00**

**448.** Nanowire array on aluminum substrate through selectively removing the barrier layer in AAO template. K. Lee, P. Banerjee, **S. A. Sherrill**, G. W. Rubloff, S. Lee

**449.** Conductive polymer nanotubes for electrochemically controlled drug delivery system. **T. M. Nguyen**, S. Kim, S. Lee

**450.** Fabrication of porous metal nanostructures and their potential application as electrochemical sensors. **M. Clay**, Q. Cui, J. Chen, **Z. Gu**

**451.** Nonaqueous redox flow battery employing redox couples with aromatic ligands. **J. Park**, M. Lee, D. Oh, D. Lee, S. Doo

**452.** Modifying electrodes with nickel-based molecular electrocatalysts for hydrogen production. **D. H. Pool**, D. L. DuBois

453. Pre-patterned nanochannel formation analysis with various inter-pore distances in anodic aluminum oxide. **S. Lee**, S. Lee

454. Understanding organosilicon-based electrolyte/graphite electrode interface in lithium-ion battery. **X. Chen**

Section G

## Bioinorganic Chemistry

S. Koch, *Organizer*

6:00 - 8:00

455. Activation of urea and carbon dioxide by several new nickel(II) complexes. **W. A. Seals**

456. Reduction potential tuning of blue copper protein by introducing histidine analog at equatorial position. **Y. Yu**, N. M. Marshall, D. K. Garner, Y. Lu

457. Carboplatin interactions with lipids and surfactants: <sup>1</sup>H NMR spectroscopy and Langmuir monolayer study. **N. Hendricks**, M. Johnson, A. G. Sostarecz, B. Baruah, E. Gaidamaskas, D. C. Crans

458. Cadmium and iron coordination in two myohemerythrins. **B. S. Russell**, A. Halfen, V. Taylor

459. Carbon monoxide and cyanide ligand biosynthesis by radical AdoMet enzyme HydG in [FeFe]-hydrogenase H-cluster maturation. **B. R. Duffus**, E. M. Shepard, S. J. George, R. C. Driesener, M. R. Challand, K. D. Swanson, P. L. Roach, S. P. Cramer, J. W. Peters, J. B. Broderick

460. Studies on the active site structure of nitrile hydratase: Asymmetric Co- and Fe-based synthetic analogs. **J. A. Rodriguez**, A. D. Vitalo, **C. J. Daley**, A. Rheingold, C. Moore

461. Synthesis, characterization, and reactivity of diamidato-bis(phosphino) nickel complexes. **D. N. Huh**, C. Moore, A. Rheingold, **C. J. Daley**

462. Development and evaluation of novel polypyridyl Ru(II) complexes as potential hypoxia-selective anticancer drugs. **Y. Chen**, J. Aslan, F. M. MacDonnell

463. Mechanism of the oxygen independent pathway of DNA cleavage by a Ru(II) polypyridyl complex. **S. A. Potet**, S. Singh, D. J. Boston, C. Griffith, F. M. MacDonnell

464. Toward modeling the active site of phosphate ester hydrolases. **R. A. Joy**, H. Arman, G. Musie

465. DFT study of the mechanism for methane hydroxylation by soluble methane monooxygenase. **S. Huang**, Y. Shiota, K. Yoshizawa

466. Synthesis of potential inhibitors of FIH Fe<sup>2+</sup> active site. **J. M. Dorhout**, C. Y. Taabazuig, M. J. Knapp

WEDNESDAY MORNING

Section B

## Coordination Chemistry

## Synthesis, Characterization, and Applications

D. Crans, *Organizer*

A. De Bettencourt Dias, R. Houser, *Presiding*

8:30 467. Uranyl sequestration: Synthesis and structural characterization of uranyl complexes with a tetradentate methylterephthalamide ligand. **C. Ni**, D. K. Shuh, K. N. Raymond

8:50 468. Recent advances in the preparation of synthetic analogs of methanobactin. **D. Rabinovich**

9:10 469. Structural diversity in luminescent pyridine-bis(oxazoline) complexes of lanthanide ions. **A. de Bettencourt-Dias**

9:30 470. Homogeneous oxo transfer to and from rhodium: Mechanistic features. N. P. Tsvetkov, J. G. Andino, H. Fan, **K. G. Caulton**

9:50 471. Coordination chemistry of dipyrrolylbenzene: N-deficient terpyridine or panacea for brightly luminescent metal complexes? **J. Williams**, L. Murphy, L. Parkes

10:10 472. Studies on mercury(II), nickel(II) and lead(II) biologically important binary complexes with  $\alpha$ -aminobutyric acid in solution. **B. B. Tewari**

10:30 473. Mixed pyridyl/phenol ligands and their copper, iron, and manganese coordination chemistry: Modeling bi- and polynuclear bioinorganic active sites. A. Jozwiuk, J. M. McClain, A. L. Myers, R. Shakya, Z. Wang, **R. P. Houser**

10:50 Intermission.

11:05 474. Ruthenium(II) complexes as potential dual action PDT agents. **R. N. Garner**, C. Turro

11:25 475. Duplex formation of ligand substituted chiral and achiral aminoethylglycine artificial oligopeptides with metal ion crosslinks. **M. B. Coppock**, M. E. Williams\*

11:45 476. Electrochemical behavior, coordination chemistry, and reactivity of octahedral Fe<sub>6</sub>N<sub>12</sub> clusters supported by a weak-field hexaamide ligand. **T. D. Harris**, Q. Zhao, R. Hernandez Sanchez, T. A. Betley

12:05 477. Reversible carbon dioxide capture in amine-functionalized microporous metal-organic framework Zn(BDP-CH<sub>2</sub>NH<sub>2</sub>) (BDP<sup>2-</sup> = 1,4-benzenedipyrazolate). **H. Choi**, J. R. Long

12:25 478. Synthesis and reactivity of an unusual acetonitrile-bridged dinuclear copper complex. **T. C. Davenport**, T. D. Tilley

Section C

## Towards Earth Abundant Solar Photocatalysis

### Young Investigators

M. Shores, *Organizer*

A. Rappe, N. Damrauer, *Organizers*, *Presiding*

8:30 479. Cu<sub>2</sub>ZnSnS<sub>4</sub> (CZTS) film electrodes fabricated through a multi-stage process. **Y. Liang**, B. A. Parkinson

8:50 480. Photophysics and photochemistry of tungsten-alkylidyne containing assemblies. **D. B. Moravec**, M. D. Hopkins

9:10 481. Controlling charge separation lifetimes in highly reducing tungsten-alkylidyne/zinc-porphyrin dyads. **D. C. O'Hanlon**, M. D. Hopkins

9:30 482. Water oxidation at a single cobalt center: Electronic tuning and secondary coordination sphere effects. **R. McGuire**, D. K. Dogutan, D. G. Nocera

9:50 483. Cobalt-dithiolene complexes for the photocatalytic and electrocatalytic reduction of protons. **W. R. McNamara**, Z. Han, P. J. Alperin, P. L. Holland, R. Eisenberg

10:10 484. Photo-assisted catalysts growth and water splitting at the metal oxide/molecule interface. **R. S. Khnayzer**, F. N. Castellano

10:30 Intermission.

10:40 485. Single pot synthesis of dyed-TiO<sub>2</sub> for hydrogen production. **D. J. Shissler**, D. C. Johnson, A. L. Prieto

11:00 486. Homogeneous cobalt electrocatalysts for solar driven hydrogen evolution from water. **B. D. Stubbert**, J. C. Peters, H. B. Gray

11:20 487. Catalytic water oxidation: DFT study of a competitive involvement of Lewis acid-Lewis base cooperation and radical coupling. **T. Privalov**, L. Sun, B. Akermark

11:40 488. Water oxidation by a polyoxometalate catalyst containing single-site cobalt center. **C. Zhao**, C. S. Kambara, J. Song, H. Lv, Y. V. Geletii, G. Zhu, J. Vickers, C. L. Hill

12:00 489. Core-shell construct featuring heterobimetallic chromophores for artificial photosynthesis. **H. Soo**, A. Agiral, H. Frei

Section E

## Organometallic Chemistry

### New Ligand Platforms

N. Radu, *Organizer*  
C. Burns, *Presiding*

8:30 490. Group 10 metal complexes incorporating anionic phosphinimine ligands for olefin polymerization. **C. T. Burns**, S. Shang, R. Thapa

8:50 491. Click-derived abnormal carbene and cyclometallated pincer ligands: New heteroleptic bistridentate ruthenium(II) complexes for potential applications in artificial photosynthesis and dye sensitized solar cells. **B. Schulze**, D. Escudero, C. Friebe, R. Siebert, H. Görls, U. Köhn, E. Altuntas, A. Baumgaertel, M. D. Hager, A.

Winter, B. Dietzek, J. Popp, L. González, U. S. Schubert

9:10 492. Efforts toward the synthesis of high oxidation state iridium complexes. **S. Whittemore**, J. Stambuli

9:30 493. Preparation of polymeric phosphine ligands by metal-catalyzed living radical polymerization and their application to hydroformylation catalysis. A. Cardozo, **R. Poli**, E. Manoury, H. Delmas, C. Julcour, J. Blanco

9:50 494. Synthesis and photophysics of platinum(II) amino-terpyridines. **L. M. Hight**, M. L. Clark-McGuire, D. R. McMillin

10:10 Intermission.

10:20 495. Photochemistry and photophysics of carbometalated Pt(II) polyimine complexes. **D. P. Lazzaro**, D. R. McMillin

10:40 496. Synthesis of chiral trinitrogen 1,3-bis(4,5-dihydrooxazol-2-ylimino)isoindoline-based pincer ligands and preliminary studies on their use in enantioselective catalysis. **C. J. Daley**, C. Moore, A. Rheingold

11:00 497. New mesoionic carbenes (MICs): Synthesis and applications of highly stable 1*H*-1,2,3-triazol-5-ylidenes. **J. Bouffard**, G. Guisado-Barrios, G. Bertrand

11:20 498. <tt class="letterText">Synthesis, characterization and properties of Rh complexes bearing a  $\pi$ -accepting PNP ligand</tt>. **Y. Zhu**, O. V. Ozerov

Section F

## Nanoscience

### Biology and Sensing

S. Wong, *Organizer*  
K. Lee, Y. Cui, *Presiding*

8:30 499. Nanoscale coordination polymers for CT imaging. **K. E. deKrafft**, L. M. Burk, O. Z. Zhou, W. Lin

8:50 500. Development of multimodal nanoparticles for imaging applications. **D. Koktysh**, W. Pham

9:10 501. Differential magnetic catch and release (DMCR): A purification technique for magnetic nanoparticles and hybrid nanocrystals. **J. S. Beveridge**, M. R. Buck, J. F. Bondi, R. Misra, P. E. Schiffer, R. E. Schaak, M. E. Williams

9:30 502. Development of a multimodal bioimaging contrast agent. **T. M. Atkins**, M. P. Singh, A. Louie, S. M. Kaulzarich

9:50 503. Magnetic core-shell nanoparticles as a highly efficient gene delivery vehicle to stem cells. **K. Lee**, S. Ghoshal, B. Shah

10:20 Intermission.

10:30 504. Biomimetic graphene nanosensing. **Y. Cui**

- 11:00 505.** Bioconjugated nanostructures of semiconducting polymers. **A. C. Kamps**, P. Park
- 11:20 506.** Using cell-delivered nanoparticles to cause local hyperthermia, increases survival in a murine metastatic pancreatic cancer model. **G. S. Abayaweera**, M. Basel, T. B. Shrestha, H. Wang, O. B. Koper, S. Balivada, S. H. Bossmann, D. L. Troyer
- 11:40 507.** Nanometric reagents for detection and neutralization of peroxide explosives. **A. Applett**, N. Materer, D. Hoel, D. Bussan
- 12:00 508.** Synthesis of core/shell Fe/Fe<sub>3</sub>O<sub>4</sub> nanoparticle-based "light switches" for determination of cancer-specific proteases in breast cancer tissue. **H. Wang**, M. Kalita, M. T. Basel, S. Balivada, T. Samarakoon, O. B. Koper, D. L. Troyer, S. H. Bossmann

Section A

### Main Group Chemistry

- N. Radu, *Organizer*  
C. Tessier, *Presiding*
- 9:00 509.** Mechanistic aspects of the main-group Lewis acid-Lewis base catalysis of the hydrogen transfer. **T. Privalov**
- 9:20 510.** Perchlorinated silanes Si<sub>2</sub>Cl<sub>6</sub> and Si<sub>3</sub>Cl<sub>8</sub> as sources of SiCl<sub>2</sub>. **F. Meyer-Wegner**
- 9:40 511.** Emerging chemistry of anionic N-heterocyclic dicarbenes. **Y. Wang**, M. Y. Abraham, Y. Xie, P. v. Schleyer, G. H. Robinson
- 10:00 512.** Electronic and molecular structures of novel dioxo technetium(V) complexes. **M. K. Edwards**, S. Chatterjee, Z. Wang, S. A. Bryan
- 10:20** Intermission.
- 10:35 513.** Interactions of Group 15 superacids with chlorophosphazenes. **Z. Tun**, M. J. Panzner, D. J. Bowers, A. J. Heston, V. Scionti, S. K. Ekanayake, C. Westdemiotis, P. L. Rinaldi, W. J. Youngs, **C. A. Tessier**
- 10:55 514.** Evidence for a S-S half bond in a Ni(II/III) cyclopentadiene complex. **S. A. Yao**, A. Baum, J. F. Berry
- 11:15 515.** Dibrigehead diphosphines that turn themselves inside-out: Molecular recognition and coordination behavior. **M. Stollenz**, M. Barbasiewicz, J. A. Gladysz

Section D

### Inorganic Catalysts

- S. Koch, *Organizer, Presiding*
- 9:00 516.** Strategies for the coordination and activation of weakly  $\pi$ -acidic, poorly reactive substrates by transition metal centers in strongly basic media. **B. G. Hashiguchi**, **M. M. Konnick**, S. M. Bischof, R. A. Periana
- 9:20 517.** Nucleophilic CH activation accelerated by strongly basic solvents.

- B. G. Hashiguchi**, K. J. Young, M. Yousuffuddin, W. A. Goddard, R. A. Periana
- 9:40 518.** Redox storage in pyridylpyrrolide-metal complex: Synthesis and reactivity. **A. K. Das**, K. Pal, C. Chun-Hsing, K. G. Caulton
- 10:00 519.** Synthesis of C<sub>3</sub>-symmetric P-stereogenic triphosphine ligands. **M. F. Cain**, R. P. Hughes, D. S. Glueck, J. A. Golen, A. L. Rheingold
- 10:20** Intermission.
- 10:25 520.** Experimental and computational design of lignin depolymerization catalysts. **S. C. Chmely**, S. Kim, Y. J. Bomble, C. Chang, L. Moens, M. R. Nimlos, G. T. Beckham
- 10:45 521.** Comparison of copper and vanadium homogeneous catalysts for aerobic oxidation of lignin models. **B. Sedai**, C. Díaz-Urrutia, R. T. Baker, R. Wu, L. A. Silks, S. K. Hanson
- 11:05 522.** Structural implications of intermediates and degradation products in the reduction of carbon dioxide using Re(bpy)(CO)<sub>3</sub>Cl. **E. E. Benson**, J. M. Smieja, F. Mariskal, C. P. Kubiak
- 11:25 523.** Mechanical effects on nanocrystal growth in solution. **C. Wang**

### Reaction Mechanisms in Environmental Organic Chemistry

- Sponsored by ENVR, Cosponsored by GEOC and INOR
- WEDNESDAY AFTERNOON**

Section A

### Organometallic Chemistry Applications to Materials and Polymer Science

- N. Radu, *Organizer*  
Z. Guan, *Presiding*
- 1:30 524.** Atom economic synthesis of functional polymers from simple monomers via late transition metal catalysis. **Z. Guan**
- 1:50 525.** Highly active multidentate alkyne metathesis catalysts and their applications in 3D molecular cage synthesis. **K. Jyothish**, Q. Wang, C. Zhang, **W. Zhang**
- 2:10 526.** Organometallic and coordination compounds as n and p dopants in organic electronics. **S. Barlow**, Y. Qi, C. K. Chan, T. Sajoto, S. Tiwari, W. Zhao, B. Kippelen, S. R. Marder, A. Kahn
- 2:30 527.** Dinuclear catalysts for the copolymerization of cyclohexene oxide and CO<sub>2</sub>. **M. R. Kember**, F. Jutz, A. J. White, A. Buchard, C. K. Williams
- 2:50 528.** Rapid and precision synthesis of sustainable polymers from naturally renewable methylene butyrolactones using organometallic catalysts. **E. Chen**
- 3:10** Intermission.
- 3:20 529.** Improvements in a novel polymerization when converting from a

- step-growth to chain-growth mechanism. **M. C. Brannock**, C. B. Gorman
- 3:40 530.** Stereocontrolled synthesis of poly(lactic acid) polymer stars. **M. P. Shaver**, D. J. Cameron
- 4:00 531.** Organometallic bioresponsive polymers and nanogel particles as MRI contrast agents. **E. A. Schopf**, J. Sankaranarayanan, J. Morachís, A. Almutairi
- 4:20 532.** Pentafluorophenyl-terpyridine metal complexes as monomers for *para*-fluoro-thiol *clicking* polymers. **A. Wild**, A. Winter, M. D. Hager, U. S. Schubert
- 4:40 533.** Alternating  $\alpha$ -olefin distributions in chromium-catalysed ethylene oligomerisation. **A. K. Tomov**, J. D. Nobbs, G. J. Britovsek\*, V. C. Gibson\*

Section B

### Chemistry of Materials

- C. Lugmair, *Organizer*  
B. Bartlett, *Presiding*
- 1:30 534.** Ordered mesoporous silicas with closed pores. **M. Mandal**, L. Huang, C. Hui, **M. Kruk**
- 1:50 535.** Role of iron in mackinawite (Fe<sub>1+x</sub>S): A theoretical study. **J. Brgoch**, G. J. Miller
- 2:10 536.** Computational study of d<sup>10</sup> trinuclear cyclic complexes for metal-organic electronics applications. **B. Chilukuri**, T. R. Cundari, M. A. Omary
- 2:30 537.** Single crystal high field magnetization measurements of the candidate spin liquid herbertsmithite, ZnCu<sub>3</sub>(OH)<sub>6</sub>Cl<sub>2</sub>. **D. E. Freedman**, T. H. Han, Y. S. Lee, D. G. Nocera
- 2:50 538.** Giant magnetoresistance in oxypnictides (La,Nd)OMnAs. **A. C. McLaughlin**, E. J. Wildmqn
- 3:10 539.** Magnetic ordering in rare-earth cobalt arsenides with ThCr<sub>2</sub>Si<sub>2</sub> structure type. **C. M. Thompson**, K. Kovnir, M. Shatruk
- 3:30** Intermission.
- 3:40 540.** Exploring the (structural) richness of materials. **M. A. Zwijnenburg**, S. T. Bromley
- 4:00 541.** New insight of the zinc oxide sulfidation reaction. **L. Neveux**, D. Chiche, D. Bazer-Bachi, J. Perez-Pellitero, L. Favergeon, M. Pijolat
- 4:20 542.** Rational design of superhalogens using Wade-Mingos rule. **B. Pathak**, **D. Samanta**, R. Ahuja, P. Jena
- 4:40 543.** From sulfur-amine solutions to metal sulfide nanocrystals: Peering into the oleylamine-sulfur black box. **J. W. Thomson**, K. Nagashima, P. M. Macdonald, G. A. Ozin
- 5:00 544.** Structure, composition, and electrochemistry of lithium manganese oxide spinel cathodes synthesized by hydrothermal methods. **B. M. Bartlett**, X. Hao, B. J. Liddle, S. M. Collins

### Towards Earth Abundant Solar Photocatalysis Water Oxidation/Splitting

- M. Shores, N. Damrauer, *Organizers*  
A. Rappe, *Organizer, Presiding*  
C. Elliott, *Presiding*
- 1:30 545.** Electrodeposition and photoelectrochemistry of CuWO<sub>4</sub> thin-film photoanodes: Toward an inexpensive, Earth-abundant water oxidation photocatalyst. **B. M. Bartlett**, J. E. Yourey
- 1:50 546.** Designing transition metal oxides for visible-light-driven direct water splitting. **P. Khalifah**, L. Wang, D. Weinstein, A. Malingowski, P. Chen, A. Orlov, D. Grills, E. Fujita, K. Maeda, K. Domen, Q. Mi, N. Lewis, M. Hybertsen
- 2:10 547.** Redox-active ligands for low-barrier O–O bond formation at later 3d metals. **J. D. Soper**
- 2:30 548.** Efforts towards multimetallic complexes for multielectronic photoinduced reactions. **C. N. Verani**
- 2:50 549.** Solar water splitting with oxide photoanodes. **D. R. Gamelin**, D. K. Zhong
- 3:20** Intermission.
- 3:35 550.** Buyer beware: Pitfalls and challenges when studying water oxidation chemistry using DFT. **A. E. Clark**, A. Ozkanlar
- 4:05 551.** Water oxidation and reduction using first-row transition metals. **S. Bernhard**, J. A. Kehl, C. Ellis, N. D. McDaniel, S. Metz, T. J. Collins
- 4:25 552.** On the mechanism of water oxidation by the blue dimer. **R. Bianco**, P. Hay, **J. T. Hynes**
- 4:55 553.** Solar fuels catalysis: An all-inorganic leaf comprising earth abundant materials. **D. G. Nocera**
- 5:25** Concluding Remarks.

Section D

### Organometallic Chemistry Synthesis and Characterization

- N. Radu, *Organizer*  
W. Bernskoetter, *Presiding*
- 1:30 554.** Reversible ruthenium molecular switch with visible/thermal actuation. **D. B. Turner**, M. Check, C. Hunter, N. Glavin, C. Turro, N. Leed
- 1:50 555.** Carbon dioxide reduction toward acrylate formation at group VI metal complexes. **W. H. Bernskoetter**
- 2:10 556.** Formation of an imide Ta(NMe<sub>2</sub>)<sub>3</sub>(=NSiMe<sub>3</sub>) through an unprecedented  $\alpha$ -SiMe<sub>3</sub> abstraction by an amide ligand. **J. Abbott**, **B. Sharma**, S. Chen, X. Chen, Z. Xue
- 2:30 557.** Ligand-dependent amido deprotonation vs. hydrogen atom transfer pathways to mononuclear

Ta(IV) terminal imidos of general formula,  $(\eta-C_5Me_5)[N(iPr)C(X)N(iPr)]Ta=N(tBu)(X = Me \text{ and } NMe_2)$ . B. L. Yonke, A. J. Keane, P. Y. Zavalij, L. R. Sita\*

**2:50 558.** Synthesis of heterotrimetallic complexes for electrocatalytic oxidation of ethanol. R. C. Walroth, S. K. Goforth, L. McElwee-White

**3:10 559.** Geometry effects on magnetic coupling in iron(III) ethynylbenzene complexes. W. A. Hoffert, A. K. Rappe, M. P. Shores

**3:30 560.** Early-late heterobimetallics: A comparison of physical properties and reactivity. J. J. Curley, R. G. Bergman, T. D. Tilley

**3:50 561.** Selective C-S bond ring-opening reaction of thietanes by heterodinuclear organotransition metal complexes. S. Komiya, N. Komine, M. Hirano

**4:10** Intermission.

**4:20 562.** Synthesis and characterization of a  $Fe_2(\mu-O)_2$  complex  $\{3,5\text{-}^iPr_2\text{-}Ar^*OFe(\mu-O)\}_2$  with a very short  $Fe \cdots Fe$  separation. C. Ni, G. J. Long, P. P. Power

**4:40 563.** Synthesis of  $[M_4L_4]X_4$  cages ( $M=Ag^I, Cu^I$ ) based on a triangular 2-substituted-benzimidazole ligand and the solution behavior. Q. He

**5:00 564.** Syntheses, X-ray crystal structures, and solution behavior of cationic, two-coordinate gold(I)  $\pi$ -diene complexes. R. E. Brooner, R. A. Widenhoefer

**5:20 565.** Cationic, two-coordinate gold(I)  $\Pi$ -allene complexes: Syntheses, X-ray crystal structures, and dynamic solution behavior. T. J. Brown, A. Sugie, R. A. Widenhoefer

Section F

## Nanoscience

### Metallic Nanostructures

S. Wong, *Organizer*

H. Patterson, S. Humphrey, *Presiding*  
**1:30 566.** Magnetic property integrated gold nanostars. E. Nalbant Esenturk, A. Hight Walker

**1:50 567.** Luminescent gold and silver clusters by chemical and electrochemical route from cationic Au clusters and Au/Ag complexes. I. Arachchige, S. Ivanov

**2:10 568.** Ambient synthesis of atomically precise  $Au_{144}(SR)_{60}$  nanoparticles. H. Qian, R. Jin

**2:30 569.** Ligand-protected gold nanoclusters as "metallic molecules". H. Häkkinen

**2:50 570.** Luminescence and simulation of Cu-Au and Cu-Ag mixed metal nanoclusters in alkali halides. H. H. Patterson, X. Li, Z. Pan, D. A. Welch  
**3:20** Intermission.

**3:40 571.** Microwave-assisted synthesis of rhodium nanoparticles and their

chemistry within mesoporous transition metal oxides. N. Dahal, S. Garcia, S. M. Humphrey

**4:10 572.** New stabilizers for ruthenium nanoparticles: Shape, size, and reactivity control. D. González-Gálvez, P. W. vanLeeuwen, B. Chaudret

**4:30 573.** Advanced materials of bismuth: 1:1 Bismuth-silver nanoalloy and multiwalled carbon nanotubes decorated and filled with nanostructured bismuth. D. Diaz, D. Velasco-Arias, I. Zumeta-Dube, P. Santiago-Jacinto

**4:50 574.** Production submicron and nano metallic particles via reductive/expansion method. H. Zea, C. Luhrs, J. Phillips

**5:10 575.** On the synthesis of cobalt-metal  $Co_xM_{1-x}$  alloy nanoparticles:  $Co_2(CO)_8$  disproportionation and ligand-controlled CoNi and CoFe phase behavior. M. M. van Schooneveld, C. Campos-Cuerva, J. D. Meeldijk, A. Meijerink, F. M. de Groot

Section E

### Coordination Chemistry Characterization and Applications

D. Crans, *Organizer*  
G. Grant, *Presiding*

**2:00 576.** Complexes as ligands: Coordination of Ru (II) diimines to bivalent metal ions. A. Perri, H. D. Gafney, P. Jagasser, G. Ibarrola, Y. Isseroff

**2:20 577.** Electronic properties of innocent compounds probed by solid-state  $^{51}V$  NMR spectroscopy: *o*-Dioxolene vanadium complexes. P. B. Chatterjee, O. Goncharov-Zapata, L. L. Quinn, G. Hou, H. Hamaed, R. W. Schurko, T. Polenova, D. C. Crans

**2:40 578.** Synthesis and reactivity of homo- and heterometallic trinuclear iron and cobalt complexes. D. R. Raad, T. M. Powers, A. R. Fout, T. A. Betley

**3:00 579.** Understanding the OEC structure via molecular Mn coordination complexes using  $^{55}Mn$  solid-state NMR and theory. P. Yang, A. Lipton, J. A. Sears, P. D. Ellis, M. Dupuis

**3:20 580.** Redox chemistry, acid reactivity and hydrogenation reactions of a new class of two-electron mixed valence dirhodium and diiridium complexes. T. S. Teets, D. G. Nocera  
**3:40** Intermission.

**3:50 581.** Pi-pi stacking interactions in cyclometalating and diimine complexes with thiacyclopentadiene ligands. G. J. Grant, N. N. Talbot, D. E. Janzen

**4:10 582.** Toward spin control in new coordination complexes. M. P. Shores, W. A. Hoffert, Z. Ni, B. S. Newell, A. M. McDaniel, S. R. Fiedler, C. M. Klug

**4:30 583.** Complexes of transition metals with an amine triselenolate tripod ligand. S. Zaman, S. A. Koch

**4:50 584.** Synthetic analogs for the active site of NiFe hydrogenase

enzymes. S. Bhattacharya, D. Amarante, M. M. Millar, S. A. Koch  
**5:10 585.** Trace metal chelation properties of the catecholate siderophore protochelin: Implications for the cycling of iron and manganese. J. M. Harrington, J. G. Roberts, A. A. Jarzecki, J. R. Bargar, L. M. Sombers, O. W. Duckworth

### WEDNESDAY EVENING

Section A

### Towards Earth Abundant Solar Photocatalysis

A. Rappe, N. Damrauer, M. Shores, *Organizers*

**6:00 - 8:00**

**586.** Free energy correlations of platinum(II) biphenyl complexes containing 1,10-phenanthroline derivatives. W. Huang, D. Rillema, K. Siam, A. J. Cruz

**587.** Nickel-thiolato complexes for the photocatalytic production of hydrogen from water in a noble metal free system. Z. Han, W. R. McNamara, M. Eum, P. L. Holland, R. Eisenberg

**588.** Synthesis, characterization, and excited state properties of polydentate Schiff base complexes of Cr(III). A. M. McDaniel, H. Tseng, E. A. Hill, N. H. Damrauer, A. K. Rappe, M. P. Shores

**589.** Chemistry of consequence to renewable energy: Multielectron photo- and electrocatalysts for energy storing applications. J. Rosenthal

**590.** Ruthenium photocatalysts for  $CO_2$  reduction. D. J. Boston, K. Huang, N. Tacconi, R. O. Lezna, F. M. MacDonnell

**591.** Selectivity of soluble all-inorganic water oxidation catalyst towards competing decomposition reactions. J. W. Vickers, Y. V. Geletii, Y. Ding, J. Song, Z. Lou, H. Lv, C. L. Hill

**592.** Totally inorganic, stable, and highly efficient cobalt/vanadium-containing molecular catalyst for visible-light-driven water oxidation. H. Lv, J. Song, C. L. Hill

**593.** Bromine photoelimination from organoplatinum(IV) centers: Exploring phosphine ligand variations. A. Raphael Karikachery, M. A. Moody, P. R. Sharp

**594.** Photocatalytic oxidation of hydrocarbons in water by ruthenium complexes. P. P. Kannam, D. Kalita, B. Radaram, B. Brooks, X. Zhao

Section B

### Organometallic Chemistry Applications to Materials and Polymer Science

N. Radu, *Organizer*

**6:00 - 8:00**

**595.** Chemistry behind the curtains: Finding the appropriate click catalyst

for the synthesis of polymers containing photochemically active metal-metal bonds. S. E. Brady, D. R. Tyler

**596.** Expanding the scope of vanadium mediated radical polymerizations. L. E. Allan, M. R. Perry, M. P. Shaver

**597.** Synthesizing and using N-O ligated palladium(II) catalysts to copolymerize functionalized norbornene and ethylene. F. Pong, S. Mandal, A. Sen

Section C

### Organometallic Chemistry Synthesis and Characterization

N. Radu, *Organizer*

**6:00 - 8:00**

**598.** Preparation of Ru(II) complexes with the strained phosphite 4-methyl-2,6,7-trioxo-1-phosphabicyclo[2,2,1]heptane: Comparison to other phosphines systems and attempted development of catalysts for olefin hydroarylation. E. E. Joslin, T. B. Gunnoe, M. Sabat

**599.** Self-assembly of 3,6-bis(4-triazolyl)pyridazines ligands with Cu(I) and Ag(I) ions: Time-dependant 2D-NOESY and ultracentrifuge measurements. A. Winter, B. Happ, G. M. Pavlov, E. Altuntas, C. Friebe, M. D. Hager, H. Görls, W. Günter, U. S. Schubert

**600.** Rational design of reactive  $M\equiv X$  ( $X = N, ML_n$  and CR) fragments supported by trianionic pincer ligands and their relevance to atom transfer, bond activation, and metathesis chemistry. S. Sarkar, S. Kuppaswamy, I. Ghiviriga, K. A. Abboud, A. S. Veige

**601.** Development of new  $^{99m}Tc/^{188}Re$ -tricarbonyl complexes with modified ML-10 ligands for molecular imaging and therapeutic agents. M. Yang, S. Park, J. Lee, H. Lee

**602.** Preparation of conductive metal complexes and their usage as paste or ink. J. Gu, H. Woo, H. Lee

**603.** Aerobic oxidation of (dpms)Pt<sup>II</sup>Me(X) complexes in water: New reaction directions and mechanistic insights ( $X = I, OH$ ). A. V. Sbergaeva, A. N. Vedernikov

**604.** Facile  $\kappa^3/\kappa^2$  interconversions for reversible C-H activation and C-C bond formation using a tris-triazolyl-based scorpionate ligand. B. E. Frauhiger, P. S. White, J. L. Templeton

**605.** Synthesis and reactions of abnormal C-4 bound NHC complexes of Pt-Sn complexes. V. Yempally, L. Zhu, D. Isrow, G. Fortman, B. Captain, C. D. Hoff

**606.** Synthesis and characterization of dirhenium-alkyne complexes. D. Esjornson

**607.** Influence of dinuclear constrained geometry catalysts containing xylene bridge with alkyl branches on ethylene

and 1-hexene copolymerization. **T. Nguyen**

**608.** Oxidative functionalization of Pt<sup>II</sup> hydrocarbyls enabled by novel anionic borate ligands. **S. Pal**, A. N. Vedernikov

**609.** Dinuclear gold(I)  $\sigma,\Pi$ -acetylide complex formation via gold(I)  $\Pi$ -alkyne complexes: Kinetics and mechanism. **T. J. Brown**, R. A. Widenhoefer

**610.** Molecular gyroscopes based on osmium via alkene metathesis in the metal coordination sphere: Synthesis and characterization. **T. Fiedler**, J. A. Gladysz

Section D

## Main Group Chemistry

N. Radu, *Organizer*

**6:00 - 8:00**

**611.** Synthesis of carborane cluster containing macrocycles for use in dye-sensitized solar cells. **C. R. Petrelli**, B. Fitzgerald, J. T. Spencer

**612.** Comparison of two solution routes to passivated silicon nanoparticles. **A. L. Holmes**, T. M. Atkins, S. M. Kauzlarich

**613.** Reductive dehalogenation of brominated and iodinated CB<sub>10</sub>H<sub>12</sub><sup>-</sup> anions with KC<sub>8</sub>. **C. Douvris**, M. T. Holden, J. Michl

**614.** Synthesis of the bifunctional ambiphilic molecule 2-(picolyl)trimethylstannane and study of its kinetics of hydrolysis. **W. Kang**, C. Balasanthiran, S. T. Pillai, J. Hoefelmeyer

**615.** Preparation of new phosphazenes via copper catalyzed Huisgen type click reactions. **C. Kumas**, P. Devulapalli, P. Wisian-Neilson

**616.** Bifunctional ambiphilic molecules featuring frustrated Lewis pairs. **J. D. Hoefelmeyer**

**617.** Addition reaction of unsaturated groups (nitrile, ketone, aldehyde and amide) to B-C(benzyl) bond of ambiphilic molecule 2-picolyl dialkyl- or diarylborane dimer. **J. Son**, J. D. Hoefelmeyer

Section D

## Organometallic Chemistry New Ligand Platforms

N. Radu, *Organizer*

**6:00 - 8:00**

**618.** Pincer-type triazolium and triazolylidene ligands: Complexes of sulfate and ruthenium(II) ions. **B. Schulze**, C. Friebe, D. Escudero, M. D. Hager, H. Görls, U. Köhn, W. Günther, L. González, U. S. Schubert

**619.** Discrepancy between large ground-to-CT state electronic coupling revealed by ultrafast visible-pump/Mid-IR-probe spectroscopy and no apparent charge transfer absorption intensity in

cofacially aligned [Ru(tpy)<sub>2</sub>]<sup>2+</sup>-quinone system. **H. Kim**, J. Park, Y. Kang, Y. Chung

**620.** Different PNP pincer type ligands: Their syntheses, metal complexes and reactivity. **Y. Zhu**, O. V. Ozerov

Section F

## Coordination Chemistry Characterization and Applications

D. Crans, *Organizer*

**6:00 - 8:00**

**621.** Silver(I) coordination polymers of bulky thiophenylether substituted aromatic compounds with porous structure. **Y. Suenaga**

**622.** Monovalent metal salts of the superweak anion B<sub>12</sub>F<sub>12</sub><sup>2-</sup>: Crystal structure transformations during reversible binding of solvent molecules. **E. V. Bukovsky**, K. W. Lui, D. V. Peryshkov, S. H. Strauss

**623.** Structures and anion exchange in layered salts of the 1,1',3,3'-Tetrakis(2-methyl-2-nonyl)ferrocenium(1+) cation. **K. Lui**, E. V. Bukovsky, S. Caamaño, G. N. Hebert, B. S. Newell, B. J. Clapsaddle, S. H. Strauss

**624.** Synthesis and characterization of mono and bimetallic Os(II) and mixed metal Os(II)/Ru(II) complexes with tppz (tppz = 2,3,5,6-tetra(2-pyridyl)pyrazine) the bridging ligand and dpop' (dpop' = 2,3-a:3',2'-j)phenazine:3',2'-j)phenazine) the terminal ligand. **R. R. Ruminski**, R. Padilla, V. A. McGinley, P. B. Williams

**625.** Rhenium and manganese compounds of di-2-pyridyl ketone hydrazones. **M. Bakir**, O. Green, C. Gyles, O. Brown

**626.** Structurally diverse Ru(II), Pt(II) and Os(II), Ru(II), Pt(II) polyazine-bridged supramolecular complexes. **J. D. Knoll**, S. M. Arachchige, K. J. Brewer

**627.** Aerial oxidation of HS<sup>-</sup> catalyzed by a mixed-valent (II/III) diruthenium complex, a near infrared molecular probe for sensitive and selective detection of HS<sup>-</sup>. **Y. Quek**, Z. Liu, C. Tan, D. Huang

**628.** Dinitrogen reduction to ammonia: Low-energy alternatives to Haber-Bosch. **C. G. Balesdent**, J. L. Crossland, D. R. Tyler

**629.** Effects of ligand perturbations on the electronic structures of peroxomanganese(III) adducts. **G. B. Wijeratne**, R. A. Geiger, T. A. Jackson

**630.** Synthesis and characterization of sterically encumbered  $\beta$ -ketoiminate complexes of iron(II) and zinc(II). **D. M. Granum**, P. J. Riedel, J. A. Crawford, T. K. Mahle, C. M. Wyss, A. K. Begej, N. Arulsamy, B. S. Pierce, **M. P. Mehn**

**631.** Investigating the anion dependence of spin crossover for tripodal hexadentate iron complexes. **C. M.**

**Klug**, A. M. McDaniel, S. R. Fiedler, M. P. Shores

**632.** Synthesis and characterization of polyoxometalates for energy storage applications. **H. D. Pratt**, D. Ingersoll, T. M. Alam, A. J. Rose, T. M. Anderson

**633.** 3D structure of vanadium framework constructed by 1,2,4,5-benzenetetracarboxylate. **O. In-noi**, G. S. Nichol, J. H. Enemark, D. L. Lichtenberger, K. J. Haller

**634.** Vanadium chemistry of a siderophore: Reporting an unprecedented solid-to-solid irreversible transformation from an oxovanadium(IV) to a *cis*-dioxovanadium(V) compound. **P. B. Chatterjee**, D. C. Crans

**635.** Synthesis and characterization of a metformium decavanadate compound. **A. Chatkon**, K. J. Haller, D. C. Crans

**636.** Effect of stability on membrane interaction and mode of action in metal-containing drugs. **A. M. Trujillo**, P. B. Chatterjee, D. C. Crans

**637.** Studies toward modeling the active site chemistry of Fe-ARD'. **C. J. Allpress**, L. M. Berreau

**638.** Photochemical nitric oxide delivery from iron sulfur nitrosyl clusters. **J. V. Garcia**, P. C. Ford, G. D. Stucky, L. Li, R. Wang, F. Zhang

**639.** Click SBA-15: Controlling immobilization of discrete metal complexes in mesoporous silica through "click" attachment, and the impact of surface density on oxidation catalysis. **B. J. Smith**, J. Nakazawa, T. P. Stack

**640.** Preparation, crystal structure, molecular magnetism and oxidation catalysis of transition metal complexes with *N,N*-bis(2-pyridylmethyl)-2-aminoethanol-ate. **J. Won Shin**, S. Kim, S. Rowthu, C. Kim, **K. Kil Sik Mina**

**641.** Self-assembly of discrete and 2D chiral coordination compounds: Structure and chiral recognition. **S. Kim**, J. Shin, S. Rowthu, J. Ryoo, **K. Min**

Section G

## Coordination Chemistry Synthesis

D. Crans, *Organizer*

**6:00 - 8:00**

**642.** Presynthesized and in situ generated tetrazolate ligand in the design of chiral cadmium coordination polymer. **K. Lu**, C. Chang, Y. Huang, S. Huang, J. Wu, Y. Liu

**643.** Calixcrown capsules: Homo- and heteromultinuclear complexes of calix[6]-*mono*-crowns. **I. Park**, K. Park, J. Vicens, S. Lee

**644.** Synthesis, structures, and characterization of dioxo-molybdenum (VI) complexes with N<sub>2</sub>O<sub>2</sub> tetradentate

ligands. **X. Lei**, M. Thummaluru, S. Mahammad

**645.** Bis(pyridyl)mercaptoimidazoles: New [N<sub>2</sub>S] mixed-donor ligands. **J. M. Hanley**, D. Rabinovich

**646.** Elemental selenium activation by nickel(I) complex and the synthesis of high-spin nickel(II) organoselenide complexes. **Y. Huang**, G. P. Yap, C. G. Riordan

**647.** Utilizing carboxylate lability in the synthesis of mixed ligand copper (II) dimers and tetramers. **T. W. Clayton**, T. Helgren, C. L. Coley, B. Murphy

**648.** Synthesis of multidentate ligands for bimetallic complexes. **Y. Tsai**, L. Luo, **Q. Zhao**

**649.** Synthesis of bipyridine derivatives and bis-bipyridine scaffolds for metal complexation and hydrogen production. **A. A. Pearson**, J. Hoberg, J. Huo, J. Buffington

**650.** Substitution stable Ru(II) nitriles exhibiting unprecedented ambient temperature luminescence. **D. J. Ceckanowicz**, K. R. Mann

## Reaction Mechanisms in Environmental Organic Chemistry

Sponsored by ENVR, Cosponsored by GEOC and INOR