INOR

Division of Inorganic Chemistry

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

SUNDAY MORNING

Section A

Renaissance Washington, DC
Downtown
Renaissance East

Fundamental Aspects of Metal Organic Framework Catalysis

MOFs for Chemical Warefare Agent Degradation

A. J. Morris, J. R. Morris, *Organizers, Presiding*

8:30 1. Robust surface-anchored UiO-66-based metal-organic-framework films on polymer fibers for rapid hydrolysis of chemical agents. **G. Parsons**, J. Zhao, D.T. Lee, H.F. Barton

9:00 2. Metal organic framework's acid dissociation constants as a robust descriptor of their morphology and reactivity: Applications to hydrolysis of warfare agents. **M. Momeni**, C.J. Cramer

9:30 Intermission.

9:45 3. Reaction of the chemical warfare agent simulant, DMMP(*g*), with zirconium (IV) MOFs: An ultrahigh-vacuum and DFT study. **G. Wang**, C.H. Sharp, A. Plonka, Q. Wang, A. Frenkel, W. Guo, C.L. Hill, C. Smith, J. Kollar, D. Troya, J.R. Morris

10:15 4. Molecular modeling insights into the adsorption and degradation of hazardous chemical warfare agents by metal-organic frameworks. **J. Harvey**, D.F. Sava Gallis, J.A. Greathouse

10:45 5. Optimizing toxic chemical removal through defect-induced UiO-66-NH_2 metal-organic framework. **G.W. Peterson**, M. Destefano, S.J. Garibay, A. Ploskonka, M. Hall, C.J. Karwacki, J.T. Hupp, O.K. Farha

Section B

Renaissance Washington, DC
Downtown
Renaissance West A

Personal & Global Energy Conversion in Chemistry & Biology

C. J. Chang, M. Kanan, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 6. Photocatalytic oxidation of bromide to bromine by using ruthenium polypyridyl complexes. **I. Chang**, K. Tsai

9:00 7. Multimetallic systems for the photocatalytic production of fuels from abundant sources. **C. Turro**

9:25 8. Thermally and photochemically activated diradicals: Applications to catalysis and nanoreagents for CO_2 reduction. **J.M. Zaleski**

9:50 9. Luminescent nanoparticles coated with metal complexes for biomedical applications. **Z. Pikramenou**

10:15 Intermission.

10:30 10. Designing and understanding catalysis with high valent metals. **A.L. Odom**, T. McDaniel, B. Billow, K. Aldrich

10:55 11. Hydrogen-atom non-innocence of an azanidodithiolate pincer ligand. **A.F. Heyduk**, K.E. Rosenkoetter, B. Charette

11:20 12. Follow the protons: Directly monitoring proton transfer mechanisms with ultrafast continuum mid-IR spectroscopy. A.M. Stingel, **P.B. Petersen**

Section C

Renaissance Washington, DC
Downtown
Grand Ballroom South

Environmental & Energy-Related Inorganic Chemistry

S. A. Koch, *Organizer*
K. L. Hull, W. R. McNamara, *Presiding*

8:30 13. Specific ion effect manifested in oxidation of ammonium salts and inorganic substrates. **K.L. Hull**, A. Cairns, M. Haq

8:50 14. Supercharging electrocatalysts for carbon dioxide reduction. S. Sung, D. Kumar, S. Park, **M. Nippe**

9:10 15. Selective partial oxidation of light alkanes using iodine oxides and halides. **N. Schwartz**, G. Fortman, S.E. Kalman, R. Fu, R.J. Nielsen, N. Boaz, W.A. Goddard, J.T. Groves, T.B. Gunnoe

9:30 16. Solar-powered biofertilizer production: An electro-augmented nitrogen and phosphorus cycle. **K.K. Sakimoto**, P.A. Silver, D.G. Nocera

9:50 17. Iron complexes for hydrogen generation from aqueous solutions. **W.R. McNamara**

10:10 18. Development of continuous high-pressure hydrogen evolution from formic acid by Iridium homogeneous catalyst and its kinetic study under pressurized conditions. **H. Kawanami**, M. Iguchi, Y. Himeda

10:30 Intermission.

10:40 19. Photochemistry of iron(III) carbenes. **L.A. Fredin**, P. Chábera, R. Lomoth, V. Sundstrom, K. Warnmark, P. Persson

11:00 20. Heterometallic molecular precursors for lithium-iron oxide cathode material. **E. Dikarev**, H. Han

11:20 21. Generalities related to reduction of nitrogen oxyanions: Ligand design aids metal reducing agents. **K.G. Caulton**, J. Seo, A. Cabelof, C. Chen, D.M. Beagan

11:40 22. Tuning the second coordination sphere of group VII polypyridyl electrocatalysts for selective reduction of CO2 to formate. **M.E. McKinnon**, K.T. Ngo, M.Z. Ertem, D.C. Grills, J.J. Rochford

12:00 23. Light-driven H_2 production by coupling Ni/Pt diimine ditiholate complexes with Pt-TiO_2. **G. Li**, M. Mark, D.W. McCamant, R. Eisenberg

12:20 24. Electrocatalytic reduction of CO_2 to formate using cobalt complexes. **P. Kang**, F. Liu

Section D

Renaissance Washington, DC
Downtown
Renaissance West B

Electronic Structure Contributions to Function: From Metals in Biology to Materials Science

From Metals in Biology to Materials Science

A. Dey, L. Quintanar, *Organizers*
P. Chen, A. E. Palmer, *Organizers, Presiding*

8:30 25. Living with oxygen. **H.B. Gray**

8:55 26. Hydroquinone ring-cleaving dioxygenases: Enzymes and model complexes. **T.E. Machonkin**

9:20 27. Structure/function relationships in cysteine and cysteamine dioxygenases. **T.C. Brunold**

9:45 28. Redox active metals In Alzheimer's disease. **S. Ghosh Dey**

10:10 29. Metal-induced aggregation of human gamma-crystallins: Relevance to cataracts disease. **L. Quintanar**, J. Dominguez-Calva, M. Perez-Vazquez, E. Martinez-Jurado, E. Serebryany, J. King

10:35 Intermission.

10:50 30. Calorimetric measurements of Zn(II) and Co(II) binding to protein sites: Can a spectroscopic probe be a thermodynamic surrogate? **D. Wilcox**

11:15 31. Rationalized design of site-differentiated Fe-S clusters in peptides and nanoclays. **R.K. Szilagyi**

11:40 32. Diatomic gas binding and sensing mechanism of hemoprotein studied by nuclear resonance vibrational spectroscopy. **T. Ohta**

12:05 33. Electronic structure contributions to molecular rectification. **M.L. Kirk**, R. Dangi, L. Ingersol, D.A. Shultz

Section E

Renaissance Washington, DC
Downtown
Grand Ballroom North

Chemistry of Materials

Materials for Energy & Catalytic Applications

C. G. Lugmair, *Organizer*
H. Djieutedjeu, *Presiding*

8:30 34. *Ab initio* assessment of $Bi_{1-x}RE_xCuOS$ (RE=La, Gd, Y, Lu) solid solution for water splitting. **S.F. Lardhi**, L. Cavallo

8:50 35. Accelerated computational design of mixed protonic and electronic conductors for H_2 separation. **Q. Bai**, Y. Zhu, X. He, E.D. Wachsman, Y. Mo

9:10 36. Effects of solution and solid state synthesis routes on the material properties of $Sr_2Fe_{1.5}Mo_{0.5}O_{6-\delta}$ solid oxide fuel cell anodes. **J. Jenkins**, B.C. Eigenbrodt

9:30 37. Probing porosity-dependent activity towards electrocatalytic CO_2 reduction on metal-decorated carbon aerogel. **X. Han**, V. Thoi

9:50 38. Electrochemical oxygen reduction on earth-abundant rich palladium alloys. **S. Hall**, D. Sun

10:10 39. High-yield ammonia synthesis via an electrochemical cycling process using N_2 and H_2O at atmospheric pressure. **J.M. McEnaney**, A. Singh, J. Schwalbe, J. Kibsgaard, J. Lin, M. Cargnello, T.F. Jaramillo, J.K. Norskov

10:30 Intermission.

10:45 40. Oxygen-evolving electrocatalysts for use in highly acidic solutions. **J. Mondschein**, R.E. Schaak

11:05 41. Size-controlled PtZn intermetallic nanoparticles for catalytic electro-oxidation. **W. Huang**, Z. Qi

11:25 42. Photocatalytic methane conversion using shape-controlled semiconductor microcrystals. **B. Sadtler**

11:45 43. Synthesis of WQ_2/CoQ_2 and WQ_2/CoQ (Q = S, Se) nanostructure for electrocatalyst and hydrogen evolution reaction. **H. Djieutedjeu**, B.S. Guiton, M. Thomas, Y. Lei

12:05 44. Enhanced cycling stability of sulfur electrodes through effective binding of pyridine-functionalized conjugated polymer. **Y. Tsao**

Section F

Renaissance Washington, DC
Downtown
Grand Ballroom Central

Organometallic Chemistry

New Ligand Platforms

N. S. Radu, *Organizer*
S. R. Daly, D. Genna, *Presiding*

8:30 45. Tridentate π-extended carbanionic donor sets for Ru^{II} polypyridyl-type photosensitizer. **M. Jaeger**, T. Schlotthauer, G. Parada, H. Goerls, S. Ott, U.S. Schubert

8:50 46. Indecisive metal: Multivalent cobalt complexes featuring hemilabile [SNS] ligands. **C.E. Hayes**, B.W. Fitchett, A.J. de Aguirre, F. Maseras, C. Bucher, W.D. Jones, R.T. Baker

9:10 47. Electron-rich organometallic platforms involving an asymmetrically anchored 6,6'-biazulenic π-linker. **M.V. Barybin**, J.C. Applegate, C.L. Berrie, N.R. Erickson, M.K. Okeowo

9:30 48. Highly active, phase-separable and recyclable bipyridine linked polyisobutylene oligomers ligands based catalysts for iridium catalyzed C-H borylation reaction. **S. Madrahimov**, H. Mamlouk, D.E. Bergbreiter

9:50 49. Synthesis and reactivity of fluorescent metal complexes. **Z.M. Heiden**, N.R. Treich

10:10 50. Asymmetric tris(2-aminoethyl)amine (tren) ligands. **D.R. Manke**

10:30 51. Cooperative ligand-centered reactivity in triaminoborane-bridged diphosphine complexes. K. Lee, C.M. Donahue, **S.R. Daly**

10:50 52. Reduction of air-stable phosphine precursors and isolation of volatile 1°, 2°, and 3° phosphines on the gram scale. N.I. Rinehart, **A.J. Kendall**, D.R. Tyler

11:10 53. Diastereoselective and enantioselective synthesis of P-stereogenic *syn*-phosphiranes from chiral epoxides: Stereochemistry and mechanism. **J.A. Muldoon**, B. Varga, M. Deegan, T. Chapp, R.P. Hughes, D.S. Glueck, C. Moore, A.L. Rheingold

11:30 54. Role of chelating P-Si ligands on group 9 metal centers: Applications in alkene functionalization. **D. Genna**

Section G

Renaissance Washington, DC
Downtown
Congressional A

Chemistry of Materials

Nanomaterials

C. G. Lugmair, *Organizer*
E. B. Cerkez, M. A. Ochoa, *Presiding*

8:30 55. Synthesis and plasmonic properties of early transition metal nitride powders and nanomaterials. **A.P. Purdy**, O.A. Baturina, B. Simpkins, S.L. Giles

8:50 56. Gold nanoclusters promote electrocatalytic water oxidation at the nanocluster/$CoSe_2$ interface. **S. Zhao**, R. Jin

9:10 57. Energy transfer, heat and dissipation in molecule-metal nanosystems. **M.A. Ochoa**, A. Nitzan

9:30 58. Orientational order controls crystalline and amorphous thermal transport in superatomic crystals. W. Ong, E. O'Brien, A. McGaughey, J. Malen, **X. Roy**

9:50 59. Synthesis of lanthanide doped nano-spinels as hosts for down-shifting phosphors. **D.A. Hardy**, G.F. Strouse

10:10 60. Synthesis and magneto-optical properties of europium sulfide-europium selenide solid solution colloidal nanocrystals. **N. Rosa**, H.A. Dalafu, D.J. James, S. Omagari, A. Kawashima, T. Nakanishi, Y. Hasegawa, S.L. Stoll

10:30 Intermission.

10:45 61. Photochemistry of gold Nanoparticle sensitized ferritin protein. **E.B. Cerkez**, K. Dutton, M. Kukulka, A. Valentine, D.R. Strongin

11:05 62. Thermoelectric performance of tetrahedrite synthesized by a modified polyol process. D. Weller, G. Kunkel, A. Ochs, D. Stevens, C. Holder, D. Morelli, **M.E. Anderson**

11:25 63. Drug delivery using layered structured nanomaterials. **J.L. Colon**, J. González-Villegas, Y. Kan, V. Bahkmutov, A. Clearfield

11:45 64. Mesoporous SiO_2 nanoparticle based thermally insulating transparent barrier coatings for single-pane windows. **Y. Yan**, S. King, M. Li, T. Galy, S.H. Tolbert

What do Synthetic Chemists Want from Their Reaction Systems?

Sponsored by CINF, Cosponsored by COMP, INOR, MEDI and ORGN

SUNDAY AFTERNOON

Section A

Renaissance Washington, DC
Downtown
Renaissance East

Fundamental Aspects of Metal Organic Framework Catalysis

A. J. Morris, J. R. Morris, *Organizers*
W. Huang, *Presiding*

1:30 65. Insights into the MOF-based degradation of organophosphates in non-aqueous media: A combined experimental-modeling study. **D.F. Sava Gallis**, C.J. Pearce, M.K. Kinnan, J.B. DeCoste, H. Jacob, J. Greathouse

2:00 66. Uptake and diffusion of chemical warfare agent simulants in Zr_6-based MOFs. **C.H. Sharp**, N.B. Jones, W. Guo, C.L. Hill, F.A. Houle, J.R. Morris

2:30 67. Metal–organic frameworks as highly functional catalytic arrays. **O.K. Farha**

3:00 Intermission.

3:15 68. Modeling reactions catalyzed by noble metal clusters deposited on metal-organic frameworks. **A. Mavrandonakis**, S.L. Pellizzeri, R. Getman, V. Bernales, A.B. Martinson, B.C. Gates, J.T. Hupp, O.K. Farha, L. Gagliardi, C.J. Cramer

3:45 69. Tandem catalysis by metal@MOFs with extremely high selectivity. **W. Huang**, X. Li, B. Zhang

4:15 70. Nanospace within metal-organic frameworks: Plenty of opportunities for heterogeneous catalysis. **S. Ma**

Section B

Renaissance Washington, DC
Downtown
Renaissance West A

Personal & Global Energy Conversion in Chemistry & Biology

C. J. Chang, M. Kanan, *Organizers, Presiding*

1:30 71. Synthetic biology approaches to new chemistry. **M. Chang**

1:55 72. Chemical approaches to studying redox biology in living systems. **C.J. Chang**

2:20 73. Controlling non-radiative decay in transition metal chromophores using structure and spin. **N.H. Damrauer**, S.M. Fatur, S. Shepard

2:45 74. How defects and proton-intercalation in WO_3 impact its activity for the photoelectrochemical oxygen evolution reaction. **B.M. Bartlett**

3:10 Intermission.

3:30 75. Catalysts for cyclic polymer synthesis. S. Nadif, S.A. Gonsales, T. Kubo, C.D. Roland, K.A. Abboud, B.S. Sumerlin, **A.S. Veige**

3:55 76. Radical control at terminal metal oxos. **J.D. Soper**

4:20 77. Metal-carbon bond forming reactions for luminescent materials. **T.G. Gray**

4:45 78. Understanding and harnessing spin in photoredox catalysis using first row transition series complexes. **M.P. Shores**

Section C

Renaissance Washington, DC
Downtown
Grand Ballroom South

Organometallics Distinguished Author Symposium in honor of Alexander Miller

P. J. Chirik, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 79. Using catalysis, mechanistic inquiry and collaboration to find sustainable methods for the production of chemicals and fuels. **K.I. Goldberg**

2:10 80. Mechanism, rate, and selectivity consequences of sulfur ligands in cross-dehydrogenative coupling. **B.P. Carrow**, L. Wang, B. Gorsline, P. Ren

2:45 Intermission.

3:00 81. Excited state behavior of platinum(II) charge transfer dimers. **F.N. Castellano**

3:35 82. Cation-responsive pincer-crown ether complexes for tunable and switchable catalysis. **A.J. Miller**, M.R. Kita, J.B. Smith, J. Grajeda, L. Gregor, A. Sullivan, A. Camp

Section D

Renaissance Washington, DC
Downtown
Renaissance West B

Electronic Structure Contributions to Function: From Metals in Biology to Materials Science

From Metals in Biology to Materials Science

A. Dey, A. E. Palmer, *Organizers*
P. Chen, L. Quintanar, *Organizers, Presiding*

1:30 83. Synthetic heme-O_2-copper assemblies and reductive O-O cleavage chemistry. **K.D. Karlin**

1:55 84. Iron-catalyzed cross-coupling: Intermediates and mechanism. **M.L. Neidig**

2:20 85. Modeling the active site and reactivity of flavodiiron nitric oxide reductases. **N. Lehnert**

2:45 86. Computational electrochemistry of mononuclear non-heme iron complexes: Redox properties and their contributions to reactivity. D. Bím, **M. Srnec**

3:10 87. Insight into the electronic structure of transition metal ion complexes from resonant inelastic X-ray scattering. **T. Kroll**, R. Hadt, S.A. Wilson, M. Baker, M. Lundberg, J.J. Yan, T. Weng, D. Sokaras, R. Alonso-Mori, D.M. Casa, M.H. Upton, B.G. Hedman, K.O. Hodgson, E.I. Solomon

3:35 Intermission.

3:50 88. Thermal and optical spin-state switching of surface-adsorbed iron complexes. **F. Tuczek**

4:15 89. Group 11 metal(I) polynuclear complexes with the substituted pyrazolates: New strategy to make metal...metal interaction. **K. Fujisawa**

4:40 90. Development of synthetic functional models of iron only hydrogenase. **A. Dey**

5:05 91. Extension of the redox principle in nature to synthetic systems. **K. Park**

Section E

Renaissance Washington, DC
Downtown
Grand Ballroom North

Inorganic Nanoscience Award

Financially supported by University of South Carolina NanoCenter
J. E. Goldberger, *Organizer, Presiding*

1:30 Introductory Remarks.

1:40 92. Tracking rare cells and biomolecules using nanostructured materials. **S.O. Kelley**

2:10 93. Sensors using DNA charge transport. **J.K. Barton**

2:40 94. Tailoring optoelctronic, magnetic, and topological phenomena in group 14-containing honeycomb 2D materials. **J.E. Goldberger**

3:10 95. Unlocking the materials genome through combinatoric nanoscience. **C.A. Mirkin**

3:40 Intermission.

3:55 96. Single-particle sensors for nano-bio interactions. **T.W. Odom**

4:25 97. Tuning protein display with nanoparticle surface chemistry. **C.J. Murphy**

4:55 98. Nanobiosensor arrays for multiplexed measurements of the spatiotemporal dynamics of neurotransmitters and microbiome signalomics. **P.S. Weiss**, A.M. Andrews

Section F

Renaissance Washington, DC
Downtown
Grand Ballroom Central

Organometallic Chemistry

Catalysis-Late Transition Metals

N. S. Radu, *Organizer*
L. Tahsini, A. G. Tennyson, *Presiding*

1:30 99. Synthesis, structural properties and catalytic application of pincer N-heterocyclic carbene complexes of copper(I) with small wingtip substituents. **L. Tahsini**

1:50 100. Catalytic asymmetric P-C bond formation via chiral Cu(I)-phosphido complexes. **S.K. Gibbons**, D.S. Glueck, A.L. Rheingold

2:10 101. Aerobic catalytic oxidative functionalization of methane by Pt(II)/Cu(II) bimetallic system in trifluoroacetic acid solutions. **D. Adams**, A.N. Vedernikov

2:30 102. Catalytic ester metathesis with applications to the transfer hydrogenation of esters, and the serendipitous discovery of a cyclopropanation of aliphatic esters and alcohols with a homogeneous Ru(II) catalyst. **E. Khaskin**, T. Jankins, A. Dubey, R. Fayzullin

2:50 103. Hydrophenylation of ethylene using a cationic Ru(II) catalyst: Change in selectivity based on an auxiliary ligand. **X. Jia**, S. Gu, J.B. Gary, B.A. McKeown, T.R. Cundari, T.B. Gunnoe

3:10 104. Ruthenium-PNP catalyzed cascade conversion of carbon dioxide to methanol. **D. Samblanet**, M.S. Sanford

3:30 105. Formation of a ruthenium–hydride intermediate and its ability to catalyze radical reduction in aerobic, aqueous solution. **A.G. Tennyson**

3:50 106. Structure, reactivity, and mechanism in alkyl-alkyl cross-coupling with iron-NHCs. **V.E. Fleischauer**, S.B. Muñoz, M.L. Neidig

4:10 107. Investigation of Fe-based 2+2 cycloaddition catalysts for the conversion of alkenes and dienes to fuels and lubricants. **D. Morris**, T. Groshens, R. Quintana, B.G. Harvey

4:30 108. Kinetic study of iron-catalyzed transfer hydromagnesiation using operando infrared spectroscopy. **J.A. Rogers**, B.V. Popp

4:50 109. Iridium hydride thermochemistry as an indicator of catalytic performance in a bimetallic iridium/ruthenium H_2 evolution catalyst. **K.R. Brereton**, C.L. Pitman, A.J. Miller

5:10 110. Synthesis of an organometallic iridium complex containing a dianionic, tridentate, mixed organic−inorganic ligand: A fast-acting and short-lived oxygen evolving catalyst. **A. Bloomfield**, A. Matula, B.Q. Mercado, V.S. Batista, R.H. Crabtree

Section G

Renaissance Washington, DC Downtown
Congressional A

Triplet Excited State in Inorganic Chemistry

F. N. Castellano, *Organizer*
M. Abrahamsson, A. De Bettencourt Dias, *Presiding*

1:30 111. Altering photophysics in *trans*-substituted molybdenum dimers using ligands featuring low energy triplet states. **R.R. Joyce**, F.N. Castellano

1:50 112. Triplet state in lanthanide luminescence and singlet state generation. **A. De Bettencourt Dias**

2:15 113. Oppositely polarized singlet and triplet states: A new strategy to control photo-triggered energy conversion reactions of coordination compounds. **M.J. Therien**, N. Polizzi, T. Jiang, D.N. Beratan

2:40 114. Transition metals in singlet fission. **D. Guldi**

3:05 Intermission.

3:20 115. Exchange-modulated spin polarizing triplet states. **M.L. Kirk**, B.W. Stein, C. Tichnell, D.A. Shultz

3:45 116. Implications of triplet state surface shapes in photophysics and photochemistry. **M. Abrahamsson**

4:10 117. Ultrafast and sustainable coherent wave-packet motions in excited state Pt dimers. P. Kim, S.E. Brown-Xu, A. Chakraborty, M.S. Kelley, X. Li, G.C. Schatz, F.N. Castellano, **L.X. Chen**

4:35 118. Solvent and excitation wavelength-dependent dynamics in the excited-state evolution of ^{3}MLCT states: The role of charge distribution in solvent-solute coupling. M.C. Carey, **J.K. McCusker**

Section H

Renaissance Washington, DC Downtown
Congressional B

Chemistry of Materials

Metal Organic Frameworks

C. G. Lugmair, *Organizer*
R. Comito, D. R. Manke, *Presiding*

1:30 119. Halide-assisted synthesis of metal-organic frameworks. **D. Genna**

1:50 120. Bimetallic and actinide-based metal-organic frameworks (MOFs). **O.A. Ejegbavwo**, E.A. Dolgopolova, M.D. Smith, N.B. Shustova

2:10 121. Transparent and monolithic glassy metal organic framework with accessible internal surface. **Y. Zhao**, S. Lee, O.M. Yaghi, C. Angell, N. Becknell

2:30 122. Secondary building unit as metalloligand: Structural and mechanistic insight into catalysis at metal-organic framework nodes. **R. Comito**, D. Mircea, R. Dubey, E. Metzger, Z. Wu, G. Zhang, J. Miller

2:50 123. Incorporation of multifunctionalities into stable metal-organic frameworks *via* one-pot synthesis. **Y. Sun**, H. Zhou

3:10 124. Structural diversity and reactivity of metal-organic frameworks assembled from diphosphine pincer complexes. **C.R. Wade**, N. Mucha, A. Kassie

3:30 Intermission.

3:45 125. Synthesis and characterization of ZIF-8 encapsulated biomaterials. **S. Li**, Z. Chen, M. Dharmarwardana, J.J. Gassensmith

4:05 126. Covalent Metal-Organic Networks (CMONs) through protecting group syntheses. **D.R. Manke**

4:25 127. Bottom-up construction of a superstructure in a porous uranium–organic crystal. **P. Li**, N. Vermeulen, C. Malliakas, D. Gómez-Gualdrón, A. Howarth, L. Mehdi, A. Dohnalkova, N. Browning, M. O'Keeffe, O.K. Farha

4:45 128. Metal organic frameworks as templates for materials synthesis. M. Li, F. Claire, G. Contreras, S. Tenney, **T.J. Kempa**

5:05 129. Development of fabrication methods to tailor surface morphology of metal-organic framework thin films and powders. A. Trojniak, L. Brower, B. Bowser, M.L. Ohnsorg, **M.E. Anderson**

Science Communications: The Art of Developing a Clear Message

Sponsored by PRES, Cosponsored by BIOL, CARB, CEI, CELL, CEPA, CINF, COLL, CPRC, CTA, DAC, I&EC, INOR, ORGN, PROF, SCHB and YCC

What do Synthetic Chemists Want from Their Reaction Systems?

Sponsored by CINF, Cosponsored by COMP, INOR, MEDI and ORGN

SUNDAY EVENING

Section A

Walter E. Washington Convention Center
Hall D

Inorganic Catalysts

S. A. Koch, *Organizer*

5:30 - 7:30

130. NSF / CHE: Data-driven discovery in chemistry (D3SC). **L. He**, **S. Atlas**, **R.J. Cave**, **D.A. Rockcliffe**, **A.K. Wilson**

131. National Science Foundation (NSF) / Division of Chemistry (CHE): Important updates on proposal preparation. **S. Albin**, **C.A. Bessel**, **K.J. Covert**, **M. Jenkins**, **K. Moeller**, **K. Moloy**, **T. Patten**, **J. Papanikolas**, **A. Schmoltner**, **S. Tam-Chang**

132. National Science Foundation (NSF): New opportunities in the chemical sciences. **S. Atlas**, **M. Bushey**, **R.J. Cave**, **K. Cook**, **M. Funk**, **E. Goldfield**, **L. He**, **T. Li**, **C.A. Murillo**, **D.A. Rockcliffe**

133. Synthesis and reactivity of chromium complexes for N_2 reduction. **A.J. Kendall**, M.T. Mock, R. Bullock

134. Mechanistic study of hydrodeoxygenation reaction on lignin beta-5 model compounds using earth abundant metal catalyst. **H. Luo**

135. Modified tris(2-pyridylmethyl)amine (TPMA) and tris[2-(dimethylamino)ethyl]amine (Me_6TREN) hybrid ligands for use in copper-mediated atom transfer radical addition (ATRA). **A.J. Rupprecht**, T. Pintauer

136. Discrete air-stable nickel-palladium(II) complexes as catalysts for Suzuki-Miyaura reactions. T. Zhao, P. Ghosh, **Z. Martinez**, X. Liu, X. Meng, M.Y. Darensbourg

137. ω-Functionalized self-assembled monolayers of phosphonates as a pathway to tethered electrocatalysis. S. Heisey, B.A. Andrews, P.R. Sunder, A.A. Keefer, **K.N. Crowder**

138. Simple structural analog ([{Zr(μ-OH)(H_2O)(α_2-$P_2W_{17}O_{61}$)}$_2$]$^{14-}$) to zirconium hydroxide for CWA simulant decomposition. **S.L. Giles**, J. Lundin, P. Pehrsson, R. Balow, J.H. Wynne

139. Engineering of RuMb: Towards a green catalyst for carbene insertion reactions. **M. Wolf**, D. Vargas, N. Lehnert

140. Novel and highly efficient copper catalysts for atom transfer radical addition (ATRA) of monohalogenated compounds. **M. Novak**, T. Pintauer

141. Inverse frustrated Lewis pair (FLP) approach for catalytic metal-free hydrogenation of imines. **S. Mummadi**, D. Kenefake, R. Diaz, C. Krempner

142. Intermolecular approach to bimetallic photocatalytic systems: Synthesis, characterization, and reactivity. **A. Forney**, H.R. Lucas

143. Water oxidation electrocatalysis by transition metals supported onto zirconium phosphate nanoparticles. **M. Ramos-Garces**, J. Sanchez, I. Narkeviciute, T.F. Jaramillo, J. Colón

Section B

Walter E. Washington Convention Center
Hall D

Fundamental Aspects of Metal Organic Framework Catalysis

A. J. Morris, J. R. Morris, *Organizers*

5:30 - 7:30

144. Kinetically guided one-pot synthesis of heterogeneous core-shell metal-organic frameworks. **X. Yang**, S. Yuan, L. Zou, Y. Zhang, J. Qin, H. Zhou

145. Development of novel catalytically active metal organic frameworks for water splitting. **B.J. Gibbons**, A.J. Morris

146. Removal of Pb ions from water using thiophene-containig metal-organic frameworks. **A. Geisse**, D. Genna

147. *In situ* studies of DMMP interaction with Zr-based metal organic frameworks. **W.O. Gordon**, A.M. Plonka, A. Balboa, Q. Wang, S.D.

Senanayake, C.H. Sharp, D. Troya, W. Guo, A. Frenkel, C.L. Hill, J.R. Morris

148. Efficient and recyclable functionalized nano-size zirconium based UiO-66 MOF catalysts for successive C-C and C-N bond formation. **P. Elumalai**, S.T. Madrahimov

149. Small molecule activation with iron(II)-based metal-organic polyhedra. **G.R. Lorzing**, B.A. Trump, C.M. Brown, E.D. Bloch

150. Chiral ruthenium aminophosphine (*PN*) and phosphine iminopyridine (*PNN*) complexes: Synthesis and application to asymmetric hydrogenation and transfer hydrogenation. **L. Scarlet**, P.T. Maragh, T.P. Dasgupta, K. Abdur-Rashid

Section C

Walter E. Washington Convention Center
Hall D

Bioinorganic Chemistry

Proteins & Enzymes & Model Systems

S. A. Koch, *Organizer*

5:30 - 7:30

151. Fold upon binding: A tale of copper(II) binding to the N-terminal region of human carbonic anhydrase II. **F. Voges-Haupt**, K.D. McConnell, J.P. Emerson

152. Understanding proteome dependent cellular zinc trafficking to form native Zn-proteins. **A. Mahim**

153. Bioinspired water-soluble Mn-porphyrin complex as catalase mimic for antioxidative activity. **R. Kubota**, S. Asayama, H. Kawakami

154. Isolation of a synthetic nitrogenase-relevant iron-molybdenum/interstitial-carbide cluster. **C. Joseph**, S. Kuppuswamy, M.J. Rose

155. Structural characterization of heme proteins mineralized within the ZIF-8 metal organic framework. **D. Grassie**, R.W. Larsen

156. Characterization of KmtR from *Mycobacterium tuberculosis*. **K.A. Higgins**, V. Surette, G. Swanson, A. Miller, K. Gonzalez, M. McGowan, S. Lewis

157. Mechanistic insights into heme-protein carbenoid chemistry using stopped flow spectroscopy. **C.B. Monroe**, J.T. Groves

158. Studies toward the development of a more accurate structural model of the nitrile hydratase active site. **W.I. Chow**, **R.R. Markham**, C. Moore, A.L. Rheingold, C.J. Daley

159. Cyanide ligands as docking agents in [FeFe]-hydrogenase biomimetics. **M. Quiroz**, P. Ghosh, M.Y. Darensbourg, N. Bhuvanesh, X. Meng

160. Modeling of halogen bonding interactions to PBDEs as a mechanism for thyroid disruption. **E.S. Marsan**, C.A. Bayse

161. Extended broken symmetry approach to modeling structures and spectroscopic properties of oxidized and reduced 2Fe-2S clusters from mitoNEET. **R.A. Wheeler**, A.M. Koval

162. Synthesis and reactivity of an anthracene-bridged dimer as a model of mono-iron hydrogenase. **S.A. Kerns**, A. Magtaan, M.J. Rose

163. Molybdenum pyranopterin dithiolene complexes: Synthesis and applications. **N. Nguyen**, **H.H. Varnum**, **V.R. Berke**, D. Gisewhite, S.J. Nieter Burgmayer

164. Substitution reactions of iron(II) carbamoyl-thioether complexes related to mono-iron hydrogenase. **Z. Xie**, M.J. Rose

165. Nitric oxide and hydrogen sulfide cross-talk mediated by zinc. **V. Hosseininasab**, T.H. Warren

166. Role of metal complexation in the metastable conformation of α-Synuclein. **R.D. Fernandez**, H.R. Lucas

Section D

Walter E. Washington Convention Center
Hall D

Electronic Structure Contributions to Function: From Metals in Biology to Materials Science

P. Chen, A. Dey, A. E. Palmer, L. Quintanar, *Organizers*

5:30 - 7:30

167. What can the relationship between ligand donor strength and spin-state energetics reveal about the electronic structure of Fe(II) polypyridine complexes? **D. Ashley**, E. Jakubikova

168. New diiron complex capable of reducing NO to N_2O mimics the reactivity of FNORs. **H.T. Dong**, C. White, N. Lehnert

169. Design of copper catalysts for electrochemical production of NO on demand. **A. Batka**, A. Hunt, N. Lehnert

170. Mechanistic studies of iron-catalyzed C-H functionalization. **T.M. Baker**, S.H. Carpenter, M.L. Neidig

171. Iron catalyzed cross-coupling with TMEDA. **J. Sears**, M.L. Neidig

172. Graphitic surfaces for small molecule functionalization of semiconductors. **M.M. MacInnes**, N. Lehnert, S. Maldonado

173. Molecular property analysis of phosphoryl-containing compounds: A theoretical approach. **A. Balboa**, M. Hurley

174. Electronic structure and bonding in cobalt(II)-*N*-heterocyclic carbene complexes. **T. Iannuzzi**, M.L. Neidig

175. Synthesis and spectroscopic characterization of ferric heme-thiolate complexes as models for cytochrome P450nor. **A.P. Hunt**, N. Lehnert

176. Synthesis, characterization, and reactivity studies of a flavodiiron nitric oxide reductase model complex. **C. White**, A. Speelman

Section E

Walter E. Washington Convention Center
Hall D

Triplet Excited State in Inorganic Chemistry

F. N. Castellano, *Organizer*

5:30 - 7:30

177. Photophysical studies of molecules with thermally activated delayed fluorescence for application in organic light emitting diodes. **T. Palmeira**, E. Torres, M. Esteves, M. Brites, M.B. Berberan-Santos

178. Phasor representation and singlet-triplet interconversion diagram in thermally activated delayed fluorescence. **L. Martelo**, T. Palmeira, M.B. Berberan-Santos

179. Molecular photophysics of Ir(III) MLCT excited states bearing hydrides. **C. Taliaferro**, F.N. Castellano

180. Pushing the limits of metal-metal interaction in dinuclear Pt(II) complexes. **J. Yarnell**, A. Chakraborty, F.N. Castellano

Section F

Walter E. Washington Convention Center
Hall D

Coordination Chemistry

Characterization & Applications

S. A. Koch, A. Larsen, *Organizers*

5:30 - 7:30

181. Surface synthesis of molecular assemblies: Application in energy conversion. **U. Mathiyazhagan**, J.W. Jurss, T.J. Meyer

182. Luminescent zirconium(IV) complexes as a molecular photosensitizers for visible light photoredox catalysis. **Y. Zhang**, C. Milsmann

183. Molecular characterization and thermal studies of cationic lanthanide complexes. **P.K. Yuen**, C. Lau, N. Ho, H. Chan, C. Law, F. Shek, A.K. Yuen

184. Rapid, machine-assisted syntheses of substituted iridium(III)-pyrazolate complexes with tunable luminescence. **L.M. Groves**

185. Synthesis and characterisation of *β*-diketonate and *β*-ketoiminate metal compounds: Potential applications in ring opening metathasis polymerisation of lactide. **R.M. Lord**, F. Janeway, P. McGowan

186. Molecular dyads and triads comprising phenothiazine or exTTF donors, Ru(II) bisterpyridine complexes and polyoxometalates. **A. Winter**, K. Barthelmes, M. Sittig, U.S. Schubert

187. Design and synthesis of cationic metal-organic polyhedra for gas storage applications. **G.E. Decker**, E.D. Bloch

188. Interaction of five coordinated copper complexes with cysteine: Theoretical and experimental studies. C.A. Huerta-Aguilar, **T. Pandiyan**, J. Gracia Mora

189. Conductometric confirmation of formation of 2:1 complexes of $[PW_{11}O_{39}]^{7-}$ with divalent metal cations. **N. Sveshnikov**, M.T. Pope

190. Hyperpolarized molecular tags as a novel strategy for developing imaging probes. **J. Bae**, Z. Zhou, K. Shen, J. Colell, T. Theis, W.S. Warren, Q. Wang

191. Effect of geometry and sterics of bipyridine ligands on catalytic performance. **C.L. Boelke**, **S. Lense**

192. NIR absorbance of Ru(II) and Ir(III) photosensitizers containing a merocyanine π-acceptor. **P. Catsoulis**, J.J. Rochford

193. Chiral mer-coordinating bis(4,5-dihydrooxazol-2-ylimino)isoindoline-based pincer ligands: Attempted synthesis optimization, characterization, and preliminary enantioselective catalysis studies. **L.M. Baldauf**, C. Moore, A.L. Rheingold, **C.J. Daley**

194. Synthesis, characterization, and reactivity of platinum indazole complexes with potential anti-cancer activity. **K.W. Barwick**, A.J. Bachman, K.A. Wheeler, **R.E. Bachman**

195. Light-driven H_2 production by attaching Ni/Pt diimine dithiolate dyads and catalysts on TiO_2. **G. Li**, M. Mark, D.W. McCamant, R. Eisenberg

196. Electronic structure and multi-catalytic features of redox-active Bian (bis-(arylimino)acenaphthene) derived ruthenium complexes. **A. Singha Hazari**, G.K. Lahiri

Section G

Walter E. Washington Convention Center
Hall D

Center for Enabling New Technologies through Catalysis: Transforming Catalysis through Collaboration

A. Goldman, N. E. Gruhn, E. Ison, S. W. Krska, L. T. Thompson, *Organizers*

5:30 - 7:30

197. Aerobic oxidation of hydrocarbons catalyzed by $[Ir]^{III}$ complexes. **S.B. Rubashkin**, Z.H. Syed, A. Wright, K.I. Goldberg

198. Ethylene oligomerization-dehydrogenation co-catalyzed by (phebox)Ir(OAc)(H) and Na^+ cation. **Y. Gao**, A. Goldman

199. Pincer Ir^{III} complexes for aerobic alkane functionalization. **K. Smoll**, K.I. Goldberg

200. Synthesis and reactivity of Iridium(III) PCP-pincer acetate complexes. **A. Shada**, A.S. Goldman

201. Alkane oxidation utilizing a novel iridium υ-oxo complex. **C.M. Perry**, E.A. Ison

202. Investigation of the non-thermodynamic factors governing metal-ligand bond dissociation rates. **B. Gordon**, **S. Malakar**, T. Zhou, S. Biswas, K. Krogh Jespersen, A.S. Goldman

203. Immobilized pincer-ligated iridium catalysts characterized via in situ UV-visible and Fourier transform infrared spectroscopy. **A.M. Pennington**, B. Sheludko, M.T. Cunningham, A.S. Goldman, F.E. Celik

204. Side chain design in brush block copolymer photonic crystals. **A.L. Liberman-Martin**, C. Chu, R.H. Grubbs

205. Glycerol deoxygenation catalyzed by (POCOP)Ir(CO) complexes. **B. Bark**, K.I. Goldberg, D.M. Heinekey

206. Heterogeneous catalysts for the aldehyde water shift reaction: Comparative investigation of molybdenum carbide, cerium oxide, and aluminum oxide supported Cu, Pt and Au. **W. Wen**, L.T. Thompson

207. Late transition metal catalysts for hydrogenolysis reactions. **L.M. Guard**, J.M. Goldberg, T. Lekich, K.I. Goldberg, D.M. Heinekey

208. Insights of iridium pincer coordination chemistry enabled by a new synthetic method for dimethyl heteroleptic phosphines. **T. Lekich**, P. Askleson, R. Burdick, L.M. Guard, J.M. Goldberg, D.M. Heinekey

209. Reductive elimination of alkylamines from phosphine-ligated alkylpalladium(II) amido complexes. **D.M. Peacock**, Q. Jiang, J.F. Hartwig, T.R. Cundari

210. Mechanistic investigation of palladium-catalyzed C(sp^3)-N bond formation with DFT methods. D. Peacock, **Q. Jiang**, T.R. Cundari, J.F. Hartwig

211. Combining Rh-catalyzed diazocoupling and enzymatic reduction to efficiently synthesize enantioenriched 2-substituted succinate derivatives. **Y. Wang**, M.J. Bartlett, C. Denard, H. Zhao, J.F. Hartwig

212. Homogenous catalytic reduction of CO_2 to MeOH at moderate temperatures. **W. Chu**, K.I. Goldberg

213. Base-free hydrogenation of esters using pincer-ligated iridium complexes and dihydrogen. **Z. Culakova**, L.M. Guard, K.I. Goldberg

214. Interrogating ligand electronic effects and the influence of solvation on thermodynamic hydricity (relevant to aqueous organometallic catalysis). **K.R. Brereton**, C.N. Jadrich, C.L. Pitman, A.J. Miller

215. Oxidative electrochemistry of pincer complexes. **A.G. Walden**, N. Lease, A.S. Goldman, A.J. Miller

216. Efforts toward the synthesis of γ'-Fe_4N. **T.E. Stevens**, C.J. Pearce, S. Atcitty, T.C. Monson

217. Mechanistic insights into the electrochemical scission of dinitrogen by a pincer rhenium complex. **B.M. Lindley**, A.J. Miller

218. Oxidative chemistry of a pincer-supported Re(V)-nitride derived from dinitrogen. **G.P. Connor**, N. Lease, A. Goldman, P.L. Holland, J.M. Mayer

219. Molybdenum pincer complexes for nitrogen reduction to ammonia. **A. Casuras**, N. Lease, A.S. Goldman

220. Leveraging science center partnerships to educate the public about catalysis. **E. Perara**, N.E. Gruhn, K.I. Goldberg

Section H

Walter E. Washington Convention Center
Hall D

Organometallic Chemistry

Catalysis

N. S. Radu, *Organizer*

5:30 - 7:30

221. Fast electrocatalytic production of hydrogen by thiophenedithiolate bridged butterfly [2Fe-2S] clusters. **M.O. Talbot**, L.M. Stratton, D.H. Evans, R.S. Glass, D.L. Lichtenberger

222. Unraveling the role of ligand variation on the effectiveness of group 7 in the electrocatalytic reduction of CO_2. **Y. Hameed**, G. Rao, B. Gabidullin, D.S. Richeson

223. Synthesis and reactions of polymer-bound Styker's reagent. S.A. Oreilly, **B. Masingo**, O. Arogbokun

224. Ni(II) catalyzed hydrophosphonylation of alkynes with a P(III) source. **R. Islas-Vigueras**, J.J. Garcia

225. Silylated cobalt catalysts for alkene functionalization. **J.E. Pallone**, D. Genna

226. Mechanistic studies of the iridium-catalyzed ortho C-H borylation of benzylic amines. **C.M. Oliver**, **A. Samoshin**, K.A. McGarry, H. Guan, T.B. Clark

227. Phosphine-directed C-H borylation reactions: New catalyst development and synthetic utility. S.E. Wright, **S. Richardson-Solorzano**, E.E. Albitz, **C. Miller**, T.B. Clark

228. Investigating rhodium catalyzed C-H borylation: Evaluating selectivity through catalyst design. **M. Mantell**, M.S. Sanford

229. Transfer hydrogenation of ketones catalyzed by novel arene ruthenium iminophosphonamides. I.S. Sinopalnikova, T.A. Peganova, A.M. Kalsin, E. Deydier, **R. Poli**

230. Investigation the path way of amines react with a tris(pyrazolyl)borate rhodium complex. **J. Yuwen**, W. Brennessel, W.D. Jones

231. Air stable molybdenum(0) catalysts for selective alkene isomerization. **J. Becica**, O.D. Glaze, G. Dobereiner

232. Macrocyclic bidentate N-heterocyclic carbene ligands for group 10 metals for catalysis. **R. Thapa**, S.M. Kilyanek

233. Towards catalytic ammonia oxidation with Mo and Ru- ammonia complexes. **P. Bhattacharya**, **E.S. Wiedner**, Z.M. Heiden, S.I. Johnson, S. Raugei, R. Bullock, M.T. Mock

Section I

Walter E. Washington Convention Center
Hall D

Organometallic Chemistry

Applications to Organic Transformations

N. S. Radu, *Organizer*

5:30 - 7:30

234. Cu(I) Complexes of pincer pyridine-based N-heterocycliccarbenes with a small wingtips substituents: Synthesis, characterization and application in Sonogashira coupling reactions. **D. Domyati**, **L. Tahsini**

235. Kinetics of the decarboxylation of well-defined copper(II) benzoate complexes. **G. Thomas**, J.M. Hoover

236. Copper-catalyzed arylation, vinylation and alkynylation of sp^2 and sp^3 C–H bonds with iodonium salts. **C. Liu**

237. Kinetic studies of the decarboxylation of silver benzoate complexes. **R.A. Crovak**, J.M. Hoover

238. Mechanistic investigation of copper-catalyzed boracarboxylation of alkenes. **N.N. Baughman**, B.V. Popp

239. Construction of benzofluorenones via 5-exo-dig carbocupration of phenylene ethynylenes: Tandem copper(I) mediated cycloaromatizations. **T.S. Hughes**, K. Gillespie, M. Lieu, J. Cobb, K. Allen

240. Highly enantioselective epoxidation of olefins with H_2O_2 catalyzed by bioinspired N4 manganese complexes. **W. Sun**

241. Alkyne diboration catalyzed by iridium/CO/^{t}BuNC system. **Q. Lai**, O. Ozerov

Section J

Walter E. Washington Convention Center
Hall D

Chemistry of Materials

C. G. Lugmair, *Organizer*

5:30 - 7:30

242. Ruthenium(II)-polypyridyl doped zirconium(IV) metal-organic frameworks as solid-state electrochemiluminescence detectors. **M. Cai**, A.J. Morris

243. Layered siloxene sheets and their composites for photocatalytic applications. **H. Kang**, K. Lee, S. Kye, S. Lee, N.H. Hur

244. Structural resolutions of magic-size $(CdSe)_{13}$ twin clusters. T. Hsieh, C. Hsieh, T. Yang, S. Huang, Y. Yeh, C. Chen, E.Y. Li, **Y. Liu**

245. Development of plasmonically enhanced TiO_2 substrates directed for ethanol oxidation reactions. **J. Boltersdorf**, J.P. McClure, D.R. Baker, C. Lundgren

246. Radiation detection and dosimetry using Y_2O_3:Eu/Li nanoscintillators. **B.W. Langloss**, I.N. Stanton, M. Belley, J. Dooley, S.X. Chang, O. Craciunescu, J.P. Chino, T.T. Yoshizumi, M.J. Therien

247. Reproducible synthesis of free-standing porous silicon membranes for energy storage applications. **M.L. Anger**

248. Establishment of heterogenous multi-step synergy biocatalytic platform by biomimetic and imobilization of enzymes. S. Zhang, H. An, Z. Zhang, **Y. Chen**

249. Design and synthesis of new types of porous imide organic cages. Z. Wang, **Z. Zhang**

250. Small molecule activation utilizing carboxylate based metal-organic polyhedra. **C.A. Rowland**, E.D. Bloch

251. Synthesis, characterization, and photophysical properties of Bi(III)-thiophenecarboxylate materials. **A.K. Adcock**, J.A. Bertke, K.E. Knope

252. Selective gas adsorption in an isostructural series of pillared metal-organic polyhedra. **E. Gosselin**

253. Pulse laser deposition of oxynitride thin films for photoelectrochemical measurements. **N.B. King**, W. Wong-Ng

254. Microwave-assisted routes for bismuth nanostructures. **P. Corio**, J.d. de Souza, F. Hirata, M. Chapina

255. Functionalization of zeolitic imidazolate frameworks for enhanced carbon dioxide selectivity. N. Khazeni, A. Bandegi, M. Garcia, J. Rastegary, A. Ghassemi, **R. Foudazi**

256. Energy transfer studies on mixed-ligand PCN-223 metal organic frameworks. **S. Shaikh**, A.J. Morris, N. Mayhall

257. Ionic liquid crystalline related to the perovskite solar cell materials: Synthesis and characterization of systems utilizing multi-chain aliphatic ammonium cations and metal complex anions. **P.C. Berger**, **R.E. Bachman**

258. Tunable electronic properties in a 2D metal-organic framework platform. **J. Park**, D. Feng, Z. Bao

259. Study of stacking faults in honeycomb lattice compounds. **L. Yin**, J. Liu, P. Khalifah

Section K

Walter E. Washington Convention Center
Hall D

Organometallic Chemistry

Synthesis & Characterization-Late Transition Metals

N. S. Radu, *Organizer*

5:30 - 7:30

260. C-C bond activation by rhenium complexes. **K. Lee**

261. Toward copper-catalyzed asymmetric P-C bond formation using chiral NHCs. **L. Mendelsohn**, S.K. Gibbons, G. Wang, A.L. Rheingold, D.S. Glueck

262. Carbon atom transfer to an iron(IV) nitride from a cyclopropenylidene carbene. **J.L. Martinez**, H. Lin, W. Lee, M. Pink, C. Chen, X. Gao, J.M. Smith

263. Cyclometalated platinum (VI) complexes with thiophene-based ligands: Synthesis and reactivity. **C.M. Anderson**, **D. Yu**, **F. Mastrocinque**, M.F. Pizzuto

264. Regioselective preparation of a flexible phosphane–borane by hydroboration with simple rhodium catalysts. **B.R. Nichols**, N. Akhmedov, J.L. Petersen, B.V. Popp

Section L

Walter E. Washington Convention Center
Hall D

Environmental & Energy-Related Inorganic Chemistry

S. A. Koch, *Organizer*

5:30 - 7:30

265. Design and practice of a long-term bactericidal system. **N. Zhan**, Q. Chang, K. Yeung

266. Design air purification filters with formulated antimicrobial agents. J. Lee, **N. Zhan**, J. Kwan, K. Yeung

267. Charge transfer-induced spin crossover manganese$^{II/III}$ redox mediators for next generation quantum dot solar cells. **M. Kessinger**, A.J. Morris

268. Synthesis and photocatalytic activity of nitrogen-doped TiO_2 microspheres wrapped with silica. **S. Kye**, H. Jung, H. Kang, K. Lee, N.H. Hur

269. Distribution and elevated solubility of lead, arsenic and cesium in contaminated paddy soil enhanced with the electro-kinetic field. **X. Mao**

270. Volatile organic compounds (VOCs) degradation and antimicrobial activities for metal doped or coupled TiO_2 nanoparticles coated on the stainless steel substrate under UV and visible light irradiation. **S. Kim**, M. Suh, C. Lee

271. Effects of solid state and sol-gel synthesis methods on the materials and electrochemical properties of $La_{0.8}Sr_{0.2}Ga_{0.8}Mg_{0.2}O_{3-\delta}$ solid oxide fuel cell electrolytes. **B.C. Eigenbrodt**, T. Marshall

272. Carbonate eutectic promoted dolomite for CO_2 removal. **X.S. Li**, C.S. Sampara, K.G. Rappe, F. Zheng, W. Liu

273. Immobilization of chromophores and catalysts to titanium dioxide via robust attachments. **N.A. Race**, M.E. Screen, W.R. McNamara

274. Second coordination sphere effects in Re(I) polypyridyl electrocatalysts for selective production of formic acid. **M.E. McKinnon**, K.T. Ngo, M.Z. Ertem, D.C. Grills, J.J. Rochford

275. Low temperature facile synthesis of α-Fe_2O_3 dispersed on Flavin mononucleotide-stabilized graphene nanosheet *via* microwave-assisted hydrothermal method. **M.E. Cabello**, E. Enriquez

276. Passivation of nanoscale zero-valent iron (nZVI) by Cr(VI): The influence of Cr(VI) concentration and environmental conditions. **X. Huang**, L. Ling, W. Zhang

277. Solution-phase synthesis and thermoelectric characterization of tetrahedrite. **A. Ochs**, G. Kunkel, D. Weller, D. Stevens, C. Holder, D. Morelli, M.E. Anderson

278. Mechanistic investigations of CO_2 reduction by manganese tricarbonyl complexes. **K. Ngo**, D.C. Grills, J.J. Rochford

279. Homogeneous and heterogeneous metal selenolate catalysts for the hydrogen evolution reaction. **C. Downes**, S. Marinescu

280. Polydopamine-coated nanocomposites of transition metal complexes supported on graphene for oxygen reduction. **H.A. Wayland**, S. Boury, B.P. Chhetri, C. Parnell, A. Ghosh

281. Determination of polycyclic aromatic hydrocarbons in Durban city road dusts. **A.D. Abdulkadir**

282. High-performance electromagnetic wave absorbing composites prepared by one-step transformation of Fe^{3+} mediated egg-box structure of seaweed. **Q. An**

Section L

Walter E. Washington Convention Center
Hall D

Inorganic Spectroscopy

S. A. Koch, V. C. Popescu, *Organizers*

5:30 - 7:30

283. To be or not to be: d^{10}-d^{10} bonding in heterometallic complexes. **K. Melancon**, B.M. Otten, M.A. Omary

284. Influences of trifluoromethyl ligands on transition metal electronic structure and their implications for metal-mediated trifluoromethylation. **J. Lukens**, I. DiMucci, K.M. Lancaster

285. Reactions of Cu^{2+} with the aromatic amino acid Phenyl alanine in aqueous solutions. **Y.Z. Hamada**

286. IR, potentiometry and UV-Vis measurements of glycine with Cu2+. **Y.Z. Hamada**

287. Photo-activated phosphorescence of gold(I) arylethynyl complexes in aerated DMSO solutions and gels. **S. Wan**, W. Lu

288. Assessing the scope and limitations of a new ^{13}C NMR approach for probing charge delocalization in electron-rich organometallics featuring the isocyanide junction unit. **Z.A. Wood**, M.D. Hart, M.V. Barybin

289. Spectroscopic and computational investigations of the ground- and excited-state properties of Cr(III) bis(4′-arylterpyridyl) complexes. **B.M. Lovaasen**, P.K. Walhout, B.D. Verble

290. Decreased polyatomic interference in the analysis of arsenic with ICP-MS after injecting methanol to sample. **J. An**, K. Nam

MONDAY MORNING

Section A

Renaissance Washington, DC Downtown
Renaissance East

Fundamental Aspects of Metal Organic Framework Catalysis

A. J. Morris, J. R. Morris, *Organizers*
D. Powers, *Presiding*

8:30 291. Controlled encapsulation of catalysts into nanoporous materials. **C. Tsung**

9:00 292. Computational study of A MOF-supported single site Ni catalyst for ethylene dimerization. **J. Ye**, A. League, D.G. Truhlar, C.J. Cramer, L. Gagliardi, V. Bernales, O.K. Farha, J.T. Hupp, Z. Li, A. Platero Prats, K.W. Chapman, D.M. Camaioni, J. Fulton, J.A. Lercher

9:30 Intermission.

9:45 293. Single-site heterogeneous catalysts for olefin upgrading enabled by cation exchange in metal-organic frameworks. R. Comito, **M. Dinca**, E.D. Metzger, R. Dubey

10:15 294. Inorganometallic catalyst design: Alkane metathesis catalysis in NU-1000 MOFs functionalized with transition metals. **B. Yang**, K. Sharkas, L. Gagliardi, D.G. Truhlar

10:45 295. Hydroxylation stereochemistry as a probe of *In-MOF* versus *On-MOF* catalysis. **D. Powers**, A. Cardenal, H. Park

Section B

Renaissance Washington, DC Downtown
Renaissance West A

Personal & Global Energy Conversion in Chemistry & Biology

C. J. Chang, M. Kanan, *Organizers, Presiding*

8:30 296. Redox distribution in multi-electron substrate activation processes. **T. Betley**

8:55 297. Charge carriers modulate the bonding of semiconductor dopants: A time-resolved x-ray study. **P.T. Snee**, A. Hassan, X. Zhang, R.D. Schaller

9:20 298. Development of BN cyloalkanes: From H_2 storage materials to molecular precursors for 2D BCN graphene. G. Chen, Z. Giustra, J. Ishibashi, W. Luo, A. Enders, **S. Liu**

9:45 299. Utilizing synthetic control in molecular complexes to understand the chemistry of solar fuels catalysis. **J.Y. Yang**

10:10 Intermission.

10:30 300. Controlling the outcome of CO_2 reduction at bismuth-film cathodes in the presence of room temperature ionic liquids. **J. Rosenthal**

10:55 301. Turning lead into gold: Materials and nanostructures in electrochemical energy conversion. **J. Bachmann**

11:20 302. Photocurrent generation in printable photovoltaic materials: Insights from ultrafast spectroscopy. **J. Hodgkiss**

11:45 303. Carbonate-catalyzed CO_2 utilization. **M. Kanan**

Section C

Renaissance Washington, DC Downtown
Grand Ballroom South

Inorganic Chemistry Lectureship

W. B. Tolman, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 304. On the trail of aminophosphinidenes. **C.C. Cummins**, M. Geeson, M. Nava, W. Transue, A. Velian

9:00 305. DNA-mediated signaling among proteins with [4Fe4S] clusters. **J.K. Barton**

9:25 306. Metal-ligand multiple bonds as viable intermediates for group transfer catalysis in C-H bond functionalization. **T. Betley**

9:50 Intermission.

10:05 307. Constructing multiple bonds between unlikely metal pairs: Niobium-iron triple bonds, and other awkward relationships. **C.M. Thomas**, G. Culcu

10:30 308. Cooperative metal-metal interactions for challenging chemical transformations. **T.D. Tilley**

10:55 309. Catalysts for solar-driven water splitting. **H.B. Gray**

11:20 310. Synthetic iron nitrogenases. **J.C. Peters**

Section D

Renaissance Washington, DC Downtown
Renaissance West B

Electronic Structure Contributions to Function: From Metals in Biology to Materials Science

From Metals in Biology to Materials Science

P. Chen, A. E. Palmer, L. Quintanar, *Organizers*
A. Dey, *Organizer, Presiding*

8:30 311. Exploring halogen bonding from fundamental principles to real-world applications. **P. Kennepohl**

8:55 312. Thermally and photothermally activated diradical architectures: From small molecule bioreagents to new material morphologies for dissolution of biopolymers. **J.M. Zaleski**

9:20 313. Characterization and control of high activity oxygen evolution reaction and carbon dioxide reduction catalysts. **A.A. Gewirth**

9:45 314. Reaction and photocurrent imaging of single semiconductor particles for solar water oxidation. **P. Chen**

10:10 Intermission.

10:25 315. High-valent states in molecular and heterogeneous oxygen-evolving catalysts and their role in O–O bond formation. **R.G. Hadt**, C. Brodsky, T. Kroll, D. Hayes, N. Li, D.K. Bediako, L.X. Chen, D.G. Nocera

10:50 316. Double exchange in linear face-sharing pentamers. **T. Glaser**

11:15 317. Design and implementation of a high resolution spectrometer and associated computational methodology for measurement of vibrational probes in proteins. **M.T. Kieber-Emmons**

11:40 318. Chemical and biological applications of synchrotron and free electron laser X-rays. **K.O. Hodgson**, B.G. Hedman

Section E

Renaissance Washington, DC Downtown
Grand Ballroom North

Many Colors of Copper

Good Cop, Bad Cop

Cosponsored by BIOL
I. Garcia-Bosch, K. D. Karlin, T. H. Warren, *Organizers*
K. J. Franz, *Organizer, Presiding*

8:55 Introductory Remarks.

9:00 319. Multiple interconnected pathological factors (copper, amyloid-β, and reactive oxygen species) in Alzheimer's disease. **M. Lim**

9:30 320. Copper vs. beta-sheets: From diabetes to cataracts disease. **L. Quintanar**

10:00 321. Transition metal signaling: Bioinorganic chemistry beyond active sites. **C.J. Chang**

10:30 Intermission.

10:45 322. New family of copper superoxide dismutases for fungal pathogens. **V. Culotta**

11:15 323. Mining for new antimicrobials with copper as the tool. A.G. Dalecki, C.L. Crawford, J.C. Lingo, **F. Wolschendorf**

11:45 324. Designing molecules to mine for cellular copper. **K.J. Franz**

Section F

Renaissance Washington, DC Downtown
Grand Ballroom Central

Center for Enabling New Technologies through Catalysis: Transforming Catalysis through Collaboration

N. E. Gruhn, E. Ison, L. T. Thompson, *Organizers*
A. Goldman, S. W. Krska, *Organizers, Presiding*

8:30 Introductory Remarks.

8:40 325. CENTC approach to electrophilic alkane oxidation. **K.I. Goldberg**, K. Allen, Y. Gao, B. Gary, D. Pahls, S.B. Rubashkin, Z.H. Syed, T. Warner, J.Z. Williams, A.M. Wright, H. Yuan, T.R. Cundari, A.S. Goldman, W.D. Jones

9:10 326. Catalytic alkane conversions based on dehydrogenation by pincer complexes. **A.S. Goldman**, M. Brookhart, K. Krogh Jespersen, R.R. Schrock, S.L. Scott

9:40 327. Light-alkane functionalization and polyethylene degradation. **Z. Huang**

10:00 328. Polyolefin catalysts for the production of ethylene based fluids. **B. Bailey**, J. Klosin, D. Arriola, T. Paine

10:20 Intermission.

10:30 329. Oxyfunctionalization with Cp*Ir(III) complexes. **E.A. Ison**

11:00 330. Immobilized pincer-ligated iridium complexes in continuous heterogeneous alkane transfer dehydrogenation. **F.E. Celik**, B. Sheludko, A.M. Pennington, M.T. Cunningham, M.E. Gliege, A.S. Goldman

11:30 331. Dehydrogenation of alkanes using pincer complexes in a continuous process. **D. Guironnet**, J. Schultz

11:50 332. Understanding the roles of metallic additives in organotransition metal catalysis. **G. Dobereiner**, K. Weerasiri, J. Becica, D. Wozniak

12:10 Concluding Remarks.

Section G

Renaissance Washington, DC Downtown
Congressional A

Triplet Excited State in Inorganic Chemistry

F. N. Castellano, *Organizer*
K. Hanson, Y. Ma, *Presiding*

8:30 333. Supramolecular strategies enabling directional energy flow from quantum dots. **S. Garakyaraghi**, C. Mongin, F.N. Castellano

8:50 334. Solid-state infrared-to-visible upconversion sensitized by colloidal nanocrystals. **M. Baldo**

9:15 335. Iridium complex for tandem 3PA-TTA photo upconversion with large anti-Stokes shift. **Y. Ma**

9:40 336. Thermally activated delayed photoluminescence from pyrenyl decorated CdSe quantum dots. **C. Mongin**, P. Moroz, N. Razgoniaeva, M. Zamkov, F.N. Castellano

10:05 Intermission.

10:20 337. Triplet states in organometallic conjugated materials. **K.S. Schanze**, S. Goswami, E. Holt, J. Wang

10:45 338. Tuning photochemistry and photophysics in metallo-supramolecular materials. **A. Ostrowski**

11:10 339. Electrophosphorescence and photophysics of heavy and not so heavy metal complexes. **M.E. Thompson**, R. Hamze, S. Shi

11:35 340. Harnessing low energy triplet states via molecular photon upconversion at organic-inorganic interfaces. S.P. Hill, T. Dilbeck, Y. Zhou, **K. Hanson**

Section H

Renaissance Washington, DC Downtown
Congressional B

Coordination Chemistry Characterization & Applications

S. A. Koch, A. Larsen, *Organizers*
D. C. Bebout, C. Milsmann, *Presiding*

8:30 341. Self-assembly of molecular thiolate-bridged group 12 metal ion complexes. W. Lai, A.A. Tran, C. Rojas Ramirez, K. Ritz, J.C. Poutsma, R.D. Pike, R. Butcher, C.A. Bayse, **D.C. Bebout**

8:50 342. Design and synthesis of molecular qubit host complexes for applications in quantum information processing. **M. Fataftah**, S.C. Coste, J. Zadrozny, D.E. Freedman

9:10 343. Solution behavior and resonance Raman spectroscopic investigation of modified salen-type subterranean fluid flow tracers. **O. Staples**, J.C. Sanchez, T.E. Tesema, J.M. Sears, T.G. Habteyes, T.M. Roper, J.A. Greathouse, T.J. Boyle, R.A. Kemp

9:30 344. Installation and reduction of nitrate using a redox-active pincer ligand. **D.M. Beagan**, N.A. Maciulis, M. Pink, K.G. Caulton

9:50 345. Joint computational and synthetic exploration into the reduction of nitrate using a novel pyrazole/pyridyl/phosphine pincer ligand. **A. Cabelof**, A.V. Polezhaev, M. Pink, K.G. Caulton

10:10 Intermission.

10:20 346. Molecular photosensitizers based on earth abundant early transition metals. **C. Milsmann**

10:40 347. Redox-active formazanate ligands on iron: Going beyond electron reservoirs. **D. Broere**, B.Q. Mercado, K.M. Lancaster, E. Bill, P.L. Holland

11:00 348. Cracking down on vapochromic materials: Vapor-induced stress in gas sensing platinum salts. **A.E. Norton**, S. Taylor, M. Abdolmaleki, R. Hart, J.A. Krause, W.B. Connick

11:20 349. Magnetic anisotropy from main group elements: Halide versus group 14 elements. **S. Coste**, D.E. Freedman, B. Vlaisavljevich

Building a Safety Culture across the Chemistry Enterprise

Institutional & Enterprise Level Efforts to Developing a Safety Culture

Sponsored by PRES, Cosponsored by BIOL, BMGT, CARB, CCS, CEI, CELL, CEPA, CHAS, CINF, COLL, CPRC, CTA, DAC, ETHX, I&EC, INOR, ORGN, PROF, SCHB and YCC

Materials Science in Nuclear Waste Disposal

Sponsored by NUCL, Cosponsored by INOR

MONDAY AFTERNOON

Section A

Renaissance Washington, DC Downtown
Renaissance East

Fundamental Aspects of Metal Organic Framework Catalysis

MOFs for Artificial Photosynthetic Catalysis

A. J. Morris, J. R. Morris, *Organizers*
S. Ott, *Presiding*

1:30 350. Functionalized metal organic frameworks for CO_2 reduction. **K. Johnson**, L. Li, J. Ye

2:00 351. Mechanistic study on CO_2 hydrogenation and photocatalytic reduction using metal-organic frameworks. **C. Wang**

2:30 Intermission.

2:45 352. Ni-cyclam-based metal-organic frameworks for electrochemical reduction of CO_2. **J. Zhu**, A.J. Morris

3:15 353. Investigations of water oxidation by catalysts incorporated metal-organic frameworks. **S. Lin**, Y. Pineda-Galvan, W.A. Maza, C. Epley, J. Zhu, M. Kessinger, Y. Pushkar, A.J. Morris

3:45 354. Molecular catalysis of energy relevance in metal-organic frameworks. **S. Ott**

Section B

Renaissance Washington, DC Downtown
Renaissance West A

Personal & Global Energy Conversion in Chemistry & Biology

C. J. Chang, M. Kanan, *Organizers, Presiding*

1:30 355. At the nexus of energy and water: Atmospheric fresh water capture

and heat transfer with a material operating at the water uptake reversibility limit. **M. Dinca**, A.J. Rieth, Y. Tulchinsky, A. Wright

1:55 356. Design of earth-abundant main group catalyst. **A.T. Radosevich**

2:20 357. Advances in quantum materials synthesis and application. **T. McQueen**

2:45 358. Approaching challenges in physics with inorganic chemistry. J.M. Zadrozny, M. Graham, J. Walsh, C. Yu, S.M. Clarke, **D.E. Freedman**

3:10 Intermission.

3:30 359. Energy transfer within nanocrystal-molecule systems. **E.J. McLaurin**

3:55 360. Group-transfer chemistry at first-row transition metal complexes in bis(alkoxide) ligand environments. **S. Groysman**, M. Yousif, A. Grass, R.L. Lord

4:20 361. Clean nanocrystals for clean energy & advanced technologies. **A.B. Greytak**, A. Roberge, M.Y. Gee

4:45 362. Molecular models of inner-sphere interfacial electron transfer. **Y. Surendranath**, M. Jackson, S. Oh, A. Murray, C. Kaminsky, S. Chu, T. Marshall-Roth

Section C

Renaissance Washington, DC
Downtown
Grand Ballroom South

Inorganic Young Investigator Awards

J. D. Protasiewicz, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 363. Role of heme redox potential in controlling enzymatic activities. **A. Bhagi**, Y. Lu

2:00 364. Excited-state metalloradicals: Luminescent cerium(III) complexes for photo-redox chemistry. **H. Yin**, Y. Jin, J. Hertzog, K.C. Mullane, P. Carroll, B. Manor, J.M. Anna, E.J. Schelter

2:25 365. Competing pathways in interfacial CO_2-to-fuels catalysis. **A. Wuttig**, M. Yaguchi, S. Hall, Y. Yoon, K. Motobayashi, M. Osawa, Y. Surendranath

2:50 366. Breaking and forming bonds through metal-borane cooperation. **B.R. Barnett**, J.S. Figueroa

3:15 Intermission.

3:25 367. Itinerant ferromagnetism driven by physical and chemical compression in $Ca_{1-x}Eu_xCo_2As_2$. **X. Tan**, M. Shatruk

3:50 368. Nanoscale metal-organic frameworks for photodynamic therapy and immunotherapy. **K. Lu**

4:15 369. Solution growth of single-crystal lead halide perovskite nanostructures and stabilization of metastable perovskites for lasing and optoelectronic applications. **Y. Fu**, H. Zhu, F. Meng, J. Zhai, M. Shearer, X. Zhu, S. Jin

4:40 370. Tailoring properties of metal-organic frameworks. **J. Park**, D. Feng, Z. Bao, H. Zhou

Section D

Renaissance Washington, DC
Downtown
Renaissance West B

Coordination Chemistry

Characterization & Applications

S. A. Koch, A. Larsen, *Organizers*
S. Pope, M. Shatruk, *Presiding*

1:30 371. Molecular spintronics devices utilizing inorganic molecules as the device elements. **P. Tyagi**, T. Goulet, E. Friebe

1:50 372. Simple method to predict the electronic spin configuration of Fe(II) tris-diimine complexes. H. Phan, J.J. Hrudka, **M. Shatruk**

2:10 373. Synthesis, structure, and luminescence of Cu(I) halide complexes of chiral bis(phosphines), $[Cu(diphos*)(X)]_2$. **S.K. Gibbons**, R.P. Hughes, D.S. Glueck, A.T. Royappa, A.L. Rheingold, R.B. Arthur, A.D. Nicholas, H.H. Patterson

2:30 374. Ligand-functionalized nanoreactors: Synthesis and coordination chemistry. **F. Gayet**, A. Joumaa, S. Chen, E. Manoury, M. Lansalot, F. D'Agosto, R. Poli

2:50 375. Exploration of the electrochemistry and catalytic activity of a flexible half porphyrin cobalt complex. **S. Saund**, S. Goldschmid, V. Thoi

3:10 Intermission.

3:20 376. Networking nanoswitches for communication and catalysis using coordination chemistry. **M.J. Schmittel**, N. Mittal, S. Gaikwad, A. Goswami, I. Paul, S. Pramanik, S. De

3:40 377. Complexes based on fluorescent 1,8-naphthalimide derivatives and applications in bioimaging. **S. Pope**

4:00 378. Novel, luminescent, cyclometalated Pt(II) complexes: From fundamental studies to heterometallic bimodal imaging agents. **S. Pope**

4:20 379. Novel, luminescent 1,8-naphthalimide-NHC ligands and their Au(I) complexes for imaging and therapeutics. **L.M. Groves**

Section E

Renaissance Washington, DC
Downtown
Grand Ballroom North

Many Colors of Copper

Proteins & Models

Cosponsored by BIOL
K. J. Franz, I. Garcia-Bosch, T. H. Warren, *Organizers*
K. D. Karlin, *Organizer, Presiding*

1:45 Introductory Remarks.

1:50 380. Copper-sulfide clusters that activate nitrous oxide and other small molecules. **N.P. Mankad**, B. Johnson, S. Bagherzadeh, C. Hsu

2:20 381. Tale of bonding and reactivity by tricopper cyclophanates. **L.J. Murray**

2:50 382. Is PqqB, a protein of unknown function within the PQQ biosynthetic pathway, a novel copper enzyme? **J. Klinman**, E. Koehn, J. Lathan, R.L. Evans III, X. Tu, D.V. Sundaram, C. Wilmot

3:20 Intermission.

3:35 383. Oxygen activation by Cu sites. **E.I. Solomon**

4:05 384. Structure, function and spectroscopy studies of *lytic polysaccharide monooxygenases*. **P. Walton**

4:35 385. RGB copper azurins: Engineered azurins that display a wide range of colors, reduction potentials and enzymatic activities. **Y. Lu**, P. Hosseinzadeh, S. Tian, C. Cui

Section F

Renaissance Washington, DC
Downtown
Grand Ballroom Central

Center for Enabling New Technologies through Catalysis: Transforming Catalysis through Collaboration

A. Goldman, N. E. Gruhn, E. Ison, S. W. Krska, L. T. Thompson, *Organizers*
M. Brookhart, K. I. Goldberg, *Presiding*

1:30 Introductory Remarks.

1:35 386. Tandem catalysis for carbon dioxide hydrogenation. **M.S. Sanford**

2:05 387. High-throughput chemistry for the development of photoredox-catalyzed hydroxymethylation of heteroaromatic bases. **C.A. Huff**, R. Cohen, K. Dykstra, E. Streckfuss, D. DiRocco, S.W. Krska

2:25 388. Bridging the gap between homogeneous and heterogeneous catalysis at Argonne National Laboratory. **E. Bunel**

2:45 389. Hydrogen transfer reactions of metal-oxide and metal-nitride materials. **J.M. Mayer**, S.M. Laga, D. Damatov, J. Castillo-Lora, R. Mitsuhashi, C. Valdez, B.A. McKeown, E.A. Mader, J. Peng, L.T. Thompson, B. Wvyratt, J.R. Gaudet, T. Cundari, D. Pardue, A. Marton, W.D. Jones, M. Wilklow-Marnell, A.J. Miller, A.G. Walden, A. Goldman, N. Lease

3:15 Intermission.

3:25 390. Thermodynamic hydricity as a tool for interpreting and predicting catalyst performance. **A.J. Miller**, K.R. Brereton, C.L. Pitman, C.N. Jadrich, H. Fallah, T.R. Cundari

3:55 391. Design and synthesis of carbide supported metal catalysts. Y. Chen, B. Wvyratt, S. Eady, W. Wen, **L.T. Thompson**

4:25 392. Investigation of sulfur tolerance in supported Pt-Pd catalysts for aromatic saturation. **M.P. Lanci**, S.L. Soled, S. Miseo, C.E. Kliewer, P.A. Stevens, Y.V. Joshi

4:45 393. Single-facet anatase TiO_2 nanomaterials as model catalysts for alcohol dehydration. **Y. Chen**, L. Zhang, H. Wang, F. Gao, Y. Wang

5:05 Concluding Remarks.

Section G

Renaissance Washington, DC
Downtown
Congressional A

Triplet Excited State in Inorganic Chemistry

F. N. Castellano, *Organizer*
P. C. Glazer, T. S. Teets, *Presiding*

1:30 394. Acetylide versus allenylidene: Excited state properties of photoluminescent Pt(II) zwitterionic acetylide complexes. **C. Zou**, J. Lin, F. Peng, M. Xie, J. Xia, X. Chang, W. Lu

1:50 395. Photophysics and photochemistry of complexes with conjugated ligands containing sulfur-based functional groups. C.M. Brown, P.R. Christensen, M. Kitt, T. Wright, **M.O. Wolf**

2:15 396. Mechanisms of photochemical H_2 evolution from organometallic iridium hydrides. **A.J. Miller**, M.B. Chambers, C.L. Pitman, D.A. Kurtz

2:40 397. Controlling triplet energies and dynamics in bis-cyclometalated iridium complexes via ancillary ligand modification. **T.S. Teets**, H. Na, P. Lai, A. Maity, J. Kölsch

3:05 398. Interconfigurational electronic transitions of cerium(III) complexes: Photophysics and photochemistry. **E.J. Schelter**, Y. Qiao, H. Yin, Y. Jin, B. Manor, P. Carroll, J.M. Anna

3:30 Intermission.

3:45 399. Population of multiple triplet states for drug photorelease and sensitization of singlet oxygen. **C. Turro**

4:10 400. Triplet excited states and metal based covalent cytotoxic agents. **P.C. Glazer**

4:35 401. Harvesting triplet excited states in Ru(II) and Cu(I) complexes for photodynamic therapy of cancer. **R.S. Khnayzer**

5:00 402. Tuning triplet excited state lifetimes in CuHETPHEN complexes. **K.L. Mulfort**, L. Kohler, D. Hayes, R. Hadt, L.X. Chen

Building a Safety Culture across the Chemistry Enterprise

Grassroots Approaches to Developing a Safety Culture

Sponsored by PRES, Cosponsored by BIOL, BMGT, CARB, CCS, CEI, CELL, CEPA, CHAS, CINF, COLL, CPRC, CTA, DAC, ETHX, I&EC, INOR, ORGN, PROF, SCHB and YCC

Transformative Research & Excellence in Education Award

Sponsored by COMSCI, Cosponsored by BIOL, COLL, COMP, ENFL, INOR, PHYS and PRES

Materials Science in Nuclear Waste Disposal

Sponsored by NUCL, Cosponsored by INOR

Undergraduate Research Posters

Inorganic Chemistry

Sponsored by CHED, Cosponsored by INOR and SOCED

MONDAY EVENING

Section A

Walter E. Washington Convention Center
Halls D/E

Sci-Mix

S. A. Koch, N. S. Radu, *Organizers*

8:00 - 10:00

130-132, **137**, **144-146**, **148-149**, **154**, **157**, **163**, **165**, **167**, **172**, **178**, **184**, **190**, **193**, **196-197**, **202**, **204**, **211**, **236**, **239**, **242**, **245-246**, **253**, **256-257**, **261**, **271**, **274**, **278**. See previous listings.

524, **528**, **532-533**, **536**, **538**, **540**, **542-543**, **549**, **552**, **559**, **562**, **566**, **568**, **570**, **575-577**, **581-582**, **585**, **588**, **597**, **607**, **613**, **615**, **617**, **621-623**, **625-626**, **631-632**, **635**, **637-638**, **641**, **645**, **648-649**, **668**, **670-672**. See subsequent listings.

TUESDAY MORNING

Section A

Renaissance Washington, DC Downtown
Renaissance East

Fundamental Aspects of Metal Organic Framework Catalysis

A. J. Morris, J. R. Morris, *Organizers*
S. Marinescu, *Presiding*

8:30 403. Probing framework-restricted metal axial ligation and spin state patterns in iron-porphyrin-based metal–organic framework catalysts. **J.V. Lockard**, P. Kucheryavy, N.O. Lahanas, C. Sun

9:00 404. Development of highly stable metal-organic frameworks for applications in catalysis. **P. Usov**, A.J. Morris

9:30 Intermission.

9:45 405. Metal dithiolene frameworks with tunable physical and chemical properties. **S. Marinescu**

10:15 406. Enhancement in molecular catalysis through redox hopping metal organic framework scaffold. **A.J. Morris**

10:45 407. Photophysical properties of crystalline self-assembled porous materials: Contribution of interchromophoric interactions and environment. **P. Deria**

Section B

Renaissance Washington, DC Downtown
Renaissance West A

Chemistry of Materials Lectureship & Best Paper Award

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

8:30 Introductory Remarks.

8:45 408. Perovskite photovoltaics: Materials, cells and modules. **K. Zhu**

9:30 409. Extrinsic ion migration in perovskite solar cells. **Z. Li**

10:10 410. Halide ion exchange and migration in mixed halide lead perovskites. **P.V. Kamat**, S.J. Yoon

10:40 Intermission.

11:00 411. Pb-free and less Pb perovskite thin-film solar cells: Theory and device. **Y. Yan**

11:30 412. Time-resolved optical studies of perovskite polycrystalline films, single crystals and their surfaces. **M.C. Beard**, Y. Yang

12:00 413. Tailoring of microstructures and grain-boundary networks in hybrid-perovskite thin films for efficient, stable solar cells. Y. Zhou, S. Pang, K. Zhu, **N.P. Padture**

Section C

Renaissance Washington, DC Downtown
Grand Ballroom South

Bioinorganic Chemistry

Proteins & Enzymes & Model Systems

S. A. Koch, *Organizer*
G. T. Cheek, H. C. Fry, *Presiding*

8:30 414. Acyl-containing small molecule mimics of [Fe]-hydrogenase: Ligand effect on structure and reactivity. **Y. Cho**, D. Gummadi, M.J. Rose

8:50 415. Electrochemical studies of cysteine/zinc interactions in aqueous media. **G.T. Cheek**, M.Y. Doan

9:10 416. Direct observation of oxygen rebound in an iron-hydroxide complex. **J. Zaragoza**, D.P. Goldberg

9:30 417. Biometal-induced structural perturbations of αSynuclein upon aggregation. **D.L. Abeyawardhane**, H.R. Lucas

9:50 418. Triiron clusters containing mixed bridging ligands for the study of dinitrogen reduction. **R.B. Ferreira**, L.J. Murray

10:10 Intermission.

10:20 419. DNA-processing repair proteins containing redox-active [4Fe4S] metallocofactors facilitate DNA lesion detection. **E. Tse**, J.K. Barton

10:40 420. Peptide assembly influence on metalloporphyrin function. **H.C. Fry**, L.A. Solomon

11:00 421. Artificial metalloproteins with Co_4O_4 cubane active sites: Exploiting secondary sphere interactions to control electronic and molecular structure. **L. Olshansky**, R.H. Lavorie, A.I. Nguyen, T.D. Tilley, A. Borovik

11:20 422. Generation of a metastable, nonheme $\{FeNO\}^8$ complex: Reduction of $\{FeNO\}^7$, production of N_2O, and nitroxyl (NO^-) based reactivity. **A.M. Confer**, A. McQuilken, D.P. Goldberg

Section D

Renaissance Washington, DC Downtown
Renaissance West B

Organometallic Chemistry

New Ligand Platforms: Pincer Ligands

N. S. Radu, *Organizer*
R. Wright, *Presiding*

8:30 423. Exploring ion-controlled substrate access to pincer-crown ether catalysts. **J.B. Smith**, S.H. Kerr, A.J. Miller

8:50 424. Multifunctional redox-active and electrophile-responsive pincer ligand supporting multiple oxidation states of Co and Fe on a way to CO_2 activation. **A.V. Polezhaev**, A. Cabelof, C. Chen, K.G. Caulton

9:10 425. Facile metal-ligand cooperative nitride to ammonia conversion on a pincer ruthenium framework using weak chelating acids. **B.M. Lindley**, Q.J. Bruch, F. Hasanayn, A.J. Miller

9:30 426. New ligand architecture to enable aerobic C-H oxidation at a platinum center. **D.B. Watts**, D. Wang, P.Y. Zavalij, A.N. Vedernikov

9:50 427. Multiple metal-boron interactions in carboranyl pincer complexes. **D.V. Peryshkov**, B. Eleazer

10:10 428. Agostic $C_{(sp2)}$-H Iron(I) pincer complex. **Q. Lai**, O. Ozerov

10:30 429. Synthesis and reactions of high-valent nitridorhenium(V) complexes bearing PNP pincer ligands. **N. Lambic**, E. Ison

10:50 430. C-H activation with PBP pincer complexes of iridium and rhodium takes advantage of a non-innocent boryl site. **O. Ozerov**, W. Shih, Y. Cao

11:10 431. Diverse reactivity of iridium pincer-crown ether carbonyl complexes. **J. Grajeda**, E.K. Nichols, A.J. Miller

Section E

Renaissance Washington, DC Downtown
Grand Ballroom North

Many Colors of Copper

Small Molecule Activation

Cosponsored by BIOL
K. J. Franz, I. Garcia-Bosch, K. D. Karlin, *Organizers*
T. H. Warren, *Organizer*, *Presiding*

8:55 Introductory Remarks.

9:00 432. Copper-catalyzed electrochemical CO reduction. **M. Kanan**

9:30 433. Hydrogenation of CO_2 using copper hydride complexes. **A.M. Appel**

10:00 434. Electrocatalytic water oxidation by a homogeneous copper catalyst disfavors single-site mechanisms. **M.T. Kieber-Emmons**

10:30 Intermission.

10:45 435. Cu(III) with imidazole ligation: Biologic relevance? **T.D. Stack**, W. Keown, L. Chiang, J.B. Gary, E.C. Wasinger

11:15 436. Copper(III) complexes relevant to possible catalytic intermediates. **W.B. Tolman**

11:45 437. Copper active site of particulate methane monooxygenase. **A.C. Rosenzweig**

Section F

Renaissance Washington, DC Downtown
Grand Ballroom Central

Center for Enabling New Technologies through Catalysis: Transforming Catalysis through Collaboration

A. Goldman, N. E. Gruhn, S. W. Krska, *Organizers*
E. Ison, L. T. Thompson, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 438. New elementary reactions, catalytic reactions, and combinations of catalytic reactions. **J.F. Hartwig**

9:05 439. Process inspired method development: New chemistries of sulfuryl fluoride. **P.S. Hanley**, M. Ober, A.L. Krasovskiy, T.P. Clark

9:25 440. Concurrent tandem catalytic methodologies for the hydrodehalogenation, cyanation, and amidation of aryl halides using a multifunctional copper catalyst. S. Lin, **A.H. Roy MacArthur**

9:45 441. Valuable skills I learned at CENTC that prepared me for a career in industry. **J.M. Villalobos**

10:05 Intermission.

10:15 442. Exploring the synergy between biological catalysis and chemical catalysis. **H. Zhao**

10:45 443. Dicarbofunctionalization of olefins by cross-coupling. **R. Giri**

11:05 444. Ru(II) complex catalyzed tandem C-C and C-N bond formation: Sustainable strategy for the utilization of alcohols as alkylating agents. K. Chakrabarti, B. Paul, B.C. Roy, S. Shee, **S. Kundu**

11:25 445. Cyclometallation reactions of alkynes, alkenes, ketones, and biphenylene with iridium pincer complexes. M. Wilklow-Marnell, D.A. Laviska, B. Li, T. Zhou, K. Krogh

Jespersen, W. Brennessel, A.S. Goldman, **W.D. Jones**

11:55 Concluding Remarks.

Section G

Renaissance Washington, DC Downtown
Congressional A

Electrochemistry

B. L. Lucht, *Organizer*
I. F. Cheng, B. Helms, *Presiding*

8:30 446. Toward a molecular level understanding of electrochemical interfaces in lithium–sulfur batteries. **B. Helms**

8:50 447. Resolving the mechanism of capacity fading in Li-ion solid-state batteries. **C. Gong**, Z. Jadidi, F.E. Gabaly, E.J. Fuller, A.A. Talin, M.S. Leite

9:10 448. Graphene from the University of Idaho thermolyzed asphalt reaction (GUITAR) is it an amorphous carbon, graphite or a new carbon allotrope? **I.F. Cheng**, D. Estrada, P. Davis, A. Clearfield, J. Foutch, K. Livingston, K. Yocham, T. Pandhi, C. Nwamba, Y. Kan, A. Blumenfeld, H. Kabir

9:30 449. Rhenium and manganese complexes with proton relays in the secondary coordination sphere for the electrocatalytic reduction of carbon dioxide. **V. Yempally**, C.A. Caputo

9:50 450. Effect of metal cations on the redox behavior of naphthalene diimides. **C.R. Wade**, B.R. Reiner

10:10 451. Probing the tunable redox nature of vertex-differentiated dodecaborate clusters. **A.I. Wixtrom**, A.M. Spokoyny

10:30 452. Nontraditional porphyrinoid scaffolds as efficient electrocatalysts for the oxygen reduction reaction. **J. Rosenthal**

10:50 453. Using rotating ring-disk electrode voltammetry to study the influence of organic solvents on the oxygen reduction reaction in Li-O_2 battery electrolytes. **J. Chen**, M. Cheng

11:10 454. Electrodeposition of Si thin film on HOPG from $SiCl_4$ in $BMImTf_2N$ at room temperature. N.K. Shah, A. Ray*, R.K. Pati, **I. Mukhopadhyay**

11:30 455. Electrochemical quantification of hormone disruptors with a bacterial biosensor. **A.L. Furst**, M.B. Francis

11:50 456. Naturally synthetic: Using biology to connect inorganic particles. **M.A. Allen**, E. Barannikova, S.J. Riley, A. Winton

Understanding the Chemistry of Our Planet

Chemistry's Role in our Earth System

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Materials Science in Nuclear Waste Disposal

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Non-Conventional Building Blocks in Conjugated Materials: Innovative Designs & New Applications

Aromatic, Antiaromatic & Non-Aromatic Systems

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TUESDAY AFTERNOON

Section A

Renaissance Washington, DC Downtown
Renaissance East

Fundamental Aspects of Metal Organic Framework Catalysis

A. J. Morris, J. R. Morris, *Organizers, Presiding*

1:30 457. Tune the catalytic selectivity of core-shell metal-organic frameworks (MOFs) by changing the length of the linker in the shell. X. Yang, **H. Zhou**

2:00 458. Multi-component metal−organic frameworks as cooperative bimetallic catalysts. **S. Yuan**

2:30 Intermission.

2:45 459. CuPd mixed-metal MOFs characterized by UHV-FTIRS and HR-XPS. **P. Guo**, M. Muhler, Y. Wang

3:15 460. Metal-organic frameworks as micromotors with tunable engines and brakes. **X. Yu**, J. Li, J. Wang, S. Cohen

3:45 461. Impact of metal substitution on stability and adsorption properties of MOF-74. **K.S. Walton**

Section B

Renaissance Washington, DC Downtown
Renaissance West A

Memorial Symposium Honoring Justine Roth: Oxygen & Isotope Effects in Mechanisms, from Enzymes to Small Molecules

Cosponsored by BIOL
A. M. Angeles Boza, J. M. Mayer, *Organizers*
K. D. Karlin, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 462. Analyzing hydrogen atom transfer reactions with Marcus theory. **J.M. Mayer**

2:00 463. Dioxygen activation by human indoleamine 2,3-dioxygenase, isoform-1 (hIDO1): The role of ferryl derivatives in catalysis. **V.V. Smirnov**

2:25 464. Differences in carbon and oxygen isotope discrimination during the catalytic activation of small molecules. **A.M. Angeles Boza**

2:50 465. Reactivity in situations where life's control over coordination is weak or non-existent. **A.T. Stone**

3:15 Intermission.

3:35 466. Fire without Flint: Cofactorless strategies for converting biopolymers into useful chemical precursors. **J. DuBois**, G.C. Moraski, G. Beckham

4:00 467. Using isotope effects to follow the chemical step along enzyme evolution. P. Singh, D. Hilvert, **A. Kohen**

4:25 468. Addition of HX across Ni amide bonds: Synthesis and reactivity of Ni hydroxide complexes. **J.M. Boncella**, N.H. Anderson, A.M. Tondreau

4:50 469. Enormous, temperature independent kinetic deuterium isotope effects in the proton-coupled electron transfer reaction catalyzed by soybean lipoxygenase. **J. Klinman**, S. Hu, A. Soudackov, S. Hammes-Schiffer

Section C

Renaissance Washington, DC Downtown
Grand Ballroom South

Chemistry of Materials

Nanomaterials

C. G. Lugmair, *Organizer*
P. Tyagi, J. G. Werner, *Presiding*

1:30 470. Molecular spintronics device based magnetic metamaterials. **P. Tyagi**, C. D'Angelo, C. Baker

1:50 471. Fluorescence preservation and solidification of semiconducting polymer-dots by hybridization with layered double hydroxides. **X. Liu**, W. Wang, Y. Chen, S. Kuo, Y. Chan, C. Chen

2:10 472. Manganese and iron oxo-clusters as potential contrast agents for magnetic resonance imaging. **V. Dahanayake**, W. Hickling, O. Rodriguez, C. Albanese, S.L. Stoll

2:30 473. Plasmonic photoelectrochemistry for catalytic functionality. **D.R. Baker**, K. Grew, J.P. McClure, J. Boltersdorf, C. Lundgren

2:50 474. Core-shell mesoporous silica nanoparticles embedded with X-ray dense nanocrystals for CT imaging and drug delivery. **S. Chakravarty**, B. Blanco-Fernandez, E.M. Shapiro

3:10 475. Nano-integrated ordered three-dimensional multifunctional hybrid for all-solid-state energy storage. **J.G. Werner**, G.G. Rodríguez-Calero, H.D. Abruna, U.B. Wiesner

3:30 Intermission.

3:45 476. Cesium lead bromide perovskite nanocube superlattices and the pressure-induced change in its structure and optical properties. **Y. Nagaoka**, O. Chen, K. Hills-Kimball, Z. Wang, R. Li

4:05 477. Synthesis and fluorescence properties of carbon quantum dots and core-shell superparamagnetic Fe@C-CN_x particles. **V.N. Khabashesku**, S. Murugesan, R. Suresh, O. Kuznetsov

4:25 478. Extension of confined-yet-coupled design to 2D semiconductors. **T.W. Farnsworth**, A. Woomer, J. Thompson, S.C. Warren

4:45 479. Design and use of upconverting $NaYF_4$:Yb/Er nanocrystals for 3D tissue imaging in optical emission computed tomography. **B.W. Langloss**, P. Yoon, M. Oldham, M.J. Therien

5:05 480. Giant PbS/CdS/CdS quantum dots: Effect of shell thickness on structure, ensemble and single-dot stability, and device performance. **S. Krishnamurthy**, Z. Hu, A. Singh, M. Sykora, J. Casson, D. Williams, H. Htoon, A. Malko, J.A. Hollingsworth

Section D

Renaissance Washington, DC Downtown
Renaissance West B

Coordination Chemistry

Synthesis & Characterization

S. A. Koch, A. Larsen, *Organizers*
C. R. Graves, W. Lee, *Presiding*

1:30 481. Aluminum complexes of redox-active ligands. **C.R. Graves**

1:50 482. Synthesis, structure, and computations of an isolable magnesium diphosphaethynolate complex. **R.J. Gilliard**, D. Heift, Z. Benkö, A.L. Rheingold, J.D. Protasiewicz, H. Grützmacher

2:10 483. Synthesis, characterization and tyrosinase enzyme inhibition studies of titanium complexes. **U. Ashiq**, Z. Shaikh, R. Jamal, M. Mahroof-Tahir

2:30 484. Synthesis and characterisation of polydentate imino phosphonate complexes of Co(III). **N. Daniel Ekekwe**, M. Polson, J. Wikaira, R. Hartshorn

2:50 485. Tetra-aza-anthraquinone: A biologically-inspired redox-active ligand bridging homogeneous and heterogeneous catalysis toward the reduction of small molecules. **I.J. Huerfano**, A.V. Polezhaev, M. Pink, C. Chen, K.G. Caulton

3:10 486. Low-coordinate heterocyclic thione and selone complexes of copper(I) and silver(I). **A. Allen**, D. Rabinovich

3:30 Intermission.

3:40 487. Synthesis, reactivity, and compositional analysis of trinuclear clusters. **C. Juda**, T. Betley

4:00 488. Synthesis, characterization, and reactivity of iron and cobalt complexes with an asymmetric nacnac ligand. **W. Lee**, E.A. Weerawardhana, C.M. Stanek, M. Zeller

4:20 489. Redox-active pincer ligands on chromium: Carbonate formation from a neglected metal. **N. Labrum**, C. Chen, M. Pink, K.G. Caulton

4:40 490. Re(CO)$_3$-templated scorpionate synthesis through nitrile activation. **A.J. Osinski**, C.J. Ziegler

5:00 491. Mechanistic study of the pH-dependent assembly/disassembly of nanojars. **B. Ahmed**, G. Mezei

Section E

Renaissance Washington, DC Downtown
Grand Ballroom North

Many Colors of Copper

Catalysis

Cosponsored by BIOL
K. J. Franz, K. D. Karlin, T. H. Warren, *Organizers*
I. Garcia-Bosch, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 492. Copper catalyzed C-H functionalization: Method development via enabling intermediates. **T.H. Warren**

2:05 493. Development of copper catalysts for the selective oxidation of C-H bonds under mild conditions. **I. Garcia-Bosch**

2:35 494. Driving synthesis by oxidation. **J. Lumb**

3:05 Intermission.

3:20 495. Fundamental redox processes in model platforms for Cu-catalyzed C-heteroatom bond forming transformations. **X. Ribas**

3:50 496. Copper-catalyzed amino difunctionalization of alkenes. **Q. Wang**

4:20 497. Revealing the mechanisms of copper-catalyzed synthetic methods. **J.F. Hartwig**

Section F

Renaissance Washington, DC Downtown
Grand Ballroom Central

Center for Enabling New Technologies through Catalysis: Transforming Catalysis through Collaboration

A. Goldman, N. E. Gruhn, E. Ison, S. W. Krska, L. T. Thompson, *Organizers*
W. D. Jones, M. S. Sanford, *Presiding*

1:30 Introductory Remarks.

1:35 498. Hydrogenolysis of carbon-oxygen bonds. **D.M. Heinekey**, K.I. Goldberg, J.M. Goldberg, B. Bark

2:05 499. Aldehyde water shift reaction: Integrating theory and experiment to deconvolute a catalytic transformation. **T.R. Cundari**, T. Brewster, W. Ou, J.C. Tran, W. Wen, J.M. Goldberg, K.I. Goldberg, S.K. Hanson, D. Thorn, D.M. Heinekey, L.T. Thompson

2:35 500. Synthesis and characterization of bifunctional transition metal complexes. **T. Brewster**, T.J. Yokley, C.E. O'Connell, T.H. Nguyen, M.M. Reynolds

2:55 501. Details towards the mechanism of base-free transfer hydrogenation catalyzed by Cp*Ir(pyridinesulfonamide)Cl complexes. **A.R. O'Connor**, T.M. Townsend, A. Ruff, G.L. Heard, C. Goldberg

3:15 502. Enabling new technology with catalysis at Eastman Chemical. **R.T. Hembre**

3:35 Intermission.

3:45 503. Cheaper by the Baker's dozen: Towards base-metal Guerbet catalysts for selective butanol production. C.E. Hayes, N. Kulkarni, W.D. Jones, **R.T. Baker**

4:15 504. Towards biomass as sustainable feedstock: Understanding mechanisms in halide and solid acid catalysis. **M. Emmert**

4:35 505. Production of long chain alcohols through the '+1' pathway: Combining enzyme engineering, strain development and fermentation optimization to accelerate development. P. Bhosale, S. Delaplane, M. Devarapalli, S. Greenwalt, R. Hill, P. Sanghani, C. Stowers, **D.C. Rosenfeld**

4:55 506. Apeel Sciences: Going with the flow… (but not really). **R. Alamillo**, M. Aronson, L. Perez

5:15 Concluding Remarks.

Section G

Renaissance Washington, DC Downtown
Congressional A

Chemistry of Materials

Synthesis & Properties

C. G. Lugmair, *Organizer*
E. Doud, *Presiding*

1:30 507. One-pot synthesis of gold microbars for optical circuitry applications. **E. Hobbs**, M. Devadas

1:50 508. Metal coordination complexes in mechanically responsive systems. **K. Hall**, M.H. Horst, S.W. Telford, K.J. Franz

2:10 509. *In-situ* structure-tracking aided design in synthesis of energy-storage materials. **F. Wang**, J. Bai

2:30 510. Aerosol assisted chemical vapor deposition of WS_2 from a single source precursor. **N. Richey**, L. McElwee-White

2:50 511. Exfoliation and doping of layered two-dimensional rhenium and molybdenum chalcohalide networks. **B. Choi**

3:10 Intermission.

3:25 512. Conductance of NHC-based single-molecule junctions formed *in situ* via (NHC)AuCl complexes. **E. Doud**, M. Inkpen, G. Lovat, L. Venkataraman, X. Roy

3:45 513. Design and synthesis of fluorinated tungsten (VI) oxo-alkoxide complexes bearing β-diketonate and β-ketoesterate ligands for chemical vapor deposition of WO_x. **D.C. Bock**, N. Ou, T.J. Anderson, L. McElwee-White

4:05 514. Synthesis and luminescent behavior of lanthanide thiophenemonocarboxylate-based materials. **R. Batrice**, A.K. Adcock, R.L. Ayscue, P. Cantos, J.A. Bertke, K.E. Knope

4:25 515. Synthesis and characterization of photoluminescent bismuth organic materials. **K.E. Knope**

Section H

Renaissance Washington, DC Downtown
Congressional B

Lanthanide & Actinide Chemistry

A. De Bettencourt Dias, *Organizer*
C. G. Gianopoulos, M. Nippe, *Presiding*

1:30 516. Heterometallic lanthanide-transition metal gomplexes: Synthesis, magnetism, and redox properties. T.P. Latendresse, C. Dickie, C. Burns, **M. Nippe**

1:50 517. Probing crystal chemistry properties that impact flotation selectivity: Collector-mineral interaction experiments in synthetic REE-orthophosphate systems. **J. Gamage McEvoy**, Y. Thibault

2:10 518. Thermal charge-transfer reduction of uranyl UO_2^{2+}(VI) to UO_2^{+}(V) by methanol and other functionalized organic compounds. **X. Sun**, D. Kolling, S. Deskins

2:30 intermission.

2:45 519. Description of uranium-halogen bonding based on charge-density studies at 20 K. **C.G. Gianopoulos**, V.V. Zhurov, S.G. Minasian, E.R. Batista, C. Jelsch, A.A. Pinkerton

3:05 520. Luminescent behavior of bismuth halide organic complexes and their lanthanide doped analogs. **R.L. Ayscue**, J.A. Bertke, K.E. Knope

3:25 521. Magnetic resonance imaging contrast agent for in-vivo copper imaging. **N.N. Paranawithana**, A.F. Martins, G. Meloni, D. Sherry

3:45 522. Lanthanide podand complexes as potential bioimaging agents based on multidentate poly-acac motifs. **T.L. King**, G. Ibarra, R.A. Jones, E.L. Que

4:05 523. Investigation of the electronic structure and evaluation of the covalency of cerocene, $(C_8H_8)_2Ce$, using carbon K-edge X-ray absorption spectroscopy. **D.E. Smiles**, S.G. Minasian, J.M. Keith, E.R. Batista, S.A. Kozimor, R.L. Martin, D.K. Shuh

Understanding the Chemistry of Our Planet

Human Impacts to our Planet

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Chemistry Past Curium

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Non-Conventional Building Blocks in Conjugated Materials: Innovative Designs & New Applications

Heteroatom Systems

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TUESDAY EVENING

Section A

Walter E. Washington Convention Center
Hall D

Chemistry of Materials

C. G. Lugmair, *Organizer*

5:30 - 7:30

524. Aqueous sol-gel route towards selected quaternary metal oxides with single and double perovskite type structure containing tellurium or tungsten. **I. Derd**, B. Markovic, J. Bijelic, N. Filipovic, B. Matasovic, E. Kovac Andric, J. Popovic, Z. Skoko, Z. Jaglicic, D. Pajic, S. Mal, T. Weller, R. Marschall, P. Voepel, C. Suchomski, B. Smarsly

525. Synthesis of hafnium oxide and its thermal treatment. **I.B. Polovov**, Y.S. Bataev, V.A. Volkovich, A. Chukin, Y.D. Afonin, A.I. Rakhmatullin, M. Boca

526. Phase transfer directed synthesis of hollow metal-organic frameworks nanocages. **B. Yu**, J. Gong

527. Electrochemical etching for MXene. **W. Sun**

528. Magnetic diluted semiconductors in 2D nanosheet crystals. S. Hsu, T. Hsieh, T.S. Lin, **Y. Liu**

529. Sized controlled synthesis of hollow sphere metal oxides for metastable intermolecular composites. **A.M. Morey**, S.T. Iacono

530. New methods to fabricate anti-fooling Ag@silica catalyst for the reduction of 4-nitrophenol. **J. Hou**, J. Gong

531. Bimetallic amino acid complexes as precursors for nickel molybdate. **F. Alqahtani**, A.W. Apblett

532. Effective charge separations in Ag_2S-CdS-ZnS 1D heterostructures. H. Chen, Y. Chen, H. Fan, **Y. Liu**

533. Stability of metal-organic frameworks for high pressure confined chemical vapor deposition. **B. Laubacker**, J.V. Badding

534. Aerosol route to various iodine oxide/iodic acid microparticles, and their performance as oxidizers in thermite systems. **T. Wu**, X. Wang, M.R. Zachariah

535. Light absorption and energy transfer in thin film metal-organic frameworks. **J. Rowe**, A.J. Morris, E.M. Soderstrom

536. Growths of highly ordered mesoporous graphene-oxide thin films (MGTFs). Z. Dai, H. Chang, **Y. Liu**

537. Synthesis and characterization of a new copper ruthenium polypyridyl complex based coordination polymer. **M. Polapally**, B. Yan

538. Effect of molecular dipole on phase behavior of pyridinium derivatives of [*closo*-1-$CB_{11}H_{12}$]$^-$. **A.C. Friedli**, B.D. Lukasik, M.O. Ali, K.L. King, P. Kaszynski

539. Study of nanostructured composites Nd(Ti,Zr)O/Si(B)CO for optical and nuclear waste storage application. **V. Proust**, T.E. Albrecht-Schmitt

540. Synthetic deconvolution of interfaces and material components in hybrid nanoparticles. **J.L. Fenton**, R.E. Schaak

Section B

Walter E. Washington Convention Center
Hall D

Main Group Chemistry

T. W. Hudnall, *Organizer*

5:30 - 7:30

541. Luminescent azepane-substituted β-diketones and difluoroboron complexes. **F. Wang**, C.A. DeRosa, M. Daly, D. Song, C.L. Fraser

542. Difluoroboron β-diketonates for ratiometric oxygen imaging with a color camera. **M. Zhuang**, C.A. DeRosa, F. Wang, C.L. Fraser

543. Luminescent piperidine-substituted dibenzoylmethane derivatives and their difluoroboron complexes. **D. Song**, F. Wang, C.A. DeRosa, C.L. Fraser

544. Radiosyntheses of [^{18}F]fluoroarenes *via* hypervalent iodoarene precursors. **J. Chun**, J. Son, J. Park, M. Yun

545. Sb@Ni_{12}@Sb_{20}^m and Sb@Pd_{12}@Sb_{20}^n cluster anions where m=+1, -1, -4; n = +1, -1, -3, -4: Multi-oxidation state clusters of interpenetrating platonic solids. **Y. Wang**, M.M. DeBusk, L. Stevens, J. Hu, P.Y. Zavalij, K.H. Bowen, B.I. Dunlap, E. Glaser, B.W. Eichhorn

546. Heterobimetallic aluminum-alkali metal complexes of tetraanionic chiral ligands. **R. Mosneanu**, C.R. Graves

Section C

Walter E. Washington Convention Center
Hall D

Solid-State Inorganic Chemistry

C. G. Lugmair, V. Poltavets, *Organizers*

5:30 - 7:30

547. IONiC connection: Increasing interactions in the inorganic community. **B.A. Reisner**, **J.L. Stewart**, A.K. Bentley, H.J. Eppley, E.R. Jamieson, A.R. Johnson, S. Lin, C. Nataro, K. Plass, S.R. Smith, L.A. Watson, N. Williams

548. Synthesis and characterization of new alkali metal and divalent transition metal materials derived from the the hydortris(3,5-dimethyl-1,2,4-triazolyl)borate ligand. **E.C. Krist**, E. Roberts, B.C. Chan, **B.A. Reisner**

549. Halogen mediated synthesis of noninterpenetrated metal organic frameworks (MOFs). **J.L. Strozier**

550. From a layer to a ring: A kinetic study for the ion-exchange reactions of a new tellurite, $Li_2Mo_3TeO_{12}$ using the powder X-ray diffraction. **S. Oh**, K. Ok

551. Investigation of relaxor ferromagnets. **C. Chin**, P.D. Battle, E.C. Hunter, M. Avdeev, J. Hadermann, R. Paria Sena

Section D

Walter E. Washington Convention Center
Hall D

Coordination Chemistry

Synthesis & Characterization

S. A. Koch, A. Larsen, *Organizers*

5:30 - 7:30

552. Bottom-up assembly of self-supporting metal-organic layers. **L. Cao**, C. Wang, W. Lin

553. Facile route synthesis and structural characterization of anionic lanthanide-salen complexes. **P.K. Yuen**, C. Lau, N. Ho, W. Chan, H. Chan, A.K. Yuen

554. Studies of dinuclear metal complexes as models for inhibited metallohydrolases. **A.H. Gad**, H.I. Nimir

555. Redox interconversion of non-oxido vanadium complexes accompanied with thiol and thiolate transformations. **H. Hsu**, J. Yan

556. Carbon-hydrogen bond activation via a bis(pyrrolyl)pyridine iron complex: Evidence for iron nitrene intermediates. **B.M. Hakey**, C. Milsmann

557. Synthesis and characterization of dioxomolybdenum(VI) complexes containing nitrogen rich ligands and their potential use in thin films growth and oxygen transfer reactions. **O. El-Kadri**

558. Anionic indium-derived metal organic frameworks. **S.E. Springer**, D. Genna

559. Amine-functionalized trispyrazolylborate iron spin crossover complexes: A key element for the preparation of electrically addressable molecular magnetic quantum bit. **C. Ma**, C. Besson

560. Synthesis of 1,3,6-trisubstituted fulvene coordination complexes as versatile building blocks for supramolecular architectures and functional materials. **S.K. Adas**

561. Simple, efficient synthetic route to 2-2'-bipyrazine derivatives from bromo-pyrazine for making rhenium and ruthenium dyes. **D.P. Rillema**, V. Komreddy, H. Nguyen

562. Synthesis and characterization of heterobimetallic Cu(I)-X complexes supported by substituted trispyridylphosphines. **J. Leonard**, M. Bezpalko, W.S. Kassel

563. Aluminum complexes of nitroxide-based redox active ligands. **A. Woodside**, C.R. Graves

564. Spectroscopic characterization of copper(II)-alkylperoxo complexes. **B. Pella**

565. Construction of variable dimension $CdCl_2$ complexes from topologically linear pentadentate ligands. **A. Gerhard**, D.B. Tice, R.D. Pike, **D.C. Bebout**

566. Recent developments in the chemistry of dicopper(I)-naphthyridinediimine crescent complexes hosting various bridging ligands. **R. Conger**, S. Fox

567. Synthesis and coordination chemistry of functionalized pyridylphosphine ligands with late transition metals. **M. Bezpalko**, W.S. Kassel

568. Synthesis and characterization of ruthenium complexes of tris(2-pyridyl)phosphine. **L. Wilkinson**, M. Bezpalko, W.S. Kassel

569. Ligand-based phase control in low-dimensional metal-organic frameworks. **O. Barreda**, **E.D. Bloch**

570. Synthesis and characterization of organic-inorganic conjugate dyes designed for solar energy harvesting. **B.C. Biermann**, M.R. Leidy, S. Parks, **R.E. Bachman**

571. Synthesis, characterization, and reactivity of cobalt complexes bearing the nitrogen-based pip_2NNN ligand. **J. Webb**, B. Hakey, M. Sabat

572. Tripodal transition metal beta-diketonate complexes. **G. Ibarra**, T.L. King, R.A. Jones, E.L. Que

573. Synthesis and characterization of rhodium(III) complexes using mixed polypyridyl ligands. P. Nunez, **D. Amarante**

Section E

Walter E. Washington Convention Center
Hall D

Bioinorganic Chemistry

DNA, RNA & Inorganic Drugs

S. A. Koch, *Organizer*

5:30 - 7:30

574. Metal catalysts as novel molecular tools and potential therapeutics: From G-quadruplex-targeting nucleases to chimeric fucosidases. **Z. Yu**, J.A. Cowan

575. Electron-deficient organometallic compounds: Potential anticancer drug candidates against human colon cancer. **R.M. Lord**, A. Saidykhan, A. Pitto-Barry, N. Barry

576. Synthesis, DNA binding study and anticancer activity of organorhenium sulfonato compounds on hormone-dependent MCF-7 and hormone-independent triple-negative MDA-MB-231 breast cancer cells. **T. Odebode**, A.J. Winstead, S.K. Mandal

577. Photodynamic therapy metal organic frameworks (PDT-MOFs). **N. Azbill**, A.G. Giacalone, R.W. Larsen

578. Towards photodynamic therapy MOFS: Encapsulation of photoactive Ru(II)(2,2'-bipyridine)$_2$(bio-active molecules)$_2$ into metal organic frameworks. **A.G. Giacalone**, L. Wojtas, R.W. Larsen

579. DNA binding studies of organorhenium picolinato, nicotinato, and tryptophanato complexes. **M. Stevenson**, S. Pramanik, S.K. Mandal

580. DNA binding studies of organorhenium mefenamato and tolfenamato complexes. **T.V. Hinton**, S. Pramanik, S.K. Mandal

Section F

Walter E. Washington Convention Center
Hall D

Many Colors of Copper

K. J. Franz, I. Garcia-Bosch, K. D. Karlin, T. H. Warren, *Organizers*

5:30 - 7:30

581. Electrocatalytic water oxidation by a copper(II) complex with an oxidation-resistant N,O-donor ligand. **K.J. Fisher**, K. Materna, B.Q. Mercado, R.H. Crabtree, G.W. Brudvig

582. Targeting drug-resistant bacteria with enzyme-activated prochelators. **A.C. Jackson**, J. Zaengle-Barone, D. Besse, K.J. Franz

583. Molecular basis of polysaccharide cleavage by lytic polysaccharide monooxygenases. **L. Ciano**, K. Frandsen, T. Simmons, P. Dupree, J. Poulsen, G. Hemsworth, E.M. Johnston, M. Tovborg, K. Johansen, P. von Freiesleben, L. Marmuse, S. Fort, S. Cottaz, H. Driguez, B. Henrissat, N. Lenfant, F. Tuna, A. Baldansuren, G. Davies, L. Lo Leggio, P. Walton

584. Examination of NO reduction at monometallic sites. **C.M. Greene**, T.H. Warren

585. Investigating the role of copper in the cytotoxic mechanism of enzyme-activated prochelators. **J.M. Zaengle-Barone**, K.J. Franz

586. Cu-directed hydroxylation of sp^2 and sp^3 C-H bonds. **R. Trammell**

587. Prostate cancer targeted prodrug based on copper prochelator. **A. Dharani**, S. Bakthavatsalam, T. Zhang, K.J. Franz

588. Copper catalyzed C-H amidation. **I. Jayasooriya**, A. Bakhoda, T.H. Warren

589. Copper complexes featuring tris(pyrazolyl)borate ligands that mediate H-bonding interactions with bound functionalities. **C.R. Cobb**, E.J. Gardner, T.H. Warren

590. Trinuclear copper pyrazolates as precursors for di- and tetra-nuclear copper adducts. **R. Dias**

Section G

Walter E. Washington Convention Center
Hall D

Center for Enabling New Technologies through Catalysis: Transforming Catalysis through Collaboration

A. Goldman, N. E. Gruhn, E. Ison, S. W. Krska, L. T. Thompson, *Organizers*

5:30 - 7:30

591. Aerobic oxidation of KA oil to adipic acid with Ir^{III} complexes. **Z.H. Syed**, S.B. Rubashkin, A.M. Wright, K.I. Goldberg

592. Comparision of the reactivity of (^{dm}Phebox)Ir(CO_2R)$_2$(H_2O) complexes with octane. **H. Yuan**, **W.D. Jones**

593. Pincer-ligated iridium(III) complexes for alkane dehydrogenation. **K.E. Kim**, K.I. Goldberg

594. Synthesis and catalytic activity of a novel pincer-osmium complex. **S. Murugesan**, X. Zhou, A.S. Goldman

595. Synthesis, characterization, and reactivity of a ruthenium complex of a new PSP pincer ligand. **X. Zhou**, S. Murugesan, A.S. Goldman

596. Continuous-flow heterogeneous alkane transfer dehydrogenation catalyzed by immobilized pincer-ligated iridium complexes. **B. Sheludko**, M.T. Cunningham, M.E. Gliege, A.S. Goldman, F.E. Celik

597. Cross-dehydrogenative-coupling of styrene with non-functionalized aromatics and alkene. **B. Li**, M. Wilklow-Marnell, W.D. Jones, A.S. Goldman

598. Iridium hydride and dihydrogen complexes relevant to biomass deoxygenation. **J.M. Goldberg**, T. Lekich, L.M. Guard, B. Bark, G.W. Wong, J.C. Linehan, K.I. Goldberg, D.M. Heinekey

599. (Hexamethylbenzene) ruthenium catalysts for the aldehyde water shift reaction. **A.S. Phearman**, D. Bhagwandin, D.M. Heinekey, K.I. Goldberg

600. Ethanol upgrading to butanol and higher alcohols: A high-throughput approach using the Guerbet reaction. **C.E. Hayes**, N. Kulkarni, W.D. Jones, R. Baker

601. Catalytic upgrading of ethanol to 1-butanol via Guerbet reaction. **N. Kulkarni**, C. Hayes, R. Baker, W.D. Jones

602. Synthesis, characterization, and application of abnormal N-heterocyclic carbene complexes of palladium. **T. Yokley**, N.D. Schley, H. Kurtz, T.P. Brewster

603. Direct aniline formation through benzene and hydroxylamine. **N. Liu**, M. Sleck, W.D. Jones

604. ^{iPr}PCPIrH_4, *para*-benzoquinones, alcohols, electrons, and protons: Making everyone play nice. **M. Wilklow-Marnell**, W.D. Jones

605. Homogeneous hydrogenation of amides: Investigation of C–N vs. C–O bond cleavage in the context of CO_2 hydrogenation. **N.M. Rezayee**, M.S. Sanford

606. Heterogenization of homogeneous ester hydrogenation catalysts in metal-organic frameworks. **D. Samblanet**, M.S. Sanford

607. Heterogeneous systems for low temperature CO_2 capture and hydrogenation. **S. Eady**, T. Silbaugh, M.A. Barteau, L.T. Thompson

608. Hydricity calculation using computational methods: Potential-pKa method versus direct calculation. **H. Fallah**, K.R. Brereton, T.R. Cundari, A.J. Miller

609. Electrochemical oxidation and deprotonation of iridium pincer catalysts: Understanding key steps on the road to alkane dehydrogenation. **A.M. Brasacchio**, A.G. Walden, B.M. Lindley, N. Lease, A. Goldman, A.J. Miller

610. Synthesis of Zn(II)/SiO_2 material and the application towards the hydrofunctionalization of alkynes. **A.K. Cook-Sneathen**, C. Coperet

611. Rhenium and osmium pincer complexes for nitrogen reduction to ammonia. **N. Lease**, A. Casuras, A. Goldman

612. Electrochemical reduction of (PNP)Ru ammonia complexes produces a variety of (pincer)Ru hydrido dinitrogen complexes. **Q.J. Bruch**, B.M. Lindley, A.J. Miller

613. Cerium oxide as a hydrogen acceptor in catalytic alcohol dehydrogenation. **S.M. Laga**, T.M. Townsend, A.R. O'Connor, J.M. Mayer

Section H

Walter E. Washington Convention Center
Hall D

Electrochemistry

B. L. Lucht, *Organizer*

5:30 - 7:30

614. Electrochemical analysis of Fe-doped anatase nanoparticles for Li- and Na-ion battery applications. **J. Clapham**, S. Naik, B.D. Fahlman

615. Electrochemical study of the promoting effect of Fe on oxygen evolution at thin Ni-borate films and the poisoning effect of Al in the borate electrolyte. R. Fayad, J. Dhainy, H. Ghandour, **L.I. Halaoui**

616. Influence of deposition temperature on the morphology of electro-deposited CdTe thin films from BMImCl medium. M. Waldiya, D. Bhagat, **I. Mukhopadhyay**

617. Electrodeposited micro/nano structured lead metal on FTO substrate at room temperature. D. Bhagat, M. Waldiya, **I. Mukhopadhyay**

618. Synthesis of new hydrophobic, fluorinated, and cross-linked polymers and their use for corrosion protection of aluminum substrates. **W. Yaseen**, S. Marpu, T. Golden, M.A. Omary

619. Band-edge modulation of Si(111): The effects of surface functionalization with aromatic and electron withdrawing moieties. **D.G. Boucher**, M.J. Rose

620. Purity and stability of an electrolytically-generated hypochlorous acid solution. **L.I. Robins**, J. Williams, L. Contreras

621. Electrochemical reductive grafting studies of diazonium gold(III) salts on glassy carbon electrodes. **B. Workie**, A. Mohamed

622. Niobium speciation in chloride melts: Electrochemistry and spectroscopy. **I.B. Polovov**, G.L. Fofanov, D. Nikitin, M.V. Chernyshov, V.A. Volkovich, O.I. Rebrin

623. Mechanistic studies of NO_3^- conversion to NH_3 by a cobalt molecular electrocatalyst. **S. Xu**, D. Ashley, C. Chen, E. Jakubikova, J.M. Smith

Section I

Walter E. Washington Convention Center
Hall D

Organometallic Chemistry

New Ligand Platforms

N. S. Radu, *Organizer*

5:30 - 7:30

624. Multiyne chains as a platform for construction fused-ring metallaaromatics. **Q. Zhuo**, H. Zhang, H. Xia

625. Multidentate lariat phosphines: Synthesis and coordination chemistry. **L. Pap**, E.B. Hulley

626. Bowl-shaped sumanenyl anions: Double concave metal encapsulation. S.N. Spisak, Z. Wei, A.Y. Rogachev, T. Amaya, T. Hirao, **M.A. Petrukhina**

627. Tethered, axially-coordinating pyrrolidinone-phosphine ligands for dirhodium paddlewheel complexes. **B. Anderson**, A. Darko

628. Small molecule activation with bimetallic complexes. **N. Gardner**, E.D. Bloch

629. Improved synthetic route to heteroleptic alkyl phosphine oxides and their reduction to phosphines. N.I. Rinehart, **A.J. Kendall**, D.R. Tyler

Section J

Walter E. Washington Convention Center
Hall D

Lanthanide & Actinide Chemistry

A. De Bettencourt Dias, *Organizer*

5:30 - 7:30

630. Structural characterization of anionic rare earth metal complexes containing salen ligands. **P.K. Yuen**, C. Lau

631. Novel bimetallic lanthanide-transition metal complexes. **P.K. Yuen**, C. Lau

632. Coordination isomer analysis of the lanthanide complexes of a rigidified polymethylated DOTA ligand. **A. Opina**, M. Strickland, Y.S. Lee, N. Tjandra, R. Byrd, R.E. Swenson, O. Vasalatiy

633. Synthesis, structural analysis, and supramolecular assembly of a series of *in-situ* generated uranyl-peroxide complexes. **J.A. Ridenour**, C.L. Cahill

634. Cyclic voltammetric studies of singly-bridged lanthanum polyoxometalates in the presence of potassium and its comparison to similar lanthanide-bridged systems. **J.F. Kirby**, A. Posillico

635. Liposomal Eu complexes and zinc nanoparticles as a responsive contrast system for magnetic resonance imaging. **A. Zuhk**

636. Circularly polarized luminescence study of chiral europium and samarium BINAPO complexes. **S. Dodder**, D. Cotter, T. Hopkins

637. Halogenated $LnPc_2$ complexes as STM addressable qubits. **M. Dailey**, C. Besson

638. Synthesis and solid-state characterization of actinide and lanthanide sandwich complexes. **K.M. Wyss**, **E.E. Hardy**, A.E. Gorden

639. Behavior of uranium and rare earth elements in liquid metal systems. V.A. Volkovich, D.S. Maltsev, E.V. Raguzina, A.S. Dedyukhin, A.V. Shchetinsky, A. Chukin, **I.B. Polovov**, L.F. Yamshchikov

640. Lanthanide and actinide borates for nuclear waste. **A. Gaiser**, T.E. Albrecht-Schmitt

641. Explorations of high pressure behavior of uranyl complexes. **E. Warzecha**, T.E. Albrecht-Schmitt

642. Homobimetallic lanthanide and actinide complexes. **R. Greer**, T.E. Albrecht-Schmitt

643. Homoleptic dithiocarbamate complexes of the heavier actinides. **J.M. Sperling**

644. Toward selective lanthanide extraction utilizing carbamoylmethylphosphine oxide chelators. **A.K. Mulville**, M.G. Patterson, A.T. Henry, E.K. Connor, S.M. Biros, E.J. Werner

645. Lanthanide coordination chemistry and luminescence properties of

complexes based on a tripodal iminopyridine ligand. **S.M. Polzin**, K.H. Felix, K.R. Johnson, E.J. Werner

646. Lanthanide mixed donor complexes as potential bioimaging agents. **A. Hannaman**

Section K

Walter E. Washington Convention Center
Hall D

Organometallic Chemistry

Applications to Materials & Polymer Science

N. S. Radu, *Organizer*

5:30 - 7:30

647. Gold oligomeric light emitting materials with controllable color emission. **S.M. Gallagher**, K.S. Schanze, A.S. Veige

648. New platinum complexes for use in platinum CVD. **S. Liu**, G.S. Girolami

649. Interpenetrated triazole-based metal-organic framework with immobilized amine for CO_2 capture. **Q. Wang**

650. Core@shell-like alginate@PEI composite with exceptional adsorption capacity, recycling performance for toxic Cr(VI) removal. **S. Zhai**

651. Copolymerization of cyclohexene oxide with CO_2 catalyzed by *N*-heterocyclic carbene group 4 complexes. **L. Ralte**, K.W. Törnroos, E. Le Roux

Section L

Walter E. Washington Convention Center
Hall D

Nanoscience

B. G. Trewyn, *Organizer*

5:30 - 7:30

652. Liquid-phase production and application of boron-rich two-dimensional materials. **A. Yousaf**, A. Green

653. Green synthesis of Nd-La doped $Sr_2Cu_2Fe_{28}O_{46}$ and Nd-La doped $Sr_2Mg_2Fe_{28}O_{46}$ nanoparticles and comparison their magnetic and microwave absorbing properties with Nd-La doped $Sr_2CuMgFe_{28}O_{46}$ nanoparticles. **P. Alimard**

654. Highly selective detection of sub-ppm-level NO_2 using rGO-In_2O_3 hybrid structures on colorless polyimide substrates. **C. Na**, J. Kim, H. Kim, H. Woo, H. Kim, J. Lee

655. Bimetallic nanocrystal catalysts for hydrodeoxygenation of 5-hydroxymethylfurfural. **J.D. Lee**, J. Luo, H. Yun, C. Wang, M. Monai, P. Fornasiero, R.J. Gorte, C.B. Murray

656. Crystal Structures of fully dehydrated fully Cd^{2+}-exchanged zeolite Y (FAU) and of its H_2S sorption complex containing the cationic cadmium sulfide clusters Cd_4S^{6+} and $Cd(SHCd)_4^{6+}$. D. Moon, **Y. Kim**, J. Kim, **W. Lim**

657. Colloidal synthesis and optical characterization of $Ge_{1-x}Sn_x$ hollow quantum dots. **D. Liyanage**, I.U. Arachchige

658. Phytochemical synthesis of metal nanoparticles using extracts of plants for sensing applications. **L. Bechdel**, E. Hobbs, **M. Devadas**

659. Vanadium based type-II metamaterial superconductors. **T. Szekerczes**, **K. Langford**, V. Smolyaninova, **M. Devadas**

660. Optical and antimicrobial properties of metal nanoparticles made from Japanese maple leaves. **D. Johnson**, **L. Bechdel**, E. Hobbs, **M. Devadas**

661. Colloidal synthesis and photophysical characterization of SiGeSn alloy. **E. Eladgham**, T.A. Nakagawara, U. Ozgur, I.U. Arachchige

662. Sulfur-based nanostructures for lithium-sulfur battery applications. **T. Liu**, T. Lee

663. Gold-silver nanoshells coated with uniformly thin silica shells. **P. Srinoi**, T. Lee

664. Synthesis and characterization of plasmonic nanoparticles coated with tin oxide shells. **R. Medhi**, T. Lee

665. Synthesis of nanoscale rare earth magnetic composite for energy storage application. **B. Shen**, C. Yu, S. Sun

666. Structural and optical effects of alloying with nitrogen in GaNAsP nanowires. M. Jansson, S. Chen, R. La, J. Stehr, C. Tu, W.M. Chen, **I.A. Buyanova**

667. Dendrimer-based a dual mode fluorescent and MRI contrast agent: Noninvasive imaging of brain tumor. **M.M. Ali**, S. Gonawala, J. Ewing

668. Hard magnetic cores for exchange-spring magnets. **L. Saucedo**, D. Carnevale, M. Shatruk, G.F. Strouse

669. Janus gold-carbon nanoparticles. A. Farajallah, I. Karroun, H. Abdou, **B. Workie**, **A. Mohamed**

Section L

Walter E. Washington Convention Center
Hall D

Organometallic Chemistry

Synthesis & Characterization-Early Transition Metals

N. S. Radu, *Organizer*

5:30 - 7:30

670. Reversible ligand CH activation and isomerization at an iron(II) phosphine complex featuring pendant amines. **A.J. Kendall**, M.T. Mock, R. Bullock

671. Electrochemical investigation of CPAM group 6 dinuclear 'end-on-bridged' dinitrogen complexes and the corresponding dinuclear bis(μ-nitrido) products arising from N≡N bond cleavage. **M. Wallace**, L.M. Duman, B. Yonke, L.R. Sita

672. Comparison of the photophysical and photochemical properties of vanadium and chromium polypyridyl complexes. **R.I. Portillo**, R. Dill, S. Shepard, C. Nite, A.K. Rappe, N.H. Damrauer, M.P. Shores

WEDNESDAY MORNING

Section A

Renaissance Washington, DC Downtown
Renaissance East

Inorganic Catalysts

S. A. Koch, *Organizer*
R. Hughes, J. Panetier, *Presiding*

8:30 673. Computational study of molecular electrocatalysts for CO_2 reduction. **J. Panetier**

8:50 674. Computational investigations of nickel based electrocatalysts for CO2RR. **K. McCardle**, J. Panetier

9:10 675. Poly(3,4-ethylenedioxythiophene) (PEDOT) infused TiO_2 nanofibers for photocatalytic decontamination of mustard gas simulant. **D. Dwyer**, J.B. DeCoste, W.E. Bernier, W.E. Jones

9:30 676. Use of a multifunctional pincer in reductive conversions of carbonate. **N. Maciulis**, A.V. Polezhaev, M. Pink, C. Chen, Y. Lozovyy, R.L. Lord, K.G. Caulton

9:50 677. Probing homogenous vs. heterogeneous reactivity by surface synthesis of metal complexes of redox-active ligands. **K.G. Caulton**, I. Huerfano, A.V. Polezhaev, C.D. Tempas, T. Morris, D. Wisman, S.L. Tait

10:10 678. Beta-elimination versus reductive elimination in the Fischer-Tropsch process catalyzed on small Ru clusters. **S. Moncho Escriva**, E.N. Brothers, B.G. Janesko

10:30 Intermission.

10:40 679. Redox study for a family of oxo-bridged iridium dimers relevant to water oxidation catalysis. **S. Sinha**, L.S. Sharninghausen, D.Y. Shopov, B.Q. Mercado, D. Balcells, G.W. Brudvig, R.H. Crabtree

11:00 680. Ir(IV) and (V) and Rh(IV) with an N,O-donor ligand. **L.S. Sharninghausen**, S. Sinha, D.Y. Shopov, B.Q. Mercado, D. Balcells, G.W. Brudvig, R.H. Crabtree

11:20 681. RhRhM: The design and synthesis of multimetallic photocatalysts. **W. Kender**, C. Turro

11:40 682. Synthesis and characterization of titanium calix[5]arene complexes. **T.B. Nsekpong**, B.A. Martinez Ortega

12:00 683. Synthesis and characterization of dioxo-molybdenum(VI) heterobimetalic calix[5]arene compounds. **C. Murphy**, B.A. Martinez Ortega

12:20 684. Detrimental role of dissolved oxygen in the catalytic reduction of 4-nitrophenol by metal nanoparticles. **R. Hughes**, E. Menumerov, S. Neretina

Section B

Renaissance Washington, DC Downtown
Renaissance West A

Inorganic Spectroscopy

S. A. Koch, V. C. Popescu, *Organizers*
I. S. Butler, *Presiding*

8:30 685. Low energy absorbing dirhodium complexes: Potential application in solar energy conversion. **C. Xue**, H. Sayre, C. Turro

8:50 686. Photochemical scrubbing of oxygen from solution using transition metal chromophores. **R.M. O'Donnell**, T. Grusenmeyer, D. Stewart, T. Ensley, W. Shensky, J.E. Haley, J. Shi

9:10 687. Phosphorescent 2−, 3−, and 4−coordinate cyclic (alkyl)(amino)carbene (CAAC) Cu(I) complexes. **R. Hamze**, R. Jazzar, M. Soleilhavoup, P.I. Djurovich, G. Bertrand, M.E. Thompson

9:30 688. Investigating the role of excited-state mixing in ligand photodissociation from polypyridyl Ru(II) complexes. **L.M. Loftus**, K.L. Fillman, A. Li, J.J. Kodanko, C. Turro

9:50 689. Some recent applications of infrared and Raman spectroscopy in bioorganometallic carbonyl chemistry. **I.S. Butler**, R. Kengne-Momo, A. Vessieres, C. Policar, G. Jaouen

10:10 690. Nature of the chemical bonding in Ti-Fe bimetallic complexes. **J.T. Moore**, L.J. Clouston, V. Bernales, K.M. Lancaster, E. Bill, L. Gagliardi, C. Lu, S. Chatterjee

10:30 691. Tuning spin states and quintet MLCT excited states in Fe(II) polypyridines using sterically demanding substituents. **S.M. Fatur**, S. Shepard, R. Higgins, M.P. Shores, N.H. Damrauer

10:50 692. Femtosecond M-edge XANES of open-shell transition metal porphyrins. E. Ryland, M. Carlson, K. Benke, K. Zhang, **J. Vura-Weis**

11:10 693. Direct observation of temperature dependent excited state equilibrium in a series of Re(I) bichromophores. **J. Yarnell**, F.N. Castellano

Section C

Renaissance Washington, DC Downtown
Grand Ballroom South

Bioinorganic Chemistry

Proteins & Enzymes & Model Systems

S. A. Koch, *Organizer*
P. Basu, *Presiding*

8:30 694. pH dependence of ferricytochrome *c* conformational transitions during binding to cardiolipin

membranes: Evidence for histidine as the distal ligand at neutral pH. **B. Milorey**, D. Malyshka, R. Schweitzer-Stenner

8:50 695. Investigation of the binding affinity and kinetics of the Ti(IV) enterobactin complex. **C. Herbst-Gervasoni**, A. Valentine

9:10 696. Carbon dioxide activation at a nickel center. **Y. Lee**

9:30 697. Fe−HNO vs. (NO)Fe−H formation from hydride attack at ferric nitrosyl porphyrins. **E.G. Abucayon**, R.L. Khade, D.R. Powell, M.J. Shaw, Y. Zhang, G.B. Richter-Addo

9:50 Intermission.

10:00 698. Role of redox levels in the hemilability of $[NiN_2S_2.Fe(NO)_2]^{+/0}$ complexes as electrocatalysts for proton reduction. **P. Ghosh**, S. Ding, M.B. Hall, M.Y. Darensbourg

10:20 699. Exploring photochemical processes of [FeFe]-hydrogenase analogues using DFT and TDDFT methods. **S. Niu**, M.B. Hall

10:40 700. Kinetic and spectroscopic investigation of the conserved catalytic triad in mercaptopropinate dioxygenase (MDO) from *Aztobacter Vinelandii*. **S. Sardar**, B.S. Pierce, A. Weitz

11:00 701. Effects ligand oxidation state have on structure, electronic, and reactivity properties of DMSO reductase models. **P. Basu**

11:20 702. Chlorine oxyanion reduction by a non-heme iron system. **C. Ford**, Y. Park, E.M. Matson, Z. Gordon, A.R. Fout

Section D

Renaissance Washington, DC
Downtown
Renaissance West B

Chemistry of Materials

Nanomaterials

C. G. Lugmair, *Organizer*
M. P. Hendricks, *Presiding*

8:30 703. Structure-selective cation exchange in the synthesis of zincblende MnS and CoS nanocrystals. **J.L. Fenton**, R.E. Schaak

8:50 704. Controlled etching of rare earth fluorides for upconverting nanophosphors with tunable morphologies. **S. Najmr**, M. Zhang, A. Keller, N. Greybush, C. Murray

9:10 705. Programmable assembly of stimuli-responsive nanoparticle arrays. **J.A. Mason**, C.A. Mirkin

9:30 706. Growth of inorganic thin films by chemical bath deposition on chemically modified graphene. **W. Lee**, S. Hangarter, J.T. Robinson, S. Walton, P. Sheehan

9:50 707. Transform carbides (M_xC_y) into graphene and M-self-doped graphene by a general chlorination strategy. Z. Kou, T. Peng, **S. Mu**

10:10 Intermission.

10:25 708. Tuning sizes, morphologies, and magnetic properties of mono- *vs.* multi-core iron oxide nanoparticles through controlled addition of water in the polyol synthesis. **G. Hemery**, A.C. Keyes, E. Garayo, I. Rodrigo, J. Garcia, F. Plazaola, E. Garanger, O. Sandre

10:45 709. Using precursors to control nanomaterial synthesis: Tunable libraries of thiourea and selenourea precursors for metal chalcogenide nanocrystals. **M.P. Hendricks**, M.P. Campos, L. Hamachi, G. Cleveland, I. Jen-La Plante, J.S. Owen

11:05 710. Monolayer 2D materials-molecular superlattices. **C. Wang**, Y. Huang, X. Duan

11:25 711. Phase-controlled synthesis of iron sulfide nanoparticles via sulfur precursor reactivity. **J.M. Rhodes**, J. Macdonald

11:45 712. $Eu_{(1-x)}Gd_{(x)}S$-ZnS core-shell nanocrystals: Synthesis, magnetic, and optical properties. **D.J. James**, S.L. Stoll

Section E

Renaissance Washington, DC
Downtown
Grand Ballroom North

Many Colors of Copper

Contributed Talks

Cosponsored by BIOL
K. J. Franz, I. Garcia-Bosch, K. D. Karlin, T. H. Warren, *Organizers*
J. Cho, S. Kundu, *Presiding*

8:55 713. Intramolecular hydrogen bonding enhances stability and reactivity of mononuclear cupric superoxide complexes. **M. Bhadra**

9:15 714. Mononuclear copper-alkylperoxo complexes in stoichiometric and catalytic reactions. **J. Cho**

9:35 715. Nitric oxide promoted O–O bond cleavage of a dicopper(II)-side-on peroxide yielding a high valent dicopper(III) bis μ-oxo species. **J.J. Liu**, K.D. Karlin

9:55 716. Nitrite to nitric oxide conversion at copper(I) and copper(II) sites. **Z. Sakhaei**, S. Kundu, J. Donnelly, T.H. Warren

10:15 717. New insights into copper-nitrosyl chemistry and isolation and characterization of a *trans*-hyponitrite-bridged dicopper(II) complex. **G.B. Wijeratne**, S. Hematian, M. Siegler, K.D. Karlin

10:35 718. Modeling nitric oxide signaling chemistry via nitrite at copper sites. **S. Kundu**, W.Y. Kim, T.H. Warren

10:55 Intermission.

11:05 719. Insights into the mechanism of N_2O reduction by reductively activated N2O reductase. **S. Bagherzadeh**

11:25 720. Binding and activation of small molecules (NO, O_2) by a biomimetic heme-Cu ligand scaffold. **H. Kim**, S. Sharma, K.D. Karlin

11:45 721. Enhanced compound II reactivity in the presence of varying axial ligands and/or lewis acids: Oxidation of C-H, phenol, and imidazole substrates. **M. Ehudin**, K.D. Karlin

12:05 722. Investigation of the 4 H^+/4 e^- reduction of oxygen performed by heme-copper oxidases. **A.W. Schaefer**, S.M. Adam, M.T. Kieber-Emmons, K.D. Karlin, E.I. Solomon

12:25 723. Axial base effects on heme-peroxo-copper adduct reactivity: Evaluating the role of axial base tether and type. **P.J. Rogler**, S. Sharma, S.M. Adam, K.D. Karlin

Section F

Renaissance Washington, DC
Downtown
Grand Ballroom Central

Organometallic Chemistry

Synthesis & Characterization

N. S. Radu, *Organizer*
D. R. Weinberg, *Presiding*

8:30 724. Gold(III) complexes of 2-*tert*-butyl-1,10-phenanthroline and of *N*-(8-quinolinyl)amides: Syntheses, structures, and a green gold(III) complex. **D.R. Weinberg**, K.M. Gilmore, J.E. Thompson, M. Sleck, D. Ohlson, N.A. Curry, R.L. Marley, A.L. Rheingold

8:50 725. Organometallic chemistry of ruthenium-gold carbonyl cluster complexes containing aryl and alkyl ligands. **J. Tedder**, R.D. Adams

9:10 726. Thermal reactivity of late-metal metallacyclobutene complexes: Reversible formation of dicobalt-vinylcarbene complexes. **J.M. O Connor**, P. Qin, K.D. Bunker, R.L. Holland, K.K. Baldridge, C. Moore, A.L. Rheingold

9:30 727. Regioselective synthesis of 1,3,4-trisubstituted cobalticinium salts: Dehydroxymethylation of tetrasubstituted cyclopentadiene ligands. **J.M. O Connor**, P. Qin, M. Melaimi, C. Moore, A.L. Rheingold, R.L. Holland

9:50 728. Elucidating the mechanism of the catalase-type reaction catalyzed by a cryptand-encapsulated dicobalt complex. **S. Bernales Candia**, L. Gagliardi, M.A. Ortuno, J. Stauber, D.G. Nocera, C.J. Cramer, C.C. Cummins

10:10 729. Stable dihydrogen complexes of cobalt(-I) suggest an inverse *trans*−Influence of Lewis acidic group 13 metalloligands. **M.V. Vollmer**, J. Xie, L. Gagliardi, C. Lu

10:30 730. Synthesis and characterization of phosphorescent two-coordinate copper(I) complexes bearing diamidocarbene ligands. **S. Shi**, L. Collins, M. Mahon, P.I. Djurovich, M.E. Thompson, M. Whittlesey

10:50 731. Synthesis and characterization of homoleptic copper (I) thiolate complexes. **J.K. Pratt**, P.P. Power

Section G

Renaissance Washington, DC
Downtown
Congressional A

Main Group Chemistry

T. W. Hudnall, *Organizer*
R. E. Mulvey, *Presiding*

8:30 Introductory Remarks.

8:35 732. Synthesis and physical properties of tetrasila[2.2]thiophenophane derivatives for the luminescent and chiroptical materials. **M. Shimada**, Y. Yamanoi, K. Omoto, S. Tashiro, M. Shionoya, T. Ohto, S.T. Pham, R. Yamada, H. Tada, M. Hattori, K. Jimura, S. Hayashi, H. Koike, M. Iwamura, K. Nozaki, H. Nishihara

8:55 733. Triply-charged corannulene bowls: Experimental and computational studies. **A. Zabula**, S.N. Spisak, A.S. Filatov, A.Y. Rogachev, M.A. Petrukhina

9:15 734. $B(C_6F_5)_3$-catalyzed selective chlorination of hydrosilanes. **R. Dobrovetsky**

9:35 735. Reactions of Zintl-ion clusters: New frontiers and discoveries. **L. Stevens**, Y. Wang, J. Hu, Y. Chen, P.Y. Zavalij, K.H. Bowen, B.I. Dunlap, B.W. Eichhorn

9:55 Intermission.

10:05 736. Main group dihydropyridine surrogate hydrides: Synthesis, structures, reactivity and catalytic applications. **R.E. Mulvey**, S. Robertson, R. McLellan, S. Orr, A. Kennedy, M. Uzelac

10:25 737. Oxygen atom insertion into salen based aluminum alkyl complexes. **V. Balasanthiran**, B.A. McKeown, T.B. Gunnoe

10:45 738. Effect of water contents on arsenic stabilization in mine waste using basic oxygen furnace (BOF) slags. **S. Kim**, H. Chung, S. Jeong, K. Nam

Section H

Renaissance Washington, DC
Downtown
Congressional B

Chemistry of Materials

Materials for Energy & Catalytic Applications

C. G. Lugmair, *Organizer*
B. J. Melde, *Presiding*

8:30 739. Solid electrolyte interphase layers on sulfur cathodes in Li/Na-S batteries: Chemical compositions, functionality, the critical role of Li^+ and cation solvation structures. **L. Wang**, C. Wang, K. Xu, B.W. Eichhorn

8:50 740. Synthetic control of structural and electrochemical properties of high-Ni layered oxide cathodes for next-generation Li-ion batteries. D. Wang, M. Zhang, J. Bai, **F. Wang**

9:10 741. Developing new porous materials for fuel catalysis and energy storage devices. **V. Thoi**

9:30 742. One step low-temperature hydrothermal synthesis of $Na_3Fe_2(PO_4)_2F_3$: A new cathode for lithium- ion batteries. **D. Manna**, A. Choudhury

9:50 743. Metal-organic frameworks (COFs) and covalent organic frameworks (COFs) for energy storage. **D. Feng**, Z. Bao

10:10 Intermission.

10:25 744. Self-supported nanoarrays of binary transition metal sulfide for supercapacitor application. **S.J. Patil**, D. Lee

10:45 745. Nanoporous sorbents for improved purification of biodiesel. **B.J. Melde**, B.J. Johnson, M.H. Moore

11:05 746. Strengthening silica aerogels through thermally induced phase separation of poly(methyl methacrylate) onto the alcogel colloidal structure. H. Ma, B. Wang, K.M. Frederick, **D.A. Loy**

11:25 747. Hot carrier photodetectors using inorganic semiconductors with nanometer-scale metallic optical coatings. **L. Krayer**, J. Munday

11:45 748. Titanium(IV)-induced formation of cristobalite in titanosilicates and its potential effect on heterogeneous catalysis: Induced Impact or Spectator? **A.S. Perera**, H. Yu, J. Cockcroft, P. Trogadas, M. Coppens

Chemistry Past Curium

Sponsored by NUCL, Cosponsored by INOR

Non-Conventional Building Blocks in Conjugated Materials: Innovative Designs & New Applications

Heterocyclic Systems

Sponsored by POLY, Cosponsored by INOR and PMSE‡

WEDNESDAY AFTERNOON

Section A

Renaissance Washington, DC
Downtown
Renaissance East

Chemistry of Materials

Metal Organic Frameworks

C. G. Lugmair, *Organizer*
W. A. Maza, *Presiding*

1:30 749. Hydrogen uptake by an iron amino-borohydride Zr(IV)-metal organic framework hybrid below 300 °C. **W.A. Maza**, B.L. Chaloux, A. Epshteyn

1:50 750. Synergistic effects of metal-organic framework containing polymer membranes for military applications. **J.B. DeCoste**

2:10 751. Porous scaffolds for electrically-transduced gas sensing and capture. **K. Mirica**

2:30 752. Diffusion rates and energetics of xylene isomer transport through UiO-66. **T. Grissom**, P. Usov, A.J. Morris, J.R. Morris

2:50 753. Ammonia adsorption in acid-modified HKUST-1. **A. Sharma**, P. Forster, L. Daemen, Y. Cheng, A. Ramirez-Cuesta, M. Hartl

3:10 Intermission.

3:25 754. Small molecule storage and activation with metal-organic polyhedra-based porous liquids. E. Gosselin, G.R. Lorzing, B.A. Trump, C.M. Brown, **E.D. Bloch**

3:45 755. Chemical neutralization of warfare agents using metal-organic frameworks. **T. Islamoglu**, A. Atilgan, S. Moon, G. Peterson, J.B. DeCoste, M. Hall, J.T. Hupp, O.K. Farha

4:05 756. Effect of guests in the pores of metal-organic frameworks on the adsorption and reactivity of toxic gases and chemical warfare agents. **A. Ploskonka**, J.B. DeCoste

4:25 757. Tuning the morphology and activity of electrospun polystyrene/UiO-66-NH_2 metal-organic famework composites. **G.W. Peterson**, A. Lu, T.H. Epps

4:45 758. 3D printing polymer-MOF composites: Properties and design challenges. **M. Hartings**

Section B

Renaissance Washington, DC
Downtown
Renaissance West A

Organometallic Chemistry

Synthesis & Characterization

N. S. Radu, *Organizer*
D. Powers, J. Robinson, *Presiding*

1:30 759. Synthesis and characterisation of new fluorinated NHC transition metal complexes and their application in catalysis. **M. Jamil**, A.K. Brisdon

1:50 760. Mechanistic insight and structure determination of in-situ species in iron-catalyzed cross-coupling with aryl nucleophiles. **S.H. Carpenter**, M.L. Neidig

2:10 761. Carbolong complexes: Novel organometallic species with three to five metal-carbon bonds. **H. Xia**

2:30 762. Characterization of and group-transfer catalysis with lattice-confined reactive M−L multiple bonds. **D. Powers**, A. Das, C. Wang, W. Gao

2:50 763. Molecular engineering of blue emitting iridium (III) complexes for use in fully solution processed OLEDs. **A. Huckaba**, S. Aghazada, M. Nazeeruddin

3:10 764. Modulation of the reactivity of oxorhenium(V) complexes via coordination of Lewis acids to the oxo ligand. **C. Brown**, E. Ison

3:30 765. Nucleophilic palladium(II) carbenes: Small molecule activations. **M. Hoffbauer**

3:50 766. Photo-switchable N-heterocyclic carbene functionalized arylazopyrazole ligands and their ruthenium(II)-arene complexes: Synthesis and photo-isomerization studies. **K.Y. Ghebreyessus**, A. Almutiri

4:10 767. Reactions of palladium and platinum methyl complexes with molecular oxygen. **H.E. Zeitler**, W. Kaminsky, K.I. Goldberg

4:30 768. Formation of Ta(V) imido complexes upon cooperative Lewis acid-Lewis base C-H activation of aryl- and alkylnitriles. **D.V. Peryshkov**, M. Rahman

4:50 769. Synthesis and characterization of sterically stabilized diiron complexes. **M.R. Carlson**, P. Zhao, T.B. Rauchfuss, C. Pham, S.P. Cramer

5:10 770. Solid-state structure, solution equilibria and chemical reactivity of CPAM group 6 [M(V, d^1), M(V, d^1)] dinuclear bis(μ-nitrido) complexes for M = Mo and W that are relevant to dinitrogen fixation. **L.M. Duman**, P.Y. Zavalij, L.R. Sita

Section C

Renaissance Washington, DC
Downtown
Grand Ballroom South

Chemistry of Materials

Nanomaterials

C. G. Lugmair, *Organizer*
H. D. Magurudeniya, S. J. Smith, *Presiding*

1:30 771. Crystalline DNA-protein nanomaterials self-assembled through three types of biological interactions. **S.J. Smith**, R. Subramanian, L. Suominen, G. Cardone, T. Baker, F.A. Tezcan

1:50 772. Cascade synthesis of gold nanoparticles in a self-assembled ionic liquid polymer nanocomposite. **H.D. Magurudeniya**, B.S. Ringstrand, A. Joshi, C.J. Sheehan, M.A. Firestone

2:10 773. Conjugates of water-soluble gold-carbon nanoparticles with proteins. M. Hameed, I. Mohamed, M. Naggar, I.A. Shehadi, **A. Mohamed**

2:30 774. Low temperature growth of $ZrSe_2$/$HfSe_2$ thin film and nanostructured complex metal chalcogenide $MnSb_2Se_4$. **H. Djieutedjeu**, B.S. Guiton, M. Thomas, Y. Lei

2:50 775. Quantitative analysis of oxidation state in cerium oxide nanomaterials. **C.M. Sims**, R. Maier, A.C. Johnston-Peck, J.M. Gorham, V.A. Hackley, B.C. Nelson

3:10 Intermission.

3:25 776. Structures and properties of ultra-small TiO_2 and ZnO nanoparticles. **M. Chen**, D.A. Dixon

3:45 777. Quantiftying the impact of sterics and electronics on ligand exchange at cadmium selenide nanocrystal surfaces. **N.C. Anderson**, J.S. Owen

4:05 778. Speciation of transition metal dopants in a CdS-based cluster. **F. Kato**, K.R. Kittilstved

4:25 779. $Ge_{1-x}Sn_x$ Alloy nanocrystals: Nearly monodisperse quantum confined nanocrystals, sub 3 nm photoluminescent quantum dots, and non-confined morphologies. **V. Tallapally**, T.A. Nakagawara, D.O. Demchenko, U. Ozgur, I.U. Arachchige

4:45 780. Light-induced ambient degradation of few-layer black phosphorus: Mechanism and protection. **J. Wang**

Section D

Renaissance Washington, DC
Downtown
Renaissance West B

Nanoscience

B. G. Trewyn, *Organizer*
Z. Lin, R. Macfarlane, *Presiding*

1:30 781. Bottlebrush-like block copolymers enabled one-dimensional nanorods with precisely controlled dimensions, compositions, surface chemistry and architectures. **Z. Lin**

1:50 782. Microwave assisted synthesis and catalytic studies of palladium–gold alloy NPs. **P. Kunal**, H. Li, S. Seraj, B. Dewing, L. Zhang, K. Jarvis, C.J. Werth, G. Henkelman, S.M. Humphrey

2:10 783. Chemical functionalization and characterization of two dimensional tungsten disulfide. **A. Jinandra**, E.L. Kahn, M. Terrones

2:30 784. Synthesis of Au nanoparticle - CdSe quantum dot assemblies and study of their unique optical properties. **B. Szychowski**, M. Daniel

2:50 785. Hydrogenation catalysis by microwave-synthesized RhPd and RhPdAu nanoparticles: An experimental and theoretical examination of composition effects. **G.W. Piburn**, H. Li, P. Kunal, G.A. Henkelman, S.M. Humphrey

3:10 786. Nanostructured Au/Ag/Pd alloy aerogels as high efficiency alcohol oxidation electrocatalysts. L. Nahar, A. Farghaly, R.J. Esteves, **I.U. Arachchige**

3:30 787. Epitaxy of programmable atom equivalents. **R. Macfarlane**

3:50 788. Dispersion measurements and calculations of AlCu thin films. **A. Kaplan**, C. Gong, M. Dias, M.S. Leite

Section E

Renaissance Washington, DC
Downtown
Grand Ballroom North

Many Colors of Copper

Contributed Talks

Cosponsored by BIOL
K. J. Franz, I. Garcia-Bosch, K. D. Karlin, T. H. Warren, *Organizers*
S. Hematian, H. R. Lucas, *Presiding*

1:45 789. Photophysical property of four-coordinate copper complexes

supported by a diphosphinosilane ligand. **Y. Lee**

2:05 790. Stabilization of cupric superoxide species with intramolecular hydrogen bonding moieties. **D.E. Diaz Romero**, D.A. Quist, K.D. Karlin

2:25 791. Reactivity of Cu(II) compounds with peroxides: Roles of ligands in C-H bond activation. **A. Mukherjee**

2:45 792. Interconversion of reduced dioxygen species bound to binuclear copper complexes. **D.A. Quist**, K.D. Karlin

3:05 793. Coping with intruders: Exploitation of metals by histatin antimicrobial peptides. **S.E. Conklin**, K.J. Franz

3:25 794. Conformational changes of α-synuclein induced by copper versus iron. **H.R. Lucas**

3:45 Intermission.

3:55 795. Metals as mediators in the cross-talk between drug and fungal pathogen. **E.J. White**, K.J. Franz

4:15 796. Targeted prodrugs to manipulate copper biology of prostate cancer. **S. Bakthavatsalam**, T. Zhang, K.J. Franz

4:35 797. Spectroscopic characterization of extracellular copper transport partners for human copper transporter 1. **K.L. Haas**

4:55 798. Copper in the tree of life. **D.L. Huffman**

5:15 799. New insight into the reaction mechanism of the formylglycine generating enzyme: A spectroscopic perspective. **K.K. Meier**, M. Appel, E.I. Solomon

5:35 800. Mechanistic investigations of a recombinant laccase from *Thermus thermophilus* HB27. **S. Hematian**, B.C. Sanders, J. Shin, J.R. Winkler, H.B. Gray

Section F

Renaissance Washington, DC Downtown
Grand Ballroom Central

Main Group Chemistry

T. W. Hudnall, *Organizer*
Z. M. Heiden, *Presiding*

1:30 Introductory Remarks.

1:35 801. Synthesis and characterization of diphenylsilyl nucleophiles. **E. Marro**, E. Press, T.K. Purkait, M. Siegler, R.S. Klausen

1:55 802. Triethylammonium cyanide: A recyclable reagent for cyanophosphine synthesis. **B.L. Chaloux**, W.A. Maza, A. Epshteyn

2:15 803. Synthesis, structure, and isomerization of phosphiranium cations. **J.A. Muldoon**, D.H. Pham, R.P. Hughes, D.S. Glueck, C. Moore, A.L. Rheingold

2:35 804. It takes a second phosphorus for Wittig to meet McMurry. **S. Ott**, K. Esfandiarfard, J. Mai

2:55 Intermission.

3:05 805. Utilization of fluorescent dye molecules to introduce redox chemistry into main group complexes. **Z.M. Heiden**, I. Kieffer

3:25 806. Lewis adducts and protonation of nitriles. **T.H. Saal**, R.M. Haiges, K.O. Christe

3:45 807. Reactivity of Verkade's superbase with various strong Lewis acids. **S. Mummadi**, D. Unruh, C. Krempner

Section G

Renaissance Washington, DC Downtown
Congressional A

Lanthanide & Actinide Chemistry

A. De Bettencourt Dias, *Organizer*
S. M. Biros, D. A. Penchoff, *Presiding*

1:30 808. Hydration of heavy metal ions: A simulation study. **B. Qiao**

1:50 809. Tripodal CMPO Ln and An extraction agents. E.J. Werner, **S.M. Biros**

2:10 810. Structural variations of thorium(IV) and uranium(IV)-carboxylates isolated from aqueous solution. **N.A. Vanagas**, K.E. Knope

2:30 811. Novel impact in actinide chemistry: Thorium sulfido and selenido compounds. **M.A. Ringgold**, A.Y. Kornienko, D. Rehe, T. Emge, J. Brennan

2:50 812. Uranyl reduction facilitated by a redox-active, donor-expanded dipyrrin. **N.L. Bell**, P.L. Arnold, J.B. Love

3:10 intermission.

3:25 813. Discovery of lanthanide-based molecular corrosion inhibitors by high throughput methods. **A. Zabula**, J.R. Robinson, R. Nahas, D. Cinoman, E.J. Schelter

3:45 814. Selective extraction of lanthanides and actinides with carboxylic acids and beta diketones. **D.A. Penchoff**, C.C. Peterson, J.D. Auxier, G.K. Schweitzer, R.J. Harrison, H.L. Hall

4:05 815. Th(IV)- and U(IV)- chlorides isolated from acidic aqueous media. **J. Wacker**, M. Vasiliu, J.A. Bertke, D.A. Dixon, K.E. Knope

4:25 816. Synthesis and investigation of metal-metal interactions in heterobimetallic Ni-Lu complexes. **B.L. Ramirez**, P. Sharma, S. Dotzler, L. Gagliardi, C. Lu

Section H

Renaissance Washington, DC Downtown
Congressional B

Chemistry of Materials

Metal Organic Frameworks

C. G. Lugmair, *Organizer*
R. W. Larsen, *Presiding*

1:30 817. Proton-coupled electron transport in anthraquinone-based metal organic frameworks. **P.J. Celis-Salazar**, C. Epley, S. Ahrenholtz, W. Maza, P. Usov, A.J. Morris

1:50 818. Extended singlet excited state lifetime via excimer formation as a function of MOF topology. **J. Yu**, P. Deria

2:10 819. Transformation from an insulator to superionic conductor by structural changes in nanoporous metal-organic frameworks. **M. Yoon**

2:30 820. Heterobimetallic active sites in a metal organic framework. **S. Desai**, D. Pahls, C. Malonzo, T. Webber, L. Gallington, M. Destefano, K.W. Chapman, O.K. Farha, J.T. Hupp, R. Penn, L. Gagliardi, A. Stein, C. Lu

2:50 821. Understanding physical and chemical factors determining lithium-sulfur battery performance using metal-organic frameworks. **A. Baumann**, G. Aversa, V. Thoi

3:10 822. Guest-guest and guest-framework photoinduced electron transfer in metal organic frameworks. **R.W. Larsen**, L. Wojtas, C. McKeithan, J. Mayers

3:30 Intermission.

3:45 823. Metal organic frameworks as solid supports for catalytic aluminum species for use in transfer hydrogenations. **P. Larson**, J. Cheney, A.F. Cozzolino

4:05 824. Modification of the solution behavior of Pd12L24 metal organic nanocages via PEGylation. **H. Li**, J. Luo, T. Liu

4:25 825. Expanding the scope MOF-polymer hybrid materials toward functional textiles. **M.S. Denny**, S. Cohen

4:45 826. Synthesis and characterization of mixed-ligand metal-organometallic MIL-101 analogues incorporating $[CpM]^+$-functionalized ligands. **A.N. Ley**, K.T. Holman

5:05 827. Reproducible synthesis and high porosity of mer-$Zn(Im)_2$ (ZIF-10): Exploitation of an apparent double-eight ring template. **J. Ramirez**, H. Yang, C. Kane, A.N. Ley, K.T. Holman

Chemistry Past Curium

Sponsored by NUCL, Cosponsored by INOR

Non-Conventional Building Blocks in Conjugated Materials: Innovative Designs & New Applications

Synthetic Methodology

Sponsored by POLY, Cosponsored by INOR and PMSE‡

THURSDAY MORNING

Section A

Renaissance Washington, DC Downtown
Congressional A

Bioinorganic Chemistry

DNA, RNA & Inorganic Drugs

S. A. Koch, *Organizer*
S. H. Bossmann, C. R. Goldsmith, *Presiding*

8:30 828. Organoferrous compounds for disruption of iron homeostasis in cells. **J.M. O Connor**, M. Aubrey, C. Hoong, M. Proetto, N.C. Gianneschi

8:50 829. Killing two birds with one stone, or rather two carboxylates: Ligand modifications improve both the water stability and relaxivity response of a MRI contrast agent sensor for hydrogen peroxide. **C.R. Goldsmith**, T.E. Hutchinson, M. Yu

9:10 830. *Bis*-picolinamide metal dihalide complexes: *Trans* isomers with significantly high potency and cancer cell selectivity. **R.M. Lord**, P. Caramés-Méndez, A. Basri, R. Phillips, P. McGowan

9:30 831. Improving the efficacy of gadolinium based theranostics. **A.J. Hall**, L.M. Rendina

9:50 832. Platinum anticancer drugs: The mechanistic study and new drug design. **Y. Liu**

10:10 Intermission.

10:20 833. Metallo-supramolecular cylinders that bind unusual DNA and RNA structures: From DNA nanoscience to bio-activity. **M.J. Hannon**

10:40 834. CO-induced eradication of colorectal adenocarcinoma cells by a luminescent photoCORM grafted on biocompatible carboxymethyl chitosan. **I. Chakraborty**, P.K. Mascharak

11:00 835. Novel 5 and 6-coordinated silver complexes derived from 2,6-(pyridyl)iminodiaadamantanes for bacterial eradication. **J. Jimenez**, P. Mascharak

11:20 836. Copper-activated drugs with NNSN-motif against MRSA. **S.H. Bossmann**, H. Wang, A.P. Malalasekera, A. Delpe-Acharige, F. Rahman, F. Wolschendorf

Section B

Renaissance Washington, DC Downtown
Congressional B

Chemistry of Materials

Materials for Energy & Catalytic Applications

C. G. Lugmair, *Organizer*
A. G. Harris, J. Macdonald, *Presiding*

8:30 837. Synthesis and characterization of Pt and Ni-based bimetallic nanocrystal catalysts for biomass upgrading. **J.D. Lee**, J. Luo, H. Yun, C. Wang, M. Monai, P. Fornasiero, R.J. Gorte, C.B. Murray

8:50 838. Assembly of metal nanoparticles embedded into porous organic cages for heterogeneous catalysis. **S. Jiang**, S.K. Beaumont

9:10 839. Tandem one-pot oxidative esterification of allyl alcohol by gold nanoparticles and alcohol

dehydrogenase enzyme supported on mesoporous silica nanoparticles. **M.M. Moyer**, X. Sun, B.G. Trewyn

9:30 840. Using a materials genome initiative approach to catalyst discovery. **A.G. Harris**, M. Green

9:50 841. Modelling the defect chemistry of organohalide perovskites. **F. De Angelis**

10:10 842. Digging out of a hole problem. **J. Macdonald**, A. LaCroix, A. O'Hara, K. Reid, S. Rosenthal, S. Panetlides

10:30 Intermission.

10:45 843. Aerosol routes to fabricate highly stable perovskite solar cells under ambient conditions. **S. Kavadiya**, P. Biswas

11:05 844. Kinetically controlled thermal hysteresis forms the basis of metastability of the perovskite phase of cesium lead iodide. **S. Dastidar**, A.T. Fafarman

11:25 845. Degradation mechanisms of perovskite solar cells elucidated through in operando GIWAXS. **T. Kelly**, K. Fransishyn, S. Kundu

11:45 846. Amplification of solar energy conversion in Q-CdTe and type-II CdTe/CdSe quantum dots sensitized titania photonic crystals in selenide electrolyte. N. Beydoun, A.S. Nehme, F. Haydous, **L.I. Halaoui**

12:05 847. Charge-carrier diffusion length over one micrometer in solution-processed $CsPbI_3$. **A.T. Fafarman**

Section C

Renaissance Washington, DC
Downtown
Grand Ballroom South

Organometallic Chemistry

Catalysis-Late Transition Metals

N. S. Radu, *Organizer*
J. M. Hoover, L. Jia, *Presiding*

8:30 848. Efficient catalysis using transition metal complexes with N-heterocyclic carbene (NHC) ligands. **V. Ananikov**

8:50 849. Catalytic synthesis of linear alkenyl arenes using capping arene ligand supported Rh(I) catalysts. **J. Chen**, A.C. Cole, M.S. Webster-Gardiner, B.A. McKeown, T.B. Gunnoe

9:10 850. Hydrogenation of hindered, unfuctionalized alkenes using redox-active α-diimine nickel catalysts. **N.G. Leonard**, P.J. Chirik

9:30 851. Dual-site zwitterionic Ni(II) catalysts for carbonylative polymerization of epoxides and oefins. **L. Jia**

9:50 852. Nickel catalyzed Suzuki-Miyaura coupling of phenolic derivatives: Insight into the fate of nickel precatalysts. **A.G. Walden**, M.D. Mohadjer Beromi, R.M. Davis, N. Hazari

10:10 853. Rhodium catalyzed C-H borylation: Affecting selectivity through catalyst design. **M. Mantell**, M.S. Sanford

10:30 854. Mechanistic insights into catalytic oxidative decarboxylative coupling reactions. **J.M. Hoover**

10:50 855. Lewis-acid assisted catalytic hydrogenation of nitriles using an air-stable monoanionic biscarbene cobalt(III) pincer complex. **B. Jackson**, K. Tokmic, A. Slazar, A.R. Fout

11:10 856. Mechanistic studies of C-H amination processes mediated by dipyrrin-cobalt imidos. **Y. Baek**, T. Betley

11:30 857. Direct boronic acid transmetalation to a Pd(II) halide. L. Chen, **B.P. Carrow**

Section D

Renaissance Washington, DC
Downtown
Congressional C

Coordination Chemistry

Synthesis & Characterization

S. A. Koch, A. Larsen, *Organizers*
G. Mezei, P. Portius, *Presiding*

8:30 858. Taming binary *p*-block azides with N-heterocyclic σ-donors as precursors for the formation of nitrogen-rich tetrazolato complexes. **P. Portius**, L. James, B. Peerless, Z. Smallwood, B. Crozier

8:50 859. Ligand exchange dynamics and controlled synthesis of isomeric oxorhenium(V) complexes. **J. Liu**, C. Ren, X. Su, M. Han, J.R. Shapley, T.J. Strathmann

9:10 860. Mercaptide-bridged dicopper(I) naphthyridine-diimine complexes bearing short metal-metal distances. R. Conger, R.R. Conry, **S. Fox**

9:30 861. Synthesis, photophysical properties, and DFT studies of Cu(1,7-phen)$(PPh_3)_2PF_6$: An unusual three-coordinate Cu(I) compound. **A. Miller**, D.J. Casadonte, A.F. Cozzolino

9:50 862. Group 10 homobimetallic complexes of the Siamese-twin porphyrin. **S.J. Dorazio**, S. Dechert, C. Bruckner, F. Meyer

10:10 Intermission.

10:20 863. Discrete multinuclear coordination complexes and selective anion binding attainable only by tethering ligands together. **G. Mezei**, B. Ahmed

10:40 864. Cobalt(0) PNP complexes: Synthesis and application. **M.R. Mills**

11:00 865. Further disordering for expanded metals: The liquid Li-NH3-MeNH2 system. **A. Seel**, N. Skipper, C. Howard, P. Edwards

11:20 866. Multielectron reactivity and electronic structure of first-row transition metal trinuclear complexes. **A.K. Bartholomew**, T. Betley

11:40 867. Syntheses and structures of bimetallic complexes supported by lexible di(imino)pyridine-based macrocycles. **S. Zhang**, P. Cui, N.C. Tomson

12:00 868. Engineering a potent nickel dioxygen catalyst. **D.R. Heitger**, H.R. Lucas

Section E

Renaissance Washington, DC
Downtown
Grand Ballroom North

Nanoscience

B. G. Trewyn, *Organizer*
X. Roy, B. Sadtler, *Presiding*

8:30 869. Compositionally-induced twin defects control the shape of ternary silver halide nanocrystals. **B. Sadtler**

8:50 870. Investigating the Raman response of mono- and few-layer ReS_2. **A. McCreary**, J. Simpson, Y. Wang, D. Rhodes, K. Fujisawa, L. Balicas, M. Dubey, V. Crespi, M. Terrones, A.R. Hight Walker

9:10 871. Using Raman spectroscopy to observe the charge density wave states in metallic tantalum diselenide. **H.M. Hill**, J. Simpson, S. Chowdhury, A.R. Hight Walker

9:30 872. Mesoporous carbon nanoparticles for f-element separations. **G. Deodhar**, K. Kluherz, B.G. Trewyn

9:50 873. Synthesis and single-molecule conductance of metallocene-based electronic components. **M. Inkpen**, G. Lovat, A. Turkiewicz, X. Roy, L. Venkataraman

10:10 874. Molecular electronics using atomically precise redox-active nanoscale building blocks. G. Lovat, B. Choi, L. Venkataraman, **X. Roy**

10:30 875. Tracking the energy flow on nanoscale *via* sample-transmitted excitation photoluminescence spectroscopy. **P. Moroz**, M. Zamkov

10:50 876. Exploring energy, environmental, and biological challenges with mesoporous nanoparticle technology. **B.G. Trewyn**

Section F

Renaissance Washington, DC
Downtown
Grand Ballroom Central

Organometallic Chemistry

Applications to Materials & Polymer Science

N. S. Radu, *Organizer*
C. Cruz, G. Du, *Presiding*

8:30 877. Strategic synthesis and polymerization of a functionalized cyclohexasilane. **E. Press**, E. Marro, S. Surampudi, R.S. Klausen

8:50 878. Manganese catalysis for polysilylethers via hydrosilylation and dehydrogenative coupling. **G. Du**, S. Vijjamarri

9:10 879. Non-transition metal catalyzed polymerization of acetylenic monomers. **C. Cruz**, J.L. Barr

9:30 880. Synthesis and characterization of alkyl and fluorinated alkyl manganese pentacarbonyl complexes as models for reversible-deactivation radical polymerization (RDRP). **R. Morales Cerrada**, J. Daran, F. Gayet, C. Fliedel, V. Ladmiral, R. Poli, B.M. Ameduri

9:50 881. Synthesis of isotactic enriched polylactide from *rac*-lactide *via* a Lewis acid catalyzed ring-opening of an epoxide. **V. Balasanthiran**, M.H. Chisholm

10:10 882. Heterobimetallic catalysts for ethylene homo- and copolymerization. **Z. Cai**, L. Do

10:30 883. Well-defined nickel- and palladium-diimine catalysts supported on sulfated zirconia for ethylene (Co)polymerization reactions. **H. Tafazolian**, D. Culver, M. Conley

10:50 884. Synthesis of unusual zirconophosphaalkene through insertion of sodium phosphaethynolate, Na[OCP]. **J.M. Kieser**, R.J. Gilliard, A.L. Rheingold, H. Grützmacher, J.D. Protasiewicz

11:10 885. Investigation of electronic effects for the amidinate ligand of CPAM early transition metal complexes as catalysts for small molecule activation and olefin polymerization. **R.R. Thompson**, L.R. Sita

11:30 886. Voltage dependent light emitters from iClick and aurophilic interactions. **C. Beto**, E. Holt, Y. Yang, J. Bullock, C. Zeman, I. Ghiviriga, K.S. Schanze, A.S. Veige

11:50 887. Preparation of aurolated porphyrinic materials with potential in photovoltaics: Application of iClick chemistry. **T.A. Makal**, A.S. Veige, K.S. Schanze

Section G

Renaissance Washington, DC
Downtown
Meeting Room 12

Environmental & Energy-Related Inorganic Chemistry

S. A. Koch, *Organizer*
A. W. Apblett, T. C. Devore, *Presiding*

8:30 888. Modification of glassy carbon electrodes with Cu- and Zn-bis(thiosemicarbazones) as heterogeneous HER catalysts. **C.A. Grapperhaus**, W. Zhang, R.M. Buchanan

8:50 889. Formamidinate-bridged Rh_2(II,II) dimer as both a robust, red-light absorbing photosensitizer and a catalyst for proton reduction. **H.J. Sayre**, C. Turro

9:10 890. Dynamics of the reversible dehydration of metal salts. **T.C. Devore**, B.A. Reisner, A. Bagley, A. Morales

9:30 891. Electrochemical reduction of CO_2 to CO with cobalt macrocycles. **K. Ngo**, D.C. Grills, D.E. Polyansky, J.T. Muckerman, E. Fujita

9:50 892. Low-voltage fabrication of CZTS thin films by electrophoretic

deposition of all-inorganic nanocrystals. **A.D. Dillon**, S. Mengel, S. Dastidar, J.B. Baxter, A.T. Fafarman

10:10 893. Investigation of electrochemical hydrogen evolution by metal-selenolate catalysts and related mechanistic studies. **C. Downes**, S. Marinescu

10:30 Intermission.

10:40 894. Electrocatalytic hydrogen production and hydrogen oxidation using tetradentate nickel (II) and zinc (II) complexes with P_2S_2 ligand framework: Synthesis, characterization and mechanistic insights. **R. Jain**, A.Z. Haddad, M.S. Mashuta, R.M. Buchanan, C.A. Grapperhaus

11:00 895. Promoting the interconversion of dinitrogen and reduced nitrogen species at copper through proton-coupled electron transfer. **E.J. Gardner**, S. Zhang, C.R. Cobb, **T.H. Warren**

11:20 896. Mobilization of cationic heavy metal from mine tailings by using fuel cell technology. **W. Ju**, E. Jho, K. Nam

11:40 897. Molecular electrocatalysts for ammonia oxidation based on earth abundant metals. **M. Raghibi Boroujeni**, S. Kundu, T.H. Warren

12:00 898. Sorption of heavy metals and uranium by nanocrystalline scheelite. **A.W. Apblett**, C.K. Perkins

12:20 899. Fast single-site water oxidation catalysis by ruthenium bipyridine-phosphonate-carboxylate complexes. **D.W. Shaffer**, Y. Xie, J.J. Concepcion

12:40 900. O-O coupling: From detailed mechanistic understanding to enhanced water oxidation catalysis. **Y. Xie**, D.W. Shaffer, J.J. Concepcion

Nanoscale Sensing in Foods & Other Complex Media

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Non-Conventional Building Blocks in Conjugated Materials: Innovative Designs & New Applications

Optoelectronic Device Applications

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THURSDAY AFTERNOON

Section A

Renaissance Washington, DC
Downtown
Congressional A

Inorganic Catalysts

S. A. Koch, *Organizer*
L. Y. Kuo, X. Zhao, *Presiding*

1:30 901. Total utilization of biomass, lignin and carbohydrate: Using earth abundant nickel catalyst. **H. Luo**

1:50 902. New molybdenum complexes for sulfide oxidation and organophosphate degradation. **L.Y. Kuo**

2:10 903. Oxidative transformation of a Ru-bound ligand during chemically driven water oxidation. **H. Kagalwala**, L. Tong, R. Zong, L. Kohler, M.S. Ahlquist, T. Fan, K.J. Gagnon, R.P. Thummel

2:30 904. Electronic and steric effects on hydrogen production catalyzed by molecular Co complexes with pentadentate ligands in aqueous solution. **X. Zhao**, P. Wang, G. Liang, M. Long, D. Reese, A. Bah, C. James, Y. Sun, L. Duan, C.E. Webster

2:50 905. Tailor-made stereo-n-blocks copolymers of poly(lactic acid) by living polymerization catalysts. **T. Rosen**, I. Goldberg, V. Venditto, M. Kol

3:10 906. Earth-abundant molecular electrocatalysts for the reduction of CO_2 and O_2. **C.W. Machan**

3:30 Intermission.

3:40 907. Ag platelet-TiO2 nanocomposites for improved visible light photocatalysis of simulated chemical warfare agents. **D.L. Kuhn**, Z. Zander, B.G. DeLacy

4:00 908. Lewis acid promoted catalytic oxidations by redox catalysts. **G. Yin**

4:20 909. Computational study for the CO_2 reduction reaction using homogeneous electrocatalysts. **X. Li**, J. Panetier

4:40 910. Electrochemical reduction of CO_2 catalyzed by Re(quinolin-oxazole)$(CO)_3Cl$ complexes. **A.M. Angeles Boza**, J. Nganga

5:00 911. Reductive coupling via disproportionation of activated alcohols using oxo-vanadium catalysts. **E.M. Steffensmeier**, K.M. Nicholas

5:20 912. Copper(I)-dioxygen chemistry supported by a tetrapodal ligand with cationic character in the secondary coordination sphere. **S. McCollom**, A. Weberg, N.C. Tomson

Section B

Renaissance Washington, DC
Downtown
Congressional B

Chemistry of Materials

Synthesis & Properties

C. G. Lugmair, *Organizer*
K. V. Lawler, N. T. Plymale, *Presiding*

1:30 913. Moving beyond $La_3Ni_2SbO_9$: The search for relaxor ferromagnetism in $LaSr_2Cr_2SbO_9$ and $PrSr_2Cr_2BO_9$ (B=Sb, Ta, Nb). **E.C. Hunter**, P.D. Battle, R. Paria Sena, J. Hadermann

1:50 914. New methods of chemical vapor deposition for mid-infrared ZnSe optical fiber lasers. **M.G. Coco**, S.C. Aro, S.A. McDaniel, A.T. Hendrickson, J.R. Sparks, V. Gopalan, P.J. Sazio, G. Cook, J.V. Badding

2:10 915. $Ba_4Ni_2Ir_2O_{12}$: A new Ni(II) and Ni(IV) containing quadruple perovskite. T. Ferreira, M. Whangbo, **H. zur Loye**

2:30 916. Molecular and electronic structures of the group 7 heptoxides. **K.V. Lawler**, B. Childs, D.S. Mast, K. Czerwinski, A.P. Sattelberger, F. Poineau, P. Forster

2:50 917. Radius ratio rule rescue. **D.A. Vander Griend**

3:10 918. Reversible phase transition of NiBi: A new high-pressure modification. **S.M. Clarke**, K.M. Powderly, C. Malliakas, Y. Meng, S.D. Jacobsen, D.E. Freedman

3:30 Intermission.

3:45 919. Investigation of the radioluminescence properties of nanosized core-shell cerium doped rare earth orthosilicate materials. **E. Zhang**, A. Dickey, M.K. Burdette, I. Bandera, J. Weick, H. zur Loye, J.N. Anker, J.W. Kolis, S.H. Foulger

4:05 920. Mechanistic insights into the oxidative reaction of hydrogen-terminated Si(111) surfaces with liquid methanol. **N.T. Plymale**, M. Dasog, B.S. Brunschwig, N.S. Lewis

4:25 921. Zwitterionic derivatives of $[closo\text{-}1\text{-}CB_{11}H_{12}]^-$ as polar materials for LCD. **P. Kaszynski**, B. Lukasik, R. Zurawinski, M.O. Ali, A.C. Friedli

4:45 922. Multiple mechanisms for magnetoresistance in LnMnAsO pnictides. **E. Wildman**, A. McLaughlin

5:05 923. Properties of redox-active, ferromagnetically-coupled cobalt(III)semiquinone-containing polymers. **P. Hewitt**, D.A. Shultz

Section C

Renaissance Washington, DC
Downtown
Grand Ballroom South

Coordination Chemistry

Synthesis & Characterization

S. A. Koch, A. Larsen, *Organizers*
J. R. Miecznikowski, D. Rabinovich, *Presiding*

1:30 924. Synthesis and characterization of cobalt(II), copper(I), and copper(II) SNS pincer complexes. **J.R. Miecznikowski**, S.C. Bonitatibus, E.M. Almanza, R. Kharbouch, J.P. Jasinski, M. Kaur

1:50 925. Synthesis and characterization of porous aromatic frameworks for capturing cesium in water. **D. Parajuli**, M. Taylor, J.R. Long

2:10 926. NHC-supported imines and phosphinidenes in coordination chemistry. **M. Peters**, M. Tamm

2:30 927. Synthesis of a goldnanocluster used in metal pollution sensing. **K. Sanyal**

2:50 928. Effect of PNP pincer backbone structure on dinitrogen activation in ruthenium hydride complexes. **Q.J. Bruch**, S. Schneider, A.J. Miller

3:10 929. Synthesis, structural elucidation and cytotoxicity studies of ruthenium (II) polypyridine compounds with anionic N^O $^-$ donor ligands. **J.A. Obaleye**, A.O. Rajee, A.A. Ajibola, P.O. Obaleye

3:30 Intermission.

3:40 930. Hexa & hepta iron clusters of linked $[Fe^{III}{}_3O/OH]^{7+/8+}$ triangles with derivatized salicylaldoximes. **D.T. De Silva**, G.B. Jameson, P.G. Plieger, G.N. Jameson, E.K. Brechin

4:00 931. Synthesis and reactivity of N-heterocyclic thiones and selones with saturated backbones. J.R. Patterson, J.J. Flanagan, **D. Rabinovich**

4:20 932. Supramolecular aggregates of single-molecule magnets using dioximate linkers. **T. Ghosh**, D. Takahashi, W. Wernsdorfer, K.A. Abboud, G. Christou

4:40 933. Multinuclear copper(I), silver(I) and coordination polymers supported by the NNN-pincer ligand : Bis(3,5-dimethylpyrazolylmethyl)pyrrole. **O. Jana**

5:00 934. One-step synthesis of substituted 2-(2'-pyridyl)quinoline ligands and investigation of the solution and solid phase behavior of the corresponding gold(III) complexes. **M.D. Sterling**, L. Bishop, A.L. Rheingold, C.H. Larsen

5:20 935. Synthesis, structure and bonding in metal complexes of P-stereogenic phosphiranes. **J.A. Muldoon**, M. Deegan, R.P. Hughes, D.S. Glueck, C. Moore, A.L. Rheingold

Section D

Renaissance Washington, DC
Downtown
Congressional C

Bioinorganic Chemistry

Proteins & Enzymes & Model Systems

S. A. Koch, *Organizer*
M. I. Galinato, M. D. Pluth, *Presiding*

1:30 936. Selection of peptidic inhibitors against sortase A by using phage display library. **M. Koksal**, **N. Ersoz**, F. Dudak

1:50 937. Quantitatively probing photosystem II with a rotating ring disk electrode assembly. **N. Kornienko**, R. van Grondelle, A. Rutherford, E. Reisner

2:10 938. Fast hydrogen atom abstraction by a hydroxo iron(III) porphyrazine. **H. Gao**, J.T. Groves

2:30 939. Investigating the bioinorganic chemistry of H_2S using small molecule model systems. **M.D. Pluth**

2:50 940. OEC model complexes via application of a tunable carboxamide ligand scaffold. **N. McMillion**, J.S. Anderson

3:10 Intermission.

3:20 941. Spectroscopic and electrocatalytic reduction studies of

nitrite to NO by human serum albumin-heme. **M.I. Galinato**, E.M. Luteran, G.A. Fye, J.A. Bennett

3:40 942. Functional role for the [4Fe4S] cluster in human DNA primase as a redox switch using DNA charge transport. **E. OBrien**, M. Holt, M.K. Thompson, L.E. Salay, A.C. Ehlinger, W.J. Chazin, J.K. Barton

4:00 943. Revision of hydroxylamine oxidoreductase activities and bacterial ammonia oxidation pathways. **J.D. Caranto**, K.M. Lancaster

4:20 944. Elucidating the reactivity of ferrous heme-P460 cofactors. **M. Smith**, K.M. Lancaster

4:40 945. Metallodithiolenes revealed as unique chemical chameleons. **J.H. Enemark**, B.W. Stein, J. Yang, R. Mtei, N. Wiebelhaus, D. Kersi, D.L. Lichtenberger, M.L. Kirk

Section E

Renaissance Washington, DC Downtown
Grand Ballroom North

Organometallic Chemistry

Applications to Organic Transformations

N. S. Radu, *Organizer*
D. Lehnherr, A. N. Vedernikov, *Presiding*

1:30 946. Redox activity of carbene ligands: Convergent and divergent radical-type pathways of metal-bound carbene radicals. **B. de Bruin**

1:50 947. Cp*Ir(III)-catalyzed *ortho* halogenation of benzamides *via* C-H bond activation. **A.J. Guzman-Santiago**, E. Ison

2:10 948. Mechanistic studies of a Re-catalyzed mono-alkylation of phenols. **D. Lehnherr**, M.D. Weisel, X. Wang, Y. Lam, H. Sheng, F. Peng, J.R. Naber, K.M. Maloney, I.W. Davies

2:30 949. Bioinspired Mn(I) catalysts for CO_2 hydrogenation and transfer hydrogenation reactions. **A. Dubey**, J.R. Khusnutdinova

2:50 950. Nonprecious metal catalysts for hydrogenation, hydrofunctionalization and dehydrogenative coupling reactions. **G. Zhang**

3:10 951. Development of a switchable amide hydrogenation catalyst yielding selective C–N and C–O bond scission products. **N.M. Rezayee**, M.S. Sanford

3:30 952. Large bite angle early transition metal biphenolate complexes as tunable catalysts for amine addition to alkenes. **J. Soltys**, A. Roller, K. Hultzsch

3:50 953. Mechanistic studies of the $Zn(II)/SiO_2$-catalyzed hydroamination of alkynes. **A.K. Cook-Sneathen**, C. Coperet

4:10 954. Formation of carbazoles and indolines via oxidative intramolecular C-N coupling of amido aryl and amido alkyl Pd(II) complexes with H_2O_2 as oxidant: A mechanistic analysis. E. Abada, P.Y. Zavalij, **A.N. Vedernikov**

4:30 955. Acceleration of Pd-catalyzed amide N-arylations using co-catalytic metal triflates: Substrate scope and mechanistic study. **J. Becica**, G. Dobereiner

4:50 956. Expansion of boracarboxylated vinyl arenes: Exploring the synthetic elaboration of the carbon-boron bond through cross-coupling. **T. Perrone**, S. Knowlden, B.V. Popp

5:10 957. Synthesis of azabicylo[6.3.0]undecadienes through a Ni-catalyzed intramolecular [4+4] cycloaddition. **G.E. Greco**, E. Kativhu

Section F

Renaissance Washington, DC Downtown
Grand Ballroom Central

Bioinorganic Chemistry

DNA, RNA & Inorganic Drugs

S. A. Koch, *Organizer*
A. G. Tennyson, Y. Zheng, *Presiding*

1:30 958. Synthesis, characterization, and biological activity of DNA mismatch-targeting rhodium complexes. **K. Boyle**, J.K. Barton

1:50 959. Photoactivation of two fluorescent dyes via ruthenium(II) polypyridyl ligand exchange. **T.N. Rohrabaugh**, J.K. White, C. Turro

2:10 960. Synthesis and characterization of dinuclear ruthenium complexes as mitochondrial calcium uptake inhibitors. **S.R. Nathan**, J. Urgiles, J. Woods, J. Wilson

2:30 961. Nontraditional tetrapyrrole complexes as efficient photochemotherapeutic agents with remarkably high phototoxicity indices. **J. Rosenthal**, A.M. Potocny, M. Martin

2:50 962. Isostructural series of first row transition metal Schiff base complexes for producing contrast in MRI. **J.J. Scepaniak**, W. Kaminsky, S. Dechert, F. Meyer

3:10 Intermission.

3:20 963. Rhodium-cyanine fluorescent probes for detection and signaling of mismatches in DNA. **A. Nano**, J.K. Barton

3:40 964. Hydride donation by NAD^+ in biologically-relevant redox catalysis. **A.G. Tennyson**

4:00 965. Nanoprecipitation of metallocages for platinum-based anticancer drug delivery. **Y. Zheng**, Z. Yue, H. Wang

4:20 966. Roussin's black and Roussin's red salts: Dynamic studies of nitric oxide releasing properties in different medium and their cytotoxic activity. **T. Drummond**, T.P. Dasgupta, P.T. Maragh

Nanoscale Sensing in Foods & Other Complex Media

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