

## INOR

### INORGANIC CHEMISTRY

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

### OTHER SYMPOSIA OF INTEREST:

**2015 ACS Catalysis Lectureship** (see *CATL, Mon, Tue*)

**SABIC Young Catalysis Investigator Award: Symposium In Honor of Melanie Sanford** (see *CATL, Tue*)

**Cope Award Symposium** (see *ORGN, Tue*)

### SUNDAY MORNING

#### Section A

Boston Convention & Exhibition Center  
Room 160B

#### Main Group Chemistry

T. W. Hudnall, *Organizer*  
J. D. Protasiewicz, D. Vidovic, *Presiding*

**9:00 1.** Alternate pyrrole and isoindoline-based BF<sub>2</sub> fluorophores. **C.J. Ziegler**, L. Crandall, I. Tamgho

**9:20 2.** Polyoxaphospholes: Polymeric organophosphorus compounds with luminescent properties. **J. Gaffen**, J.D. Protasiewicz

**9:40 3.** Luminescent materials featuring multiply bonded phosphorus groups. **J.D. Protasiewicz**

**10:00 4.** Computational design and characterization of organometallic molecules with unprecedented beryllium-beryllium double bonds. **X. Wang**

**10:20** Intermission.

**10:30 5.** Tribora-cyclopropenyl dianion - a boron-based homoaromatic Hückel  $\pi$  system. **T. Kupfer**, H. Braunschweig

**10:50 6.** Synthesis and reactivity of phosphonium dication. **D. Vidovic**

**11:10 7.** Stabilization of reactive main group species by coordination to carbonyl-decorated carbenes. **T.W. Hudnall**, A. Ledet, K.M. Melancon, A.J. Torres

**11:30 8.** Redox- and anion-controlled modulation of a Au-Sb bond. **S. Sen**, I. Ke, F.P. Gabbai

**11:50 9.** Exploring the electronic structure of aluminum hydrides: X-ray absorption spectroscopic investigations of aluminum coordination complexes. **A.B. Altman**, J. Arnold, S.G. Minasian, S. Pemmaraju, D. Prendergast, D.K. Shuh, T. Tylicszczak

#### Section B

Boston Convention & Exhibition Center  
Room 159

#### Organometallic Chemistry: New Ligand Platforms

N. S. Radu, *Organizer*  
D. Mendoza-Espinosa, E. T. Papish, *Presiding*

**8:00 10.** Exploring the reactivity of Pd pincer complexes immobilized in a Zr(IV) metal-organic framework matrix. **S.A. Burgess**, C.R. Wade

**8:20 11.** Stabilizing high oxidation state first row metal complexes with a robust fluoroalkoxy carbene. A.J. Arduengo, S.P. Kelley, W.J. Marshall, **J.W. Runyon**

**8:40 12.** Heteroatom-functionalized 1,2,3-triazoliums: Ionic liquids for the Baylis-Hillman reaction and ligand precursors for MIC transition metal complexes. **D. Mendoza-Espinosa**, G. Negron-Silva, R. Gonzalez-Olvera

**9:00 13.** Synthesis and application of N-trifluoromethylated N-heterocyclic carbene ligands and their complexes. **P. Engl**, A. Toni

**9:20 14.** Tetranuclear Pd catalysts based on metal phosphonate cages for olefin polymerization. **Q. Liu**, N.D. Contrella, A.S. Filatov, R.F. Jordan

**9:40 15.** Metal-ligand cooperative pathway for intermolecular oxa-Michael additions to unsaturated nitriles. S. Perdriau, D. Zijlstra, E. Heeres, H. de Vries, **E. Otten**

**10:00 16.** New bifunctional ligands for catalysis. **E.T. Papish**, C.R. Thompson, E.A. Douglas, D.L. Gerlach

**10:20 17.** Threefold symmetric zerovalent cobalt is a potent reductant of N<sub>2</sub>. B.J. Cook, M. Pink, S. Bidwell, R.L. Lord, **K.G. Caulton**

**10:40 18.** Iridium PC(sp<sup>3</sup>)P-type complexes which exhibit unique ancillary interactions. **D.C. Babbini**, V.M. Iluc

**11:00 19.** Metal-ligand cooperativity between a new series of aryl-substituted PNP pincer-type ligands and an Ir(I/III) metal center. **S.P. Vilanova**, V.M. Iluc

**11:20 20.** Mono- and dimetalation of a tridentate bisimidazole-phosphine ligand. **S.E. Flowers**, B.M. Cossairt

**11:40 21.** Diastereoselective and enantioselective synthesis of P-stereogenic *Syn*-phosphiranes. **J. Muldoon**, B. Varga, M. Deegan, T.W. Chapp, D.S. Glueck, C. Moore, A.L. Rheingold

**12:00 22.** Pyridyl-functionalized 3H-1,2,3,4-triazaphospholes: Synthesis, coordination chemistry, and application in homogeneous catalysis. **J. Sklorz**, C. Mueller

#### Section C

Boston Convention & Exhibition Center  
Room 162B

#### Solid-State Inorganic Chemistry

C. G. Lugmair, *Organizer*  
V. Poltavets, *Organizer*, *Presiding*  
A. Choudhury, *Presiding*

**8:30** Introductory Remarks.

**8:35 23.** TiS<sub>2</sub> and TiS<sub>3</sub> layered materials: Intercalation and/or substitution to enhance the thermoelectric properties. **A. Maignan**

**9:15 24.** Magnetic anisotropy in new misfit layer compounds. **S.M. Clarke**, D.E. Freedman

**9:35 25.** Novel soft chemistry techniques for metastable materials synthesis. **V. Poltavets**, J.D. Davis, S.K. Kraemer

**9:55 26.** Controlling hard/soft magnetic exchange in core/shell nanoparticles. **D. Carnevale**, M. Shatruk, G.F. Strouse

**10:15** Intermission.

**10:30 27.** Series of magnetically frustrated quaternary chalcogenides with interpenetrating lattices. **A. Choudhury**, S. Mohapatra, K. Ghosh

**10:50 28.** Single crystal growth and X-ray observation of charge-density-wave order in Ruddlesden-Popper nickelate R<sub>4</sub>Ni<sub>3</sub>O<sub>10</sub>(R=La and Pr). **J. Zhang**, Y. Chen, H. Zheng, Y. Ren, J. Mitchell

**11:10 29.** Formation of transition metal oxide with high-aspect-ratio geometry by high pressure CVD. **Y. Liu**, V. Gopalan, J.V. Badding

**11:30 30.** Origin of superhardness in metallic tungsten monoboride. **M.T. Yeung**, J. Lei, R. Mohammadi, C.L. Turner, Y. Wang, S.H. Tolbert, R.B. Kaner

#### Section D

Boston Convention & Exhibition Center  
Room 160C

#### Environmental and Energy-Related Inorganic Chemistry

S. A. Koch, *Organizer*  
F. N. Castellano, *Presiding*

**8:00 31.** Design and synthesis of ruthenium-EDOT based coordination polymers for use in inorganic-organic hybrid dye sensitized solar cells. **S.M. Boyer**, K.H. Skorenko, A. Nandur, F.H. Schreffler, M.I. Ehrlich, B.E. White, W.E. Bernier, W.E. Jones

**8:20 32.** Enhancements to electrocatalytic reduction of CO<sub>2</sub> by cobalt phthalocyanine upon immobilization in polyvinylpyridine membrane. **W.W. Kramer**, I.M. Ferrer, C.C. McCrory

**8:40 33.** Electrocatalytic reduction of carbon dioxide to carbon monoxide by manganese carbonyl complexes containing phenanthroline-type ligands: Catalytic turnover even in the absence of Brønsted acids. **B. Dhakal**, D.A. Kurtz, R.J. Hulme, G.A. Felton

**9:00 34.** Stoichiometric production and delivery of chlorine to substrates. **A. Stastny**, A.E. Norton, J.A. Krause, W.B. Connick

**9:20 35.** Hydrogenation of CO<sub>2</sub> and dehydrogenation of formic acid using iridium catalysts based on proton-responsive azole ligands. **Y. Himeda**, N. Onishi, S. Xu, Y. Suna, Y. Manaka, J.T. Muckerman, E. Fujita

**9:40 36.** Photochemical upconversion beyond the molecule. **F.N. Castellano**

**10:00** Intermission.

**10:10 37.** Electrocatalytic reduction of CO<sub>2</sub> with manganese catalyst supported by pendant Brønsted-Lowry acid ligands. **K. Ngo**, R.P. Narayanan, B. Mahanti, B.R. Reed, S. Groysman, J.J. Rochford

**10:30 38.** Rapid water oxidation electrocatalysis by a ruthenium complex with a facially coordinating polypyridyl ligand. **A. Walden**, A.J. Miller

**10:50 39.** Electrochemical water oxidation investigations into divalent and trivalent cobalt and manganese perfluoropinacolate complexes. **J.L. Steele**, L. Tahsini, C. Sun, A.F. Long, J.W. Bacon, J.A. Golen, A.L. Rheingold, L. Doerrer

**11:10 40.** Degradation of lignin model compounds through selective C-C bond cleavage using earth abundant vanadium catalysts driven by visible light. S. Gazi, W.K. Ng, R. Ganguly, H. Hirao, **H. Soo**

**11:30 41.** Chromophore-catalyst assemblies based on porphyrin and Ru(II) polypyridyl catalysts for light driven water oxidation. **A. Nayak**, R.R. Knauf, L. Alibabaei, J.L. Dempsey, T.J. Meyer

**11:50 42.** Volatile heterometallic precursors for the low-temperature synthesis of lithium ion battery cathode material. **Z. Wei**, H. Han, A.S. Filatov, E. Dikarev

#### Section E

Boston Convention & Exhibition Center  
Room 161

#### Bioinorganic Chemistry: DNA, RNA and Inorganic Drugs

S. A. Koch, *Organizer*  
J. Liu, *Presiding*

**8:00 43.** Ru(II) polypyridyl complexes as potent photosensitizers in photodynamic therapy. C. Mari, V. Pierroz, R. Rubbiani, M. Patra, S. Ferrari, **G. Gasser**

**8:20 44.** Small peptides-Re(CO)<sub>3</sub> conjugates synthesis using new lysine linkage approach. **K. Chanawanno**, V. Kondeti, S.M. Paruchuri, J.A. Caporoso, T. Leeper, R.S. Herrick, C.J. Ziegler

**8:40 45.** Lanthanide ion dependent DNAzymes: In vitro selection and metal binding studies. **J. Liu**, P. Huang

**9:00 46.** Facile synthesis and biological evaluation of metallocenyl derivatives. **J. Hess**, M. Patra, A. Leonidova, V. Pierroz, S. Ferrari, G. Gasser

**9:20 47.** Practical and reliable method for long-term room temperature storage of RNA within silica. **M. Puddu**, W.J. Stark, R.N. Grass

**9:40 48.** Rationally designed glucose-platinum(II) conjugates for actively targeting cancer cells. **M. Patra**, T.C. Johnstone, K. Suntharalingam, S.J. Lippard

**10:00** Intermission.

**10:10 49.** Biological consequences arising from the unique binding profile of phenanthriplatin. **I.A. Riddell**, G. Park, K. Agama, Y. Pommier, S.J. Lippard

**10:30 50.** On the cytotoxic activity of Pd(II), Pt(II) and Ru(II) complexes of N, N-disubstituted-N-acyl thioureas. **A. Batista**, A. Graminha, A.M. Plutin, A. Alvarez, R. Ramos, R. Mocoelo, E. Castellano

**10:50 51.** Upconverting lipid vesicles for the red light activation of anticancer metallodrugs. **S. Bonnet**

**11:10 52.** Verstatile and remarkably stable Mn-based MR imaging probe: Application to targeted thrombus imaging. **E. Gale**, I. Atanasova, F. Blasi, P. Caravan

**11:30 53.** In silico guided design and synthesis of new high relaxivity Gd(DOTAla) derivatives. **E. Boros**, H. Kim, B. Tidor, P. Caravan, A. Horning

**11:50 54.** DNzyme sensors for cellular metal ion sensing. **K. Hwang**, Y. Lu

#### Section F

Boston Convention & Exhibition Center  
Room 162A

#### Chemistry of Materials: Materials for Energy and Catalytic Applications

C. G. Lugmair, *Organizer*  
A. Hall, *Presiding*

**8:00 55.** Graphite-conjugated pyrazines as molecularly-tunable electrocatalysts. **T. Fukushima**, Y. Surendranath

**8:20 56.** Electrocatalytic CO<sub>2</sub> reduction at ordered nanoporous metallic thin films. **A. Hall**, Y. Yoon, Y. Surendranath

**8:40 57.** Grain boundary rich metals: Synthesis and impact on electrocatalysis. **Y. Yoon**, A.S. Hall

**9:00 58.** Strain modulated electrocatalysis. **E. Benson**, D. Svedruzic, S. Ferrere, B.A. Gregg

**9:20 59.** Rhenium-based complexes and conducting metallopolymers for electrocatalytic CO<sub>2</sub> reduction. **Y. Liang**, L.A. Lytwak, **B.J. Holliday**

**9:40 60.** Imparting architecture control over colloidal nanocrystal frameworks for energy storage devices. **T.E. Williams**, A.W. Wills, B. Helms

**10:00** Intermission.

**10:10 61.** Experimental and theoretical investigation of LiFeO<sub>2</sub> – tunnel: Fe<sup>2+</sup>/Fe<sup>4+</sup> cathode for Li-ion batteries. **V. Poltavets**, J.D. Davis, S.R. Bruno, C. Blakely

**10:30 62.** Comparison of different TiO<sub>2</sub> phase structures and morphologies on dye-sensitized solar cell. **C. Tsui**, K.L. Yeung

**10:50 63.** Synthesis of mesoporous metal oxides via aerosol-assisted self-assembly pyrolysis for energy storage. **M. Sheehan**, M. Rudden, C. Tsung

**11:10 64.** Band edge control of crystalline silicon by chemical functionalization of the surface. **N.T. Plymale**, A.A. Ramachandran, A.N. Lim, B.S. Brunschwig, N.S. Lewis

**11:30 65.** Amplification of light energy conversion within the dielectric-band in a dye-sensitized solar cell coupled to an inverse opal compared with an inverse glass. **R. Fayad**, **L.J. Halaoui**

**11:50 66.** New iron-based polyanion compounds as cathode materials for rechargeable alkali-ion batteries. **H. Yaghoobnejad Asl**, A. Choudhury

#### Section G

Boston Convention & Exhibition Center  
Room 160A

#### Coordination Chemistry: Synthesis and Characterization

D. C. Crans, *Organizer*

A. R. Fout, D. Rabinovich, *Presiding*

**8:30 67.** Isolation and characterization of intermediates involved in the silylation of dinitrogen using a dicobalt catalyst. **R. Siedschlag**, V. Bernales, K.D. Vogiatzis, L. Gagliardi, C. Lu

**8:50 68.** Synthesis and reactivity of new N-heterocyclic thione (NHT) and related ligands. **D. Rabinovich**

**9:10 69.** Linear oligopyrroles as redox-active ligands: Metal coordination and redox behavior. **E. Tomat**

**9:30 70.** Redox-state effects on small molecule bin multimetallic iron complexes. **G. de Ruiter**, N.B. Thompson, T. Agapie

**9:50 71.** Robust trinuclear complexes towards reactivity with challenging small molecule substrates. **J. Teesdale**, T. Betley

**10:10 72.** Investigating the role of a tripodal H-bond donor and acceptor ligand scaffold in small molecule activation. **C. Ford**, E.M. Matson, Y. Park, A. Fout

**10:30 73.** Bioinspired  $\alpha$ -hydroxy acid containing tripodal amine chelates and photoactivity of their metal complexes. **J.E. Vernia**, M.J. Baldwin

**10:50 74.** Synthesis and characterization of trinuclear complexes featuring early transition metals. **A.K. Bartholomew**, T. Betley

**11:10 75.** Group transfer catalysis utilizing a pyrazolate-bridged Co<sub>2</sub> system. **B.J. Cook**, C. Chen, R.L. Lord, K.G. Caulton

**11:30 76.** New class of high-relaxivity Mn<sup>III</sup>-based contrast agents as platforms for targeted intracellular magnetic resonance molecular imaging. **A. Barandov**, B. Bartelle, A. Jasanoff

**11:50 77.** Synthesis and coordination chemistry of chelating guanidiny borate ligands. **N.A. Piro**, W.S. Kassel

**12:10 78.** Anion binding by cobalt complexes of an H-bond donor triguanidine ligand. **R.C. Scarrow**, J.A. Schneider, S.C. Schwartz, S. Park, T.M. Nguyen

#### Section I

Boston Convention & Exhibition Center  
Room 158

#### Coordination Chemistry: Synthesis and Characterization

D. C. Crans, *Organizer*  
A. De Bettencourt Dias, C. Thomas, *Presiding*

**8:30 79.** Linking [Fe<sup>III</sup>]<sub>3</sub> triangles with derivatised salicylaldoximes. **D.T. De Silva**, G.N. Jameson, E.K. Brechin, P.G. Plieger

**8:50 80.** Investigating the interaction and redox activity of novel polynuclear iron complexes with carbohydrates: Synthesis, structure, electrochemical, and spectroscopic investigation of their interactions with monosaccharides. **C.D. Stewart**, H. Arman, G.T. Musie

**9:10 81.** Towards selective Fe(II) optical sensors. **T.Y. Tittiris**, S.M. McLeod, J.R. Morrow

**9:30 82.** Isolation and characterization of a  $\mu^2$ -tricobalt nitride in four different oxidation states. **B. Lin**, T. Betley

**9:50 84.** Synthesis and reactivity of trinuclear Zn–Fe clusters. **C. Juda**, T. Betley

**10:10 85.** Synthesis and reactivity of a sterically demanding benzimidazole thione. **L. Hernandez**, D. Rabinovich

**10:30 86.** Synthesis and characterization of N-heterocyclic phosphonium/phosphide nickel complexes: Mono- and multimetallic. **D.A. Evers-McGregor**, M. Bezpalko, B.M. Foxman, C. Thomas

**10:50 87.** Coordination chemistry of mid-to-late first-row transition-metal complexes with tris(2-pyridyl)phosphine (PPy<sub>3</sub>) and its oxide (OPPy<sub>3</sub>). **K. Suppa**, C. Fairfield, D. Pericic, N.A. Piro, **W.S. Kassel**

**11:10 88.** Class I mixed-valent dirhenium complexes. **Y. Yan**, J.T. Mague, J.P. Donahue, **S. Sproules**

**11:30 89.** Dicarboxylate-connected and bisphosphine substituted dimolybdenum(II) coordination compounds. **D. Hoehne**, A. Pothig, E. Herdtweck, M. Cokoja, S. Haslinger, X. Cai, M. Koeberl, F.E. Kuehn, W. Herrmann

**Transition Metal Catalyzed Olefin Polymerization: Towards Structure Control**

**Tutorial**  
Sponsored by PMSE, Cosponsored by INOR<sup>‡</sup>

**SUNDAY AFTERNOON**

**Section A**

Boston Convention & Exhibition Center  
Room 160B

**Inorganic Young Investigator Awards**

J. M. Boncella, *Organizer, Presiding*

**1:30** Introductory Remarks.

**1:35 90.** Synthetic micro/nanomachines and their applications: Toward "Fantastic Voyage". **W. Gao**, **J. Wang**

**2:05 91.** Structure design of silicon anodes for high energy lithium-ion batteries. **N. Liu**, Y. Cui

**2:35 92.** Electronically doped colloidal semiconductor nanocrystals. **A.M. Schimpf**, D.R. Gamelin

**3:05** Intermission.

**3:15 93.** Gas separations in metal-organic frameworks with open metal sites. **E.D. Bloch**, J.R. Long

**3:45 94.** Organometallic palladium complexes as chemoselective bioconjugation reagents. **E.V. Vinogradova**, C. Zhang, A.M. Spokoyny, B.L. Pentelute, S.L. Buchwald

**4:15 95.** Exploring the trap state landscape of colloidal CdSe nanocrystals with cadmium halide ligands. **M.J. Greaney**, R.L. Brutchey

**4:45 96.** Models of the oxygen-evolving complex of photosystem II. **J. Kanady**, T. Agapie

**5:15 97.** Efforts toward the next generation of platinum drugs: Monofunctional complexes and nanodelivery. **T.C. Johnstone**, S.J. Lippard

#### Section B

Boston Convention & Exhibition Center  
Room 159

#### Synthetic Chemistry Approaches to Magnetic Materials

D. E. Freedman, M. A. Green, E. E. Rodriguez, *Organizers*  
D. Harris, *Organizer, Presiding*

**1:30 98.** Emergent chemical kinetics in a magnetic system. **S. Bramwell**

**2:00 99.** Ternary manganese chalcogenides: New approaches to the synthesis of layered materials with strong magnetic frustration. **C. Pak**, **M. Shatruk**

**2:20 100.** Synthetic chemical approaches to designing and understanding qubits. **J. Zadrozny**, M. Graham, M. Fataftah, S. Coste, **D.E. Freedman**

**2:40 101.** Electronic structure contributions to magnetic exchange interactions in photoexcited states. **M.L. Kirk**, D. Shultz

**3:10** Intermission.

**3:20 102.** Controlled under pressure: Understanding magnetic anisotropy in heavy atom organic radicals. **S. Hill**, K. Thirunavukkuarasu, S. Winter, C.C. Beedle, R.T. Oakley

**3:50 103.** Tunable superparamagnetism in *n*-type TM<sup>2+</sup>- and Ln<sup>3+</sup>-doped nanoparticles. **J.D. Rinehart**

**4:10 104.** Effect of optical switching on the spin states of electronically bistable magnetic materials: Photoresponsive metal clusters. **N. Frank**

**4:30 105.** Magnetic and multiferroic metal-organic frameworks. **A. Cheetham**

Section C

Boston Convention & Exhibition Center  
Room 162B

### Inorganic Catalysts

S. A. Koch, *Organizer*  
K. A. Grice, *Presiding*

**1:30 106.** Group 13 metal-containing catalysts and the development of more sustainable hydrocarbon oxidation reactions. **C.R. Goldsmith, F. Bronston, C. Koellner, N.A. Piro, W.S. Kassel, C.R. Graves**

**1:50 107.** Electrospun composite nanofibers for enhanced photocatalytic degradation of environmental toxins. **D.L. McCarthy, J. Troiano, J. Tollin, J. Liu, J.B. Decoste, W.E. Bernier, W.E. Jones**

**2:10 108.** Dehydrofluorination of 1,1,1,2,3-pentafluoropropane to produce eco-friendly refrigerant 2,3,3,3-tetrafluoropropene (HFO-1234yf) using Cr-based catalysts. **S. Lim, J. Ha, H. Kim**

**2:30 109.** Electrochemical reduction of carbon dioxide with group 6 metal complexes. **K.A. Grice, C. Saucedo, M. Sovereign**

**2:50** Intermission.

**3:00 110.** Redox-active pincer ligands on chromium: Efforts toward reductive coupling of carbon dioxide. **N.S. Labrum, C. Chen, K.G. Caulton**

**3:20 111.** Surface attachment of homogeneous CO<sub>2</sub> reduction catalysts: Re(bpy-CN)(CO)<sub>3</sub>Cl on gold. **M.L. Clark, C.W. Machan, S.A. Chabolla, T. Dang, C.P. Kubiak**

**3:40 112.** Hydrocarbon oxidation by bimetallic late transition metal complexes with dual active sites. **C. Hess, S. Lindsay**

**4:00 113.** Multinuclear palladium oxygen species related to aerobic oxidation catalysis. **A.J. Ingram, K.L. Walker, R.N. Zare, R.M. Waymouth**

**4:20 114.** Iron-catalyzed synthesis of unprotected complex N-heterocycles via direct amination of primary, secondary, and activated C-H bonds. **A. Mikhailine, T. Betley**

**4:40 115.** Facile microwave synthesis and catalytic properties of cobalt (II) porphyrinyl compounds. **C.J. McElroy, P. Jairu, S. Amorello, P.D. Voegel**

Section D

Boston Convention & Exhibition Center  
Room 160C

### Metalloenzyme Mechanisms

G. Ghirlanda, I. V. Korendovych, *Organizers, Presiding*

**1:30 116.** Using designed enzymes for mechanistic investigation of heme-copper oxidase and nitric oxide reductase. **Y. Lu, A. Bhagi, I.D. Petrik,**

**Y. Yu, J. Reed, S. Chakraborty, A. Mukherjee**

**2:00 117.** Short peptides self-assemble in the presence of metals to produce catalytic amyloids. **I.V. Korendovych**

**2:30 118.** Binding of nitrogenase substrates to an iron complex with sulfur and carbon ligands. **I. Coric, A.M. Brosnahan, B.Q. Mercado, P.L. Holland**

**3:00** Intermission.

**3:10 119.** Kinetics and mechanisms of oxygen and peroxide activation with non-heme iron enzyme models. **E. Rybak-Akimova**

**3:40 120.** Redox mechanisms of metalloenzymes, studied with protein electrochemistry. **S.J. Elliott, E.T. Judd, K. Walsh, B. Levin**

**4:10 121.** Water oxidation by photosystem II. **G.W. Brudvig**

Section E

Boston Convention & Exhibition Center  
Room 162A

### Chemistry of Materials: Metal Organic Frameworks

C. G. Lugmair, *Organizer*  
C. Mottillo, E. Tsvion, *Presiding*

**1:30 122.** Chemistry of CH<sub>4</sub> adsorption on MOFs with open metal sites. **E. Tsvion, M.P. Head-Gordon**

**1:50 123.** Tailoring the nucleophilic character of metal-organic frameworks for the reactive removal of chemical threats. **J.B. DeCoste, M.A. Browe, G.W. Wagner, G.W. Peterson**

**2:10 124.** Novel quick approach to tethering amine on metal-organic frameworks for selective CO<sub>2</sub> capture from air and flue gas. **H. Li, K. Wang, H. Zhou**

**2:30 125.** Dioxygen activation in a cobalt metal-organic framework for O<sub>2</sub>/N<sub>2</sub> separations and catalysis. **D.J. Xiao, M. Gonzalez, J.R. Long**

**2:50 126.** DFT modeling of metal-organic frameworks for oxygen-nitrogen separation: Effect of temperature and metal. **M.V. Parkes, J.A. Greathouse, T.M. Nenoff**

**3:10 127.** First-principles molecular dynamics simulations on hydrogen storage in metal-organic framework. **K. Koizumi, K. Nobusada, M. Boero**

**3:30** Intermission.

**3:40 128.** Functionalized metal-organic frameworks bearing flexible side chains: A way to tune gas sorption properties. **I. Schwedler, S. Henke, A. Schneemann, P. Llewellyn, R.A. Fischer**

**4:00 129.** New Ca-based metal organic framework selectively absorbing Xe over Kr. **X. Chen, A.M. Plonka, D. Banerjee, R. Krishna, H.T. Schaefer, S. Ghose, P.K. Thallapally, J.B. Parise**

**4:20 130.** Light gas separations and storage with MOFs via modeling, synthesis, and pressurized induced structural changes. **T.M. Nenoff, D.F. Sava Gallis, M.V. Parkes, J.A.**

**Greathouse, M. Rodriguez, K.W. Chapman**

**4:40 131.** Stability analysis of microporous zeolitic imidazolate frameworks in carbon dioxide-rich atmospheres. **C. Mottillo, T. Friscic**

**5:00 132.** Functionalized MOFs for hydrocarbon separation. **A. Schneemann, E.D. Bloch, S. Henke, P. Llewellyn, J.R. Long, R.A. Fischer**

**5:20 133.** Structural changes in M[(bdc)(ted)<sub>0.5</sub>] (M = Zn, Ni or Cu) metal organic frameworks upon thermal dispersion of LiCl and adsorption of carbon dioxide. **J. Guerrero-Medina, G. Mass-Gonzalez, L. Pacheco-Londoño, S.P. Hernandez-Rivera, R. Fu, A.J. Hernandez-Maldonado**

Section F

Boston Convention & Exhibition Center  
Room 161

### Coordination Chemistry: Synthesis and Characterization

D. C. Crans, *Organizer*  
K. G. Caulton, E. Tomat, *Presiding*

**1:30 134.** Heteroleptic formazan complexes of cyclometallated platinum. **T.S. Teets, E. Kabir**

**1:50 135.** Synthesis and reactivity of monoanionic pincer N-heterocyclic carbene iron complexes. **B. Jackson, A. Fout**

**2:10 136.** Synthesis and characterization of aluminum, gallium, tin, and chromium complexes with a non-innocent bulky diimine ligand. **R.A. Zarkesh, M. Anstey**

**2:30 137.** Fullerenes functionalized with piperazine: Building blocks for supramolecular architectures. **A. Aghabali, A.L. Balch, M.M. Olmstead**

**2:50 138.** Cooperative activation of carbon dioxide by a nucleophilic ligand backbone an oxophilic metal. **B.J. Cook, C. Chen, M. Pink, R.L. Lord, K.G. Caulton**

**3:10 139.** Ru-NHDC complexes from an abnormal Ru-NHC carbene. **M.J. Bitzer, A. Pothig, J. Kueck, C. Jandl, F.E. Kuehn, W. Baratta**

**3:30 140.** Intramolecular C-C coupling reactions in rhenium complexes triggered by ligand methyl group deprotonation. **R. Arevalo, J.A. Perez, L. Riera**

**3:50 141.** Hydroaminoalkylation of olefin catalyzed by silica supported metallaziridine. **B. Hamzaoui, J.M. Basset**

**4:10 142.** Synthesis, characterization, and reactivity of ruthenium nitrosyl complexes in oxygen-rich ligand environments. **Z.J. Tonzetich, V.M. Krishnan**

**4:30 143.** Dinuclear metallacycles with single anion bridges: Unusual magnetic and NMR properties. **D.L. Reger, A.E. Pascui, M.D. Smith, J. Jerierska, A. Ozarowski**

**4:50 144.** Can polynuclear metal clusters behave as "extended" organometallic complexes? **M. Nielsen, T. Betley**

**5:10 145.** Synthesis and photophysical properties of near-infrared Zn<sub>16</sub>Ln metallacrown complexes. **T.N. Nguyen, S.V. Eliseva, I. Martinic, C. Chow, S. Petoud, V.L. Pecoraro**

Section G

Boston Convention & Exhibition Center  
Room 160A

### Organometallic Chemistry: Catalysis

N. S. Radu, *Organizer*  
M. L. Neidig, *Presiding*

**1:30 146.** Electronic structure and bonding in iron(II)-bisphosphine complexes of relevance to iron catalyzed cross-coupling. **J.L. Kneebone, S.L. Daifuku, V.E. Fleischauer, J.A. Bailey, M.L. Neidig**

**1:50 147.** C-H bond amination mediated by high-spin iron complexes. **T. Betley, M.J. Wilding, D. Iovan, A. Mikhailine**

**2:10 148.** Spectroscopic investigation of in situ formed phenylated iron-bisphosphines and their reactivity in iron-catalyzed cross-coupling. **S.L. Daifuku, J.L. Kneebone, B.E. Snyder, M.L. Neidig**

**2:30 149.** Structure, bonding, and mechanism in iron-catalyzed cross-coupling. **M.L. Neidig**

**2:50 150.** Iron-NHC catalyzed C-C coupling by radical mechanism. **J.A. Przyojski, Z.J. Tonzetich**

**3:10** Intermission.

**3:15 151.** Mechanistic insights into C-H activation using (phebox)Ir compounds. **S.I. Johnson, R.J. Nielsen, M. Zhou, A.S. Goldman, W.A. Goddard**

**3:35 152.** Borylation chemistry with pincer complexes of iridium. **O. Ozerov, L.P. Press, C. Lee, J. Zhou, N. Bhuvanesh**

**3:55 153.** Rh(III) and Ir(III) complexes bearing protic NHCs: Synthesis and applications. **F. Aznarez, M. Iglesias, L.A. Oro, E.F. Hahn**

**4:15 154.** Iridium catalyzed base-free hydrogenation of esters and lactones. **T. Brewster, N.M. Rezaee, Z. Culaikova, M.S. Sanford, K.I. Goldberg**

**4:35 155.** Pincer (phebox)Ir (III) complexes in the C-H activation and oxidation of mesitylene. **M. Zhou, S. Johnson, R.J. Nielsen, T. Emge, W.A. Goddard, A.S. Goldman**

**4:55 156.** Liberation of hydrogen from formic acid using homogeneous palladium complexes supported by N-heterocyclic carbene ligands. **J. Eddy, P.G. Ariyananda, G.P. Yap, J. Rosenthal**

**5:15 157.** Selective heterogeneous C-H activation/halogenation reactions catalyzed by Pd@MOF composites. **V. Pascanu, F. Carson, M. Vico Solano,**

M.J. Johansson, X. Zou, B. Martin-Matute

### Transition Metal Catalyzed Olefin Polymerization: Towards Structure Control

#### Technical Session

Sponsored by PMSE, Cosponsored by INOR<sup>‡</sup>

#### SUNDAY EVENING

#### Section A

Boston Convention & Exhibition Center  
Hall C

### Bioinorganic Chemistry: DNA, RNA and Inorganic Drugs

S. A. Koch, *Organizer*

6:00 - 8:00

**158.** In vitro biological structure-activity relationship of novel dithiocarbamate phosphine gold(I) complexes: DNA binding and molecular docking studies. **A.A. Isab**  
**159.** Towards development of a minimalistic sequence specific reactivity standard for platinum-RNA interactions. **S. Elmroth**, M. Clausén, A. Alshiekh  
**160.** Synthesis of an enzyme-activated prochelator for combating antibiotic resistance. **D. Besse**, K.J. Franz  
**161.** Cytotoxic and DNA-binding properties of organorhenium-coordinated non-steroidal anti-inflammatory drugs (NSAIDs). **S. Azemati**, S. Pramanik, S.K. Mandal, A.J. Winstead

**162.** Iron complex PzPy: Triggering apoptosis from DNA intercalation. **A. Mokdad**, G. Zoppellaro, R. Zboril  
**163.** Antiparasitic activity of copper(II) complexes of metronidazole. J. Wu, J.H. Palmer, **R.K. Upmacis**

#### Section B

Boston Convention & Exhibition Center  
Hall C

### Building Innovative Solid State Materials Through Solution Chemistry

J. R. Neilson, A. J. Norquist, C. M. Oertel, *Organizers*

6:00 - 8:00

**164.** Role of noncovalent interactions templated vanadium oxides. **M. Wenny**, A.J. Norquist, J. Schrier  
**165.** Solution chemical syntheses of solid state nanoelectronic device components. **A.J. Bicchì**, A.R. Hight Walker  
**166.** Heterogenous frustrated Lewis pairs for small molecule activation. **J. Xing**, J. Buffet, D. O'Hare  
**167.** Synthesis of metal-organic frameworks containing organophosphine linkers. **R. Sternberg**, C.R. Wade

**168.** Synthesis of single crystals and nanostructures of lead oxide carboxylates with halogenated

benzoate ligands. C. Gang, V.S. Mandala, M. Zeller, **C.M. Oertel**

**169.** Rational synthesis of dimensionally reduced TiS<sub>2</sub> phases. **R.A. Morasse**, T. Li, Z. Baum, J.E. Goldberger

**170.** Ultrasonic spray synthesis as a route to shape controlled LaTiON nanoparticles. **E. Rugen**, S.E. Skrabalak

**171.** Thermodynamic investigations of actinide and lanthanide complexation: From fundamentals to applications. **P. Dau**, L. Rao

#### Section C

Boston Convention & Exhibition Center  
Hall C

### Environmental and Energy-Related Inorganic Chemistry

S. A. Koch, *Organizer*

6:00 - 8:00

**172.** Electrocatalytic reduction of carbon dioxide to carbon monoxide by manganese carbonyl complexes containing diimines: The need for greater conjugation in the dypyrromethane vs. dypyrromethene system. **N.R. Wheeler**, B. Dhakal, R.J. Hulme, G.A. Felton  
**173.** Photochemistry and redox non-innocence of electron rich *fac*-Re(I) tricarbonyl  $\beta$ -diketonate and oxyquinolate complexes: A fundamental study toward the application of CO<sub>2</sub> reduction. **K. Ngo**, B. Mahanti, N. Lee, J.J. Rochford  
**174.** Flow synthesis of magnetic metal-organic frameworks. K. He, **C. Tsui**, K.L. Yeung

**175.** Electrocatalytic CO<sub>2</sub> reduction and redox non-innocence of Mn(I) tricarbonyl oxyquinolate complexes. **M.E. McKinnon**, K. Ngo, R.P. Narayanan, J.J. Rochford  
**176.** Photoelectrochemical characterization of ruthenium flavanoid complexes in a dye-sensitized solar cell. **N. Lee**, K. Ngo, G.E. Gilligan, A. Zachary, M. Lamberto, J.J. Rochford

**177.** Recent developments for new Hg<sup>2+</sup>-fluorescence chemosensors based on 2-[4-(2-aminoethylsulfanyl)butylsulfanyl]ethanamine. **N. Wanichacheva**, T. Puangsamlee, S. Watpathomsub, S. Kraithong  
**178.** Bis(aldimino)pyridine nickel complexes as electrocatalysts for the reduction of CO<sub>2</sub>. **R.P. Narayanan**, K. Ngo, B.R. Reed, S. Groysman, J.J. Rochford  
**179.** Highly sensitive and selective chemosensor based on cyclic fluorescein for Hg<sup>2+</sup> detection in aqueous solution. **P. Piyanuch**, S. Watpathomsub, H. Nienaber, N. Wanichacheva

**180.** Structure-activity properties of curcuminoid ruthenium polypyridyl photosensitizers in dye sensitized solar cells. **G.E. Gilligan**, N. Lee, S. Bag, J.J. Rochford

**181.** Electrochemistry of cytochrome *c* from a cold-adapted microorganism. **N. Dalchand**, **M.C. Buzzeo**, **J.S. Magyar**  
**182.** Synthesis and characterization of a dimanganese Schiff-base complex as an artificial water oxidation catalyst. **S. Kal**, J.R. Buchwald, P.H. Dinolfo  
**183.** 59Co-NMR studies of Co compounds with O-donor ligands for WOC. **J. Weber**, M. Youmans, L. Doerr

#### Section D

Boston Convention & Exhibition Center  
Hall C

### Nanoscience

R. M. Richards, *Organizer*

6:00 - 8:00

**184.** Synthesis of polymer ligand stabilized fluorescent platinum nanoclusters and their applications as metal ions sensor and bio-imaging fluorophore. **X. Huang**, H. Ishitobi, Y. Inouye  
**185.** Surface chemistry and composition manipulation of germanium nanocrystals. **K. Tabatabaei**  
**186.** Highly fluorinated high-k hybrid dielectric nano materials for solution-processed electronic devices. **Y. Kim**, J. Son, J. Lee  
**187.** Synthesis of ceria-doped titanate nanosheets and nanotubes. Y. Fam, S.A. Ferdousi, **C. Tsui**, K.L. Yeung, Y. Du

**188.** Synthesis and processing of core/alloy nanoparticles with stainless interfaces. **L. Pathade**, T.L. Doane, R.D. Slaton, P. Lutz, M.M. Maye  
**189.** Synthesis and characterization of hollow Mn<sub>3</sub>O<sub>4</sub> nanoparticles. **S. Varapragasam**, C. Balasanthiran, J.D. Hoefelmeyer

**190.** Bioresorbable smart stent incorporated with therapeutic nanoparticles for endovascular diseases. **D. Lee**, T. Hyeon

#### Section E

Boston Convention & Exhibition Center  
Hall C

### Organometallic Chemistry: New Ligand Platforms

N. S. Radu, *Organizer*

6:00 - 8:00

**191.** Multi-electron charging of  $\pi$ -bowls: Structural transformations, supramolecular assembly, and metal binding trends. S.N. Spisak, **C. Dubceac**, N.J. O'Neil, Z. Zhou, A.S. Filatov, A. Zabula, M.A. Petrukhhina  
**192.** Unsymmetrical pincer-type palladium complexes containing novel pyrazolyl aminophosphine ligands. E. Cook, K. Iwasaki, J.D. Masuda, **A. Xia**  
**193.** Synthesis of 2-dimethylphosphino biaryl (Buchwald-type) ligands. **D.T. Seidenkranz**, A.J. Kendall, D. Tyler

**194.** Functionalized triazaphospholes: Intriguing phosphorus heterocycles with many perspectives. **J. Sklorz**, C. Mueller  
**195.** Synthesis, characterization, and reactivity studies of a boron-nitrogen-containing isostere of tri-*o*-tolylphosphine. **C. McConnell**, P. Memmel, C. Fristoe, P. Campbell, S. Liu

#### Section F

Boston Convention & Exhibition Center  
Hall C

### Synthetic Chemistry Approaches to Magnetic Materials

D. E. Freedman, D. Harris, E. E. Rodriguez, *Organizers*

6:00 - 8:00

**196.** Azamacrocyclic transition metal complexes for MR imaging and spectroscopy. **P.B. Tsitovich**, J.R. Morrow  
**197.** Hydride reductions to control the magnetic properties of the double perovskite Sr<sub>2</sub>FeMoO<sub>6</sub>. **N.J. Schreiber**, D.D. Taylor, E.E. Rodriguez

#### Section G

Boston Convention & Exhibition Center  
Hall C

### Lanthanide and Actinide Chemistry

A. De Bettencourt Dias, *Organizer*

6:00 - 8:00

**198.** One-step synthesis of hydrophilic up-conversion nanoparticles. **T. Wang**, L. Wang, Z. Feng, N. He, Z. Chen  
**199.** New heteronuclear lanthanide-niobium oxide clusters. **B. Yan**, D. Herrington, B. Garabato

**200.** Influence of the aryl carbonyl group in CMPO ligands for the sensitization of lanthanide luminescence. **E.G. Leach**, **A.A. Kulesza**, S.M. Biros

**201.** Experimental and computational study of lanthanide-CMPO ligand complexes. **A.J. Vanderweide**, R.L. Lord, S.M. Biros  
**202.** Series of rigid, bidentate ligands with varying degrees of hardness for the selective extraction of actinides from aqueous solutions. **J.A. Cunningham**, S.M. Biros

**203.** Synthesis and characterization of multidentate CMPO ligands for use in the complexation and extraction of f-elements. **A.R. Lear**, S.M. Biros  
**204.** Withdrawn.

**205.** Synthesis, characterization, and the near-infrared luminescence properties of Nd<sup>III</sup> and Yb<sup>III</sup> complexes containing terpyridine derivative ligand and 3d-4f type conjugated terpyridine-alkyne bridging Yb<sup>III</sup>-Co<sup>0</sup> carbonyl cluster complex. **B. Zhu**, Y. Liu, Y. Han

**206.** Effect of rotational correlation time and magnetic field strength on the

relaxivity of Eu(II)-containing complexes. **C.U. Lenora**, M.J. Allen  
**207.** Exploration of multifunctional behavior of a metallacrown 21-MC-7 species. **J.C. Lutter**, S.V. Eliseeva, J.W. Kampf, V.L. Pecoraro  
**208.** Carbazole-based coordination polymers of lanthanides and actinides. **C.E. Bien**, D.R. Manke  
**209.** Doped hydroxyapatite nanoparticles as scaffolds for multimodal imaging. **D. SantaLucia**, A. Washburn, L. Chapman, R. Tan, S. Lapi, **A.L. Eckermann**  
**210.** Electronic structure and thermodynamic studies of actinide and lanthanide complexation. **A. Dinescu**, T. Weaver

#### Section H

Boston Convention & Exhibition Center  
Hall C

#### Main Group Chemistry

T. W. Hudnall, *Organizer*

**6:00 - 8:00**

- 211.** Diels Alder cycloadditions catalyzed by aluminum based Lewis acids. **D. Vidovic**, Z. Liu  
**212.** Building a Lewis acidic phosphorus. **D. Vidovic**, M. Tay, D. Carmichael  
**213.** C-F bond activation by transient phosphonium dication. **D. Vidovic**, N. Dordevic, M. Tay, D. Dimic, S. Muthaiah  
**214.** Intramolecular P-C bond oxidation. **D. Vidovic**, G. Ilic  
**215.** Boron based nucleophilic ligands. **D. Vidovic**, B. Murugesapandian  
**216.** m-Terphenyl-stabilized boron (bis)triflates. **D. Vidovic**, D. Do, B. Tombling, S. Koo  
**217.** Preparative chemistry of potential B-N polymeric precursors. **K. Hauger**, J. Cui, R.H. Neilson  
**218.** Synthetic efforts toward diamidocarbene-supported terminal borylenes. **A. Ledet**, T.W. Hudnall  
**219.** Synthesis and characterization of carbene-stabilized arsenic(I) cations. **K.M. Melancon**, A.J. Torres, T.W. Hudnall  
**220.** Coordination of N-heterocyclic phosphonium (NHP) cations to late transition metals: NHPs as sterically and electronically tunable nitrosyl analogues. **M. Bezpalko**, C. Thomas  
**221.** 2-Trimethylsilylphosphinine derivatives: Synthesis, reactivity, and coordination chemistry. **M.H. Habicht**, C. Mueller  
**222.** Complete dehydrogenation of saturated BN-heterocycles. **Z. Giustra**, L. Chou, B. Li, D.A. Dixon, C. Tsung, S. Liu

#### MONDAY MORNING

#### Section A

Boston Convention & Exhibition Center  
Room 160A

#### Inorganic Chemistry Lectureship

W. B. Tolman, *Organizer, Presiding*  
**8:30** Introductory Remarks.

**8:35 223.** Semiconductor nanocrystals: Photophysics and technology. **M.G. Bawendi**

**9:05 224.** In situ phase transformation of colloidal nanocrystals. **P. Radovanovic**

**9:35 225.** Quantum dot-corrrole conjugates for optical oxygen sensing. **D.G. Nocera**, C. Lemon

**10:05** Intermission.

**10:20 226.** Determining band-edge potentials of colloidal quantum dots. **J.L. Dempsey**, K.J. Hammon, R.R. Knauf

**10:50 227.** Shining light on metal phosphide quantum dots: Understanding nucleation, growth, and photoluminescence enhancement. **B.M. Cossairt**, D. Gary, J. Stein

**11:20 228.** Doped semiconductor nanocrystals: An inorganic perspective. **D.R. Gamelin**

#### Section B

Boston Convention & Exhibition Center  
Room 159

#### Synthetic Chemistry Approaches to Magnetic Materials

D. Harris, E. E. Rodriguez, *Organizers*  
D. E. Freedman, *Organizer, Presiding*

**8:30 229.** New polar and magnetic corundum - type oxides, A2BB'O6:High pressure synthesis. **M.K. Greenblatt**, M. Li, M. Retuerto, Z. Deng, M. Croft, D. Vanderbilt, M. Ye, P.W. Stephens, J. Hadermann, D. Walker, J. Hemberger, C.P. Grams, C. Jin, W. Li, J.I. Jang, F.O. Saouma, V. Gopalan, H. Akamatsu

**9:00 230.** Nitrogen atom transfer for the assembly of magnetic molecules. M. Ding, H. Lin, M. Pink, Y. Lozovyj, C. Mathoniere, R. Clerac, **J.M. Smith**

**9:20 231.** Bottom-up approach to building layered iron chalcogenides for magnetism and superconductivity. X. Zhou, C. Borg, **E.E. Rodriguez**

**9:40 232.** New single-molecule magnets with high blocking temperatures. K.R. Meihaus, S. Demir, J. Zdrozny, P. Bunting, J.D. Rinehart, **J.R. Long**

**10:10** Intermission.

**10:20 233.** Accurate experimental determination of magnetic anisotropy for a rational design of single-molecule magnets. M. Perfetti, E. Lucaccini, G. Cucinotta, M. Serri, L. Sorace, **R. Sessoli**

**10:50 234.** Ca<sub>2</sub>Mn<sub>3</sub>O<sub>8</sub>: A new family of frustrated materials? **D.C. Arnold**

**11:10 235.** Strategies for room temperature multiferroic magnetoelectric oxides. **M.J. Rosseinsky**

**11:40 236.** Synthesis of benzoquinonoid radical-containing

materials with strong magnetic exchange coupling. I. Jeon, J. DeGayner, A. Gaudette, J. Park, A. Banisafar, A. Willis, **D. Harris**

#### Section C

Boston Convention & Exhibition Center  
Room 162B

#### Industrial Inorganic Chemistry: Innovation from Discovery to Applications

N. S. Radu, J. Walzer, *Organizers, Presiding*

**9:00** Introductory Remarks.

**9:05 237.** Development of high functioning, durable smart windows. **H. Turner**

**9:35 238.** Homoleptic iridium complexes of 1,2,4-riazolones as blue emitters for OLED solid-state lighting. **G.D. Vo**

**10:05 239.** Synthesis and reactivity of backfluorinated NHC carbene complexes. **R. Blanski**, R.H. Grubbs  
**10:35** Intermission.

**10:50 240.** Industrial water treatment chemistry. **C. McInnis**

**11:20 241.** Controlling ethylene/ $\alpha$ -olefin selectivity with molecular olefin polymerization catalysts. **J. Klosin**

**11:50 242.** Ethylene to 1-hexene: From HTE to continuous unit operations with cyclometallated pyridyl amine chromium catalysts. **S. Brown**, J.F. Walzer

#### Section D

Boston Convention & Exhibition Center  
Room 160C

#### Metalloenzyme Mechanisms

G. Ghirlanda, I. V. Korendovych, *Organizers, Presiding*

**8:30 243.** Controlling biological radical reactions: Lessons from radical SAM. **J.B. Broderick**, M. Horitani, A. Byer, K. Shisler, T. Chandra, B.M. Hoffman

**9:00 244.** Role of manganese in streptococcal virulence. **O. Makhlynets**, D. Rhodes, A.K. Boal, K. Crump, A.C. Rosenzweig, T. Kitten, J. Stubbe

**9:30 245.** De novo designed 2[4Fe-4S] ferredoxin mimics: Modulation of redox and ET properties. **G. Ghirlanda**, D.j. Sommer

**10:00** Intermission.

**10:10 246.** Spectroscopy of nitrogenase and CO – new spectroscopy of enzyme intermediates. **S.P. Cramer**, L.B. Gee, A. Scott, P. Nack-Lehman, C. Dapper, W. Newton

**10:40 247.** Discovery of a novel bacterial nitric oxide sensor. **E.M. Boon**

**11:10 248.** Snapshots of S-adenosylmethionine radical enzymes. **C.L. Drennan**

#### Section E

Boston Convention & Exhibition Center  
Room 161

#### Molecular Water Oxidation Catalysis

S. Bernhard, *Organizer*  
M. Albrecht, *Organizer, Presiding*

**8:00 249.** Iridium(III) bis-pyridine-2-sulfonamide complexes as efficient and durable catalysts for homogeneous water oxidation. **S. Bernhard**, M. Li, J.I. Goldsmith, K. Takada

**8:30 250.** Earth abundant metal-based catalysts for artificial photosynthesis. L. Tong, L. Kohler, R. Zong, R. Zhou, L. Wickramasinghe, A. Kopecky, **R.P. Thummel**

**9:00 251.** Crafting transition metal water oxidation catalysts. **A.D. Lobet**

**9:30 252.** In search for organic catalytic motifs for solar water splitting. **K. Glusac**

**10:00** Intermission.

**10:30 253.** Studies of the pathways open to copper water oxidation catalysts containing proximal hydroxy groups during basic electrocatalysis.

**D.L. Gerlach**, S. Bhagan, A. Cruce, M.K. Bowman, S. Pan, E.T. Papish

**11:00 254.** Molecular iron catalysts for water oxidation: Structural basis and reaction mechanism. **M. Costas**, Z. Codola, J. Lloret-Fillol, L. Gomez

**11:30 255.** Co-based molecular water oxidation catalysts. **K. Sakai**

#### Section F

Boston Convention & Exhibition Center  
Room 160B

#### Chemistry of Materials: Nanomaterials

C. G. Lugmair, *Organizer*  
M. M. Maye, P. Radovanovic, *Presiding*

**8:30 256.** Coordination complexes in carbon nanotube composites for chemiresistive sensing. **S. Liu**, L. Moh, G.T. Sazama, A.R. Petty, T.M. Swager

**8:50 257.** Fabrication of sub-cell size spiky nanoparticles for cancer cells destruction. **X. Xie**, D.G. Anderson, N.A. Melosh

**9:10 258.** Halide passivated colloidal PbS nanocrystals for application in hybrid solar cells. **H. Lu**, R.L. Brutchey

**9:30 259.** Using phase behavior and oxidation rates to control symmetry, composition, and internal microstructure in stainless nanomaterials. **M.M. Maye**, L. Pathade, T.L. Doane, P. Lutz, R.D. Slaton

**9:50 260.** Gold diazonium reduction on unusual substrates. I. Bakas, K. Jlassi, D. Aswal, M. Chehimi, M. El Naggar, I. Shehadi, **A. Mohamed**

**10:10 261.** Z-type ligand exchange at the surface of colloidal CdSe nanocrystals. **P.E. Chen**, J.S. Owen

**10:30** Intermission.

**10:40 262.** Sustained quenching of rotational diffusional motion of catalytic Janus colloids. **S. Das**, A. Garg, A. Campbell, D. Velegol, A. Sen, R. Golestanian, S. Ebbens

**11:00 263.** Mechano luminescence and aggregation induced emission of bromine and methoxy substituted naphthyl conjugated  $\beta$ -diketonate compounds. **T.P. Butler**, W.A. Morris, J. Samonina-Kosicka, C. Fraser

**11:20 264.** Centimeter long metallic nanowires: Superconductive properties and applications. **J.L. Bischof**, W. Zhao, T. Fitzgibbons, P.J. Sazio, M.H. Chan, J.V. Badding

**11:40 265.** Dendritic growth of Pd on Au nanocubes examined by in situ liquid cell scanning transmission electron microscopy. **R.G. Weiner**, D. Chen, R.R. Unocic, S.E. Skrabalak

**12:00 266.** Morphology-controlled synthesis of  $W_{18}O_{49}$  nanostructures for highly-efficient photocatalysis. **Z. Huang**, **J. Song**, **Z. Wang**, **X. Zhang**, **L. Pan**, **J. Zou**

**12:20 267.** Facile approach for the synthesis of sub-micron sized hollow and multiporous organosilica spheres. **M. Segers**, M. Sliepen, N. Arfsten, P. Buskens, M. Moller

#### Section G

Boston Convention & Exhibition Center  
Room 162A

#### Lanthanide and Actinide Chemistry

A. De Bettencourt Dias, *Organizer*  
E. Borbas, T. Sorensen, *Presiding*

**9:00 268.** Advanced microscopy applications of lanthanide centred emission. **T.J. Sorensen**

**9:20 269.** Zinc responsive MRI contrast agents for in vivo imaging. **A.F. Martins**, J. Yu, C. Preihls, V. Clavijo, P. Zhao, Y. Wu, A.D. Sherry

**9:40 270.** Tuning of the triplet-state energy of new highly luminescent Ln(III) complexes. **A. Duerrbeck**, A.T. Hor, N.J. Long

**10:00 271.** Development of volatile rare earth containing single-source precursors with proper metal ratios for low-temperature preparation of up- and down-conversion fluoride materials. **M.C. Barry**, Z. Wei, A.S. Filatov, E. Dikarev

**10:20** Intermission.

**10:30 272.** Synthesis and evaluation of a series of lanthanide chelates that act as T2ex MRI contrast agents. **I. Daryaee**, M. Moinpour, M. Pagel

**10:50 273.** Multiplex imaging with luminescent lanthanide complexes. **E. Borbas**

**11:10 274.** Molecular recognition of spermine by  $LnDOTP^{5-}$ : Toward a noninvasive staging of prostate cancer. **A.O. Olatunde**, L.L. Cheng, P.Z. Sun, P. Caravan

#### 2015 ACS Catalysis Lectureship

Sponsored by CATL, Cosponsored by INOR

#### Transition Metal Catalyzed Olefin Polymerization: Towards Structure Control

##### Technical Session

Sponsored by PMSE, Cosponsored by INOR<sup>2</sup>

#### MONDAY AFTERNOON

##### Section A

Boston Convention & Exhibition Center  
Room 162A

#### Building Innovative Solid State Materials Through Solution Chemistry

A. J. Norquist, *Organizer*  
J. R. Neilson, C. M. Oertel, *Organizers, Presiding*

**1:00 275.** Towards multicomponent chalcogenide aerogels: Effect of chalcogenide, capping agent, and crystal structure on the kinetics of assembly. **J. Davis**, S. Brock

**1:20 276.** Control over phase and plasmonic behavior of copper sulfide nanoparticles through solution chemistry. **K. Plass**

**1:50 277.** Atomic-scale derivatives of transition metal chalcogenides. **J.E. Goldberger**, T. Li, R. Morasse

**2:20 278.** Three-phase co-assembly: Tunable, highly-ordered, porous silica films for photonics and sensing applications. **J. Aizenberg**, I. Burgess, T. Shirman, K. Phillips, M. Duffy, N. Koay, T. Kay, G. England

**2:50 279.** Low temperature synthesis of (noncentrosymmetric) oxide-fluoride material. **K.R. Poeppelmeier**, K. Chang

**3:10** Intermission.

**3:20 280.** Functional nanostructured systems through solution chemistry. M. Aksit, **R.D. Robinson**

**3:50 281.** Towards magnetic or luminescent halide materials synthesized under hydrothermal conditions. **R. Gautier**

**4:10 282.** Photoelectrochemical characteristics of catalyst-modified  $WO_3$  and  $CuWO_4$  synthesized by solution-based methods. **B.M. Bartlett**, C.R. Lhermitte, J.G. Verwer

**4:30 283.** New ferrites from hydrofluxes: From zeolite to hexaferrite related structures. **H. Zur Loye**

**5:00 284.** Hybrid inorganic-organic materials with an aromatic cation and charge transfer:  $(C_7H_7)_2SnI_6$  and  $C_7H_7PbI_3$ . **A. Maughan**, J. Kurzman, J.R. Neilson

##### Section B

Boston Convention & Exhibition Center  
Room 159

#### Synthetic Chemistry Approaches to Magnetic Materials

D. E. Freedman, D. Harris, *Organizers*  
E. E. Rodriguez, *Organizer, Presiding*

**1:30 285.** Synthetic approaches to magnetically ordered organic-based magnets With  $T_c$ s as high as 400 K (127 °C) and coercive fields as high as 27,000 Oe. **J.S. Miller**

**2:00 286.** Magnetism in mixed-anion systems. **E. McCabe**, J.S. Evans, C. Stock

**2:20 287.** Strong exchange coupling in radical-bridged dlanthanide complexes. **S. Demir**, M. Gonzalez, J. Zadrozny, M. Nippe, J.R. Long

**2:40 288.** Synthetic routes to new homo- and heterometallic magnetic molecules and single-molecule magnets. **G. Christou**

**3:10** Intermission.

**3:20 289.** Modular molecular magnets: Investigation of coupling, anisotropy, and electronic factors on magnetic bistability. **K.R. Dunbar**

**3:50 290.** Application of coordination chemistry to the design and synthesis of molecular qubits. **J. Zadrozny**, J. Niklas, O. Poluektov, D.E. Freedman

**4:10 291.** Consideration of electronic structure in transition metal complexes for the design of MRI thermometers and magnets. **I. Jeon**, D. Harris

**4:30 292.** Synthetic approaches for high-blocking temperature single-molecule magnets. **M. Murugesu**

##### Section C

Boston Convention & Exhibition Center  
Room 162B

#### High-Energy Organometallic Complexes: Reactivity Driving New Synthesis and Catalysis

C. C. Cummins, M. R. Smith, *Organizers*  
R. Waterman, *Organizer, Presiding*

**1:30** Introductory Remarks.

**1:40 293.** Molecular Fe-mediated nitrogen fixation catalysis: Improving turnover and mechanistic insights. **J.C. Peters**, S.E. Creutz, T.J. Del Castillo, J. Rittle, N.B. Thompson

**2:00 294.** Chemical transformations with two-coordinate, first-row metal complexes. **T. Tilley**

**2:20 295.** New insights on electrochemically-promoted catalytic asymmetric hydrogenation. **B.T. Donovan-Merkert**

**2:40 296.** Photohydrides: Visible light-triggered hydride transfer as a strategy in catalysis. **A.J. Miller**, C.L. Pitman, S. Barrett, K.R. Brereton, S.A. Slattery

**3:00 297.** Small, but not so innocent, the redox non-innocence of multiply bonded ligands: Implications for catalysis. **T.R. Cundari**

**3:20** Intermission.

**3:30 298.** Investigation of the reactivity of low-coordinate Ni complexes stabilized by NHC ligands. **S.M. Baldwin**, S.A. Del Ciello, R. Witzke, J. Teesdale, G.L. Hillhouse

**3:50 299.** Mechanistic investigations of quantum dot nucleation and growth. M.P. Campos, L. Hamachi, M.P. Hendricks, I. Jen-La Plante, **J.S. Owen**

**4:10 300.** Modeling aspects of hydrodeoxygenation: C–O and C–C bond cleavage by electron-rich molybdenum and tungsten trimethylphosphine compounds. A. Sattler, A.A. Zuzek, D. Buccella, **G. Parkin**

**4:30 301.** Redox-active  $M[SNS]_2$  cofactors for heterobimetallic catalysts. **A.F. Heyduk**, K.E. Rosenkoetter, M. Wojnar, J.W. Ziller

**4:50 302.** Palladium complexes: An umpolung on transition metal carbenes. P. Cui, C.C. Comanescu, **V.M. Iluc**

##### Section D

Boston Convention & Exhibition Center  
Room 160C

#### Metalloprotein Inhibitors: Drugs, Drug Candidates, and New Targets at the Interface of Medicinal and Inorganic Chemistry

S. Cohen, Z. Sweeney, *Organizers, Presiding*

**1:30** Introductory Remarks.

**1:40 303.** Design and optimization of potent, selective fungal CYP51 inhibitors. **W.J. Hoekstra**, E. Garvey, C. Yates, R. Schotzinger

**2:15 304.** Specificity and regulation of metal-dependent deacetylases: Implications for biological function. **C.A. Fierke**, C.A. Pitcairn, B. Kim, E.D. Sullivan, N.A. Wolfson, J.E. Lopez

**2:50 305.** Structural studies on metal-binding pharmacophores for metalloprotein inhibitors. **S. Cohen**

**3:25** Intermission.

**3:35 306.** Novel inhibitors of iron and zinc-containing enzymes. **C. Schofield**

**4:10 307.** Drug discovery strategies toward a once daily HIV integrase strand transfer inhibitor. **A.M. Walji**

**4:45 308.** Recent advances in the development of influenza endonuclease inhibitors. **J. Bauman**, H. Sagong, D. Patel, S. Baker, R. Vijayan, A.K. Parhi, K. Das, L. Martinez-Sobrido, E. Arnold, E.J. LaVoie

##### Section E

Boston Convention & Exhibition Center  
Room 161

#### Molecular Water Oxidation Catalysis

M. Albrecht, *Organizer*  
S. Bernhard, *Organizer, Presiding*

**1:30 309.** Translating nature's principles of water oxidation to successful man-made catalysts. **G.C. Dismukes**, P. Smith, G. Gardner, C. Cady, K. Calvino, H. Chen, D.A. Case, M.K. Greenblatt

**2:00 310.** Layered calcium manganese oxides (birnessites) as bio-inspired water-oxidation catalysts. **P. Kurz**

**2:30 311.** Natural born catalysts: The great beauty of molecular photosynthesis. **M. Bonchio**  
**3:00 312.** Water oxidation with metal-organic frameworks. **W. Lin**  
**3:30** Intermission.  
**4:00 313.** Electrochemically driven water-oxidation catalysis beginning with cobalt-polyoxometalates: Determination of the true, homogeneous vs. heterogeneous catalyst. R.G. Finke, **S. Folkman**  
**4:30 314.** Bioinspired photochemical water oxidation with cobalt catalysts. **G.R. Patzke**, S. Lubner  
**5:00 315.** Low-temperature syntheses of amorphous mixed-metal oxide electrocatalysts. **C.P. Berlinguette**

Section F

Boston Convention & Exhibition Center  
Room 160B

**Chemistry of Materials: Materials for Energy and Catalytic Applications**

C. G. Lugmair, *Organizer*  
A. I. Carrillo Gomez, *Presiding*  
**1:30 316.** Examining the role of imidazolium ionic liquids in the proton-coupled electron transfer promoted conversion of CO<sub>2</sub> to CO on bismuth based materials. **J.L. DiMeglio**, J. Medina-Ramos, R.C. Puppillo, J. Rosenthal  
**1:50 317.** Mixed-metal nanosheet water oxidation catalysts made by pulsed-laser ablation in liquids – Part 1: Synthesis, characterization, and electrocatalysis. B.M. Hunter, J.D. Blakemore, H.B. Gray, J.R. Winkler, **A.M. Mueller**  
**2:10 318.** Hybrid luminescent mesoporous silica with catalytic properties. **A.I. Carrillo Gomez**, A. Lanterna, M.L. Marin, J. Scaiano, O. Reiser  
**2:30 319.** DFT study on a 2D,  $\pi$ -conjugated, nickel metallo-organic framework for ethylene purification. **S. Moncho Escriva**, E.N. Brothers, M.B. Hall  
**2:50 320.** Transition metal selenide nanostructures as highly efficient catalysts for oxygen evolution reaction. **A. Swesi**, **J. Masud**, M. Nath  
**3:10 321.** Design of silica-based hybrid catalysts and their application in alkane oxidation. **M. Yadav**, A.J. Karkamkar  
**3:30** Intermission.  
**3:40 322.** Mixed-metal nanosheet water oxidation catalysts made by pulsed-laser ablation in liquids – Part 2: Mechanistic insights gained by novel in-situ spectroscopies. **B.M. Hunter**, H.B. Gray, J.R. Winkler, A.M. Mueller  
**4:00 323.** Improving catalytic activity of copper-based inorganic materials for water oxidation. X. Liu, S. Cui, **P. Du**  
**4:20 324.** Metal organic frameworks as crystallized capping agent for metal

nanoparticle synthesis. **L. Chou**, A.P. Young, C. Tsung  
**4:40 325.** Flexible ion-conducting composite membranes for lithium batteries. **R.D. Miller**, S. Kitajima, C. Scott, K. Virwani, D. Bethune, H. Kim, L. Thompson, M. Reich, M. Schneider, W. Schmidbauer, M. Kunze, E. Jung, W. Wilcke, N. Aetukuri  
**5:00 326.** Electrochemically driven mechanical energy harvesting. **S. Kim**, S. Choi, K. Zhao, H. Yang, G. Gobbi, S. Zhang, J. Li  
**5:20 327.** Solution speciation and stability of cobalt-polyoxometalate water oxidation catalysts by X-ray scattering. **M.D. Nyman**, S. Goberna-Ferrón, J. Galan-Mascaros

Section G

Boston Convention & Exhibition Center  
Room 160A

**Bioinorganic Chemistry: Proteins and Enzymes and Model Systems**

S. A. Koch, *Organizer*  
M. I. Galinato, *Presiding*  
**1:30 328.** Fast unimolecular multiple-site CPET over a large temperature range. **M.A. Bowring**, L.R. Bradshaw, D.R. Gamelin, J.M. Mayer  
**1:50 329.** Effect of heme enzyme electronic structure modification on their nitrite reductase functionality. **M.I. Galinato**, E. Luteran  
**2:10 330.** Electronic and steric influence on the biomimetic copper(I)-nitro complexes. **S.C. Hsu**, Y. Chang, W. Chuang  
**2:30 331.** Biochemical characterization of enzymes involved in sulfur assimilation from dimethylsulfone. **D.K. Wicht**  
**2:50 332.** Superoxide dismutase mimicry by a zinc(II) complex with a redox-active organic ligand. **C.R. Goldsmith**, M. Yu, D.D. Schwartz, J.D. Gorden  
**3:10** Intermission.  
**3:20 333.** Imine-functionalized tris(pyrryl)amine ligands: A highly tunable platform for iron oxidation chemistry. **Z. Gordon**, A. Fout  
**3:40 334.** Modeling NO signaling: Reversible interaction of NO at a Copper(II) thiolate. **S. Zhang**, T.H. Warren  
**4:00 335.** Crystallographic studies of the immune-response, metal chelating protein calprotectin. **S.E. Bowman**, M. Baker, E.M. Nolan, C.L. Drennan  
**4:20 336.** Bioinspired aminopyridine transition-metal complexes derived from biperidine for epoxidation catalysis. **G. Yang**, S. Thompson, E.A. Mikhalyova, E. Rybak-Akimova  
**2015 ACS Catalysis Lectureship**  
Sponsored by CATL, Cosponsored by INOR

**Transition Metal Catalyzed Olefin Polymerization: Towards Structure Control**

**Technical Session**

Sponsored by PMSE, Cosponsored by INOR<sup>‡</sup>

**Undergraduate Research Posters Inorganic Chemistry**

Sponsored by CHED, Cosponsored by INOR and SOCED

**MONDAY EVENING**

Section A

Boston Convention & Exhibition Center  
Hall C

**Sci-Mix**

S. A. Koch, *Organizer*

**8:00 - 10:00**

**164, 166, 171, 174, 179, 183, 185, 196, 200, 211, 212.** See previous listings.

**337.** Characterization and reactivity of iron and cobalt bimetallic tris(phosphinoamide) complexes. **K.M. Gramigna**, S. Kuppaswamy, R. Mathialagan, C.M. Thomas

**338.** Lanthanide complexes for environmental and biological imaging. **P.S. Barber**, A.M. Mendez, S.L. Worters, A.M. McAdams, M. Cendejas, J.P. Guyot, L.D. Jaramillo

**497, 499, 500-502, 506, 514, 516, 524-525, 527, 532, 534-536, 540-542, 547, 550-551, 553-554, 560, 567, 573-576, 580-582, 584, 737, 741, 744-747, 750-751, 755, 759, 763, 765-766, 769, 773-776, 779-780, 786.** See Subsequent Listings.

**TUESDAY MORNING**

Section A

Boston Convention & Exhibition Center  
Room 157B

**Inorganic Nanoscience Award**

S. L. Stoll, *Organizer, Presiding*

**8:20** Introductory Remarks.

**8:30 339.** Solution-based synthesis and applications of multifunctional nanomaterials. **S.S. Wong**

**9:00 340.** Nature of the DNA bond.

**C.A. Mirkin**

**9:30 341.** Nanoelectronics meets biology: From new tools to electronic therapeutics. **C.M. Lieber**

**10:00 342.** Precise chemical, physical, and electronic nanoscale contacts. **P.S. Weiss**

**10:30** Intermission.

**10:45 343.** Zinc oxide nanocrucible arrays for magnetic nanodot synthesis via ALD-assisted block polymer lithography. **W.L. Gladfelter**, C. Lin, S. Polisetty, L. O'Brien, A. Baruth, M.A. Hillmyer, C. Leighton

**11:15 344.** Electrodeposited nanowire photonics. **R.M. Penner**

**11:45 345.** Modeling the effect of carbon nanotube functionalization on

mechanical and optical properties.

**G.C. Schatz**

**12:15** Concluding Remarks.

Section B

Boston Convention & Exhibition Center  
Room 159

**Synthetic Chemistry Approaches to Magnetic Materials**

D. E. Freedman, E. E. Rodriguez, *Organizers*

D. Harris, *Organizer, Presiding*

**8:30 346.** Magnetic properties of low-dimensional intermetallic materials.

**S.M. Clarke**, D.E. Freedman

**8:50 347.** Synthetic elucidation of design principles for long-lived electronic spin-based qubits. **M. Graham**, J. Zadrozny, M. Shiddiq, J.S. Anderson, M. Fataftah, S. Hill, D.E. Freedman

**9:10 348.** Synthetic strategies for manipulating magnetic properties in microporous manganese oxides. **A. Larson**, P. Motakef, E.E. Rodriguez

**9:30 349.** Superconducting CuSe<sub>2</sub> polymorph selection through kinetically-controlled solid-state metathesis. **A. Martinolich**, J. Kurzman, J.R. Neilson

Section C

Boston Convention & Exhibition Center  
Room 162B

**High-Energy Organometallic Complexes: Reactivity Driving New Synthesis and Catalysis**

M. R. Smith, R. Waterman, *Organizers*  
C. C. Cummins, *Organizer, Presiding*

**9:00 350.** Synthesis and reactivity of titanium nitrides. From dimers and monomers to discrete salts. **D.J. Mindiola**

**9:20 351.** New nickel(0) complexes supported by chelating N-heterocyclic carbene ligands: Unusual structures and small molecule activation. M. Reineke, M. Sampson, A.L. Rheingold, **C.P. Kubiak**

**9:40 352.** Metal nitrenes and amides in catalytic C-H functionalization. **T.H. Warren**

**10:00 353.** Transition-metal catalyzed reactions that form bonds to phosphorous. **R. Waterman**

**10:20 354.** Small molecule activation by low valent nickel complexes. **C.G. Riordan**

**10:40** Intermission.

**10:50 355.** Reduction chemistry of rare-earth metal complexes supported by ferrocene diamide ligands. **P. Diaconescu**

**11:10 356.** M-M interaction in low-valent Ni(II)-Ni(II) species and their use in small molecule activation. **F. Olechnowicz**, G.L. Hillhouse, R.F. Jordan

**11:30 357.** Tandem catalytic processes for light alkane upgrading and ethylene

polymerization. **J.E. Bercaw**, D.C. Leitch, A. Sattler, J.A. Labinger  
**11:50 358.** Generation of late metal imido and carbene fragments via cooperative reactions across metal-metal bonds in early/late heterobimetallics. **C.M. Thomas**, S.L. Marquard, B. Wu, J. Krogman, K.M. Gramigna

**12:10 359.** Characterization and reactivity of a series of macrocyclic cobalt-Mabiq compounds. **C. Hess**

**12:30 360.** When three's a crowd: Reactivity of low-coordinate Ni–NHC polyfluorometalacycles. **R. Baker**

#### Section D

Boston Convention & Exhibition Center  
Room 160C

### Environmental and Energy-Related Inorganic Chemistry

S. A. Koch, *Organizer*  
M. Emmert, *Presiding*

**8:00 361.** Structural requirements for interfacial proton-coupled electron transfer. **M. Jackson**, Y. Surendranath

**8:20 362.** Dinuclear cobalt(III) complexes as pH dependent catalysts for water oxidation and water reduction. **M. Youmans**, L. Doerr

**8:40 363.** Green chemistry design for rare earth recycling. **M. Emmert**

**9:00 364.** Activation of challenging C–O bonds through anion catalysis. **M. Emmert**

**9:20 365.** High-performance aqueous redox flow battery using nontoxic organic-inorganic electrolyte. **K. Lin**, Q. Chen, M.P. Marshak, M.R. Gerhardt, L. Tong, L. Eisenach, R.G. Gordon, M.J. Aziz

**9:40 366.** Photoelectrochemical characterization of non-innocent ligand ruthenium  $\beta$ -diketonate complexes in dye-sensitized solar cells. **N. Lee**, K. Ngo, G.E. Gilligan, A. Zachary, J.J. Rochford, M. Lamberto

**10:00** Intermission.

**10:10 367.** Selective carbon dioxide reduction on rhenium grafted to a glassy carbon surface. **S. Oh**, Y. Surendranath

**10:30 368.** Copper(II) bis-perfluoropinacolate complex for electrochemical reduction of nitrate in water. **S.F. Hannigan**, L. Doerr, L. Tahsini

**10:50 369.** Elucidating biological energy transduction from ammonia: Electronic structure studies of ammonia monooxygenase and hydroxylamine oxidoreductase. **K.M. Lancaster**, J. Caranto, M. Smith, A. Vilbert, R. Walroth

**11:10 370.** Effects of solvent on the ionic liquid mediated electrocatalytic conversion of CO<sub>2</sub> to CO at a Bi-based electrode. **T.P. Keane**, J.L. DiMeglio, J. Rosenthal

**11:30 371.** Investigating the interface between nanostructured black silicon and hydrogen-evolution reaction

catalysts: Mapping the semiconductor/metal junction. **N.C. Anderson**, J. Aguiar, N.R. Neale

**11:50 372.** Selective electrocatalytic CO<sub>2</sub> reduction by a polypyridyl–iron complex. **D.Z. Zee**, M. Nippe, A.E. King, C.J. Chang, J.R. Long

#### Section E

Boston Convention & Exhibition Center  
Room 161

### Molecular Water Oxidation Catalysis

M. Albrecht, *Organizer*

S. Bernhard, *Organizer, Presiding*

**8:30 373.** Cp\*Ir and Ir(CO)<sub>2</sub> precatalysts for water oxidation. **R.H. Crabtree**, G.W. Brudvig, U. Hintermair, J.D. Blakemore, D.M. Tiede, S.W. Sheehan, J. Thomsen, S. Hashmi, M. Zhou, D. Huang

**9:00 374.** In situ characterization of molecular water oxidation catalysts. **D. Hetterscheid**

**9:30 375.** From molecular-defined to nanostructured catalysts for water-splitting. **M. Beller**

**10:00** Intermission.

**10:30 376.** Computational models applied to homogeneous water oxidation catalysis: What's the value proposition? **C.J. Cramer**

**11:00 377.** Chemical and light-driven oxidation of water catalyzed by iridium complexes. **A. Macchioni**, A. Bucci, I. Corbucci, L. Fagiolari, G. Pastori, C. Zuccaccia

**11:30 378.** Molecular water oxidation catalysis with iridium triazolylidene complexes -- enhancing catalytic performance. **M. Albrecht**, A. Petronilho

#### Section F

Boston Convention & Exhibition Center  
Room 160B

### Chemistry of Materials: Metal Organic Frameworks

C. G. Lugmair, *Organizer*

R. S. Forgan, A. B. Thompson, *Presiding*

**8:30 379.** Kinetically tuned dimensional augmentation (KTDA) method to synthesize robust Fe-MOFs with various applications. **K. Wang**, H. Zhou

**8:50 380.** Synthesis, structure, magnetic and nonlinear optical (NLO) properties of Mn(II), Cu(II), and Ni(II) complexes of 3-(2-pyridyl)-5,6-diphenyl-1,2,4-triazine-4, 4'-disulfonate. **O.A. Odunola**, O.A. Ibrahim, E.O. Onawumi, M. Hong

**9:10 381.** Defect Engineered mixed valence Ru-MOFs: Study on the influence of defect metal sites. **W. Zhang**, M. Kauer, R. Wagner, D.J. Xiao, K. Epp, O. Kozachuk, Y. Wang, R.A. Fischer

**9:30 382.** Stability through flexibility: Mechanical properties of Zr and Hf

MOFs from single crystal techniques. **R.S. Forgan**, R. Marshall, C. Hobday, C. Morrison, T. Bennett, S. Moggach

**9:50 383.** Derivatives of MOF-5 via solvothermal and cation exchange techniques. **A.W. Stubbs**, C. Brozek, M. Dinca

**10:10** Intermission.

**10:20 384.** Synthesis of metal-organic materials (MOMs) using a microwave reactor. **C.V. Gauthier**, J.J. Flanagan

**10:40 385.** Synthesis of freestanding metal-organic-framework (MOF) aerogels. **Z. Liu**, W. Han, K.L. Yeung

**11:00 386.** Design and synthesis of metal-organic frameworks from bipyrazole ligands. **Q. Jia**, Q. Li

**11:20 387.** Grafting heterobimetallic complexes onto the metal organic framework NU-1000. **A.B. Thompson**, T. Wang, J.T. Hupp, O.K. Farha, R. Penn, A. Stein, C. Lu

**11:40 388.** Quantitative direct and indirect mapping of linker distributions in mixed linker MOFs via STEM-EDX. **C. Wiktor**, M. Meledina, S. Turner, G. van Tendeloo, R.A. Fischer

#### Section G

Boston Convention & Exhibition Center  
Room 160A

### Electrochemistry

B. L. Lucht, *Organizer, Presiding*

**8:30 389.** Optimizing the electrocatalytic reduction of CO<sub>2</sub> by Re- and Mn-based bipyridine complexes with supramolecular assembly. **C.W. Machan**, S.A. Chabolla, C.P. Kubiak

**8:50 390.** Low cost electrocatalysts with pendant functionality: The mechanism of enhanced electrocatalytic activity for CO<sub>2</sub> reduction. **G. Neri**, C. Wilson, J.J. Walsh, **A.J. Cowan**

**9:10 391.** Quinone electrochemistry in acidic and alkaline solutions and its application in large-scale energy storage. **M.R. Gerhardt**, Q. Chen, K. Lin, M.P. Marshak, L. Tong, C. Galvin, R.G. Gordon, M.J. Aziz

**9:30 392.** Graphene as a protective layer for silicon in an aqueous PEC cell. **A. Nielander**, N.S. Lewis

**9:50 393.** Mechanistic insights into proton coupled electron transfer activation of CO<sub>2</sub> catalyzed by pure metal surfaces. **A. Wuttig**, Y. Surendranath

**10:10 394.** Role of 1, 3-propane sultone and vinylene carbonate in solid electrolyte interface (SEI) formation and gas generation. **B. Zhang**, **B.L. Lucht**, M. Metzger, S. Solchenbach, H. Gasteiger, S. Meini

**10:30 395.** Improved performance of graphite/ LiNi<sub>0.5</sub>Mn<sub>1.5</sub>O<sub>4</sub> cells cycled to high voltage (4.8 V) with electrolyte additives. **Y. Dong**, **B.L. Lucht**, M. Xu, L. Zhou, F. Chesneau

#### Section H

Boston Convention & Exhibition Center  
Room 162A

### Chemistry of Materials: Synthesis and Properties

C. G. Lugmair, *Organizer*

P. J. Cappillino, *Presiding*

**8:30 396.** Anion sensing using a platinum(II) complex. **A.E. Norton**, J.A. Krause, W.B. Connick

**8:50 397.** Synthesis and characterization of tungsten nitrido precursors for deposition of WN<sub>x</sub>C<sub>y</sub> films. **A. Koley**, K. McClain, M. Nolan, C. O'Donohue, T. Anderson, L. McElwee-White

**9:10 398.** Effects of alpha substitution and strapped structure on the mechanochromic luminescence and aggregation-induced emission behavior of difluoroboron  $\beta$ -diketonate dyes. **W.A. Morris**

**9:30 399.** Effect of nitrate concentration on the properties of solution-processed Al<sub>2</sub>O<sub>3</sub> thin films. **C. Perkins**, J.C. Ramos, D. Park, B. Fulton, D.W. Johnson, D.A. Keszler

**9:50 400.** Synthesis of nanostructured, bimetallic, noble metal powders using Atomic Layer Electroless Deposition (ALED). **P.J. Cappillino**, J.D. Sugar, F. el Gabaly, T.Y. Cai, Z. Liu, J.L. Stickney, D.B. Robinson

**10:10 401.** InP quantum dots with tunable emission by post-synthetic modification with Lewis acids. **J. Stein**, B. Cossairt

**10:30** Intermission.

**10:40 402.** Supercritical fluid electrodeposition of germanium. **P. Bartlett**, C. Cummings, M. Hasan, A.L. Hector, W. Levason, **D. Pugh**, G. Reid, D. Smith, J. Spencer

**11:00 403.** Porous carbon coated metal nanoparticles for electrocatalysis. **M. Sheehan**, M. Rudden, C. Tsung

**11:20 404.** Dual electrically conducting spin-crossover bifunctional molecular materials based on cobalt-TCNQ radical salts. **X. Zhang**, Z. Wang, H. Xie, K.R. Dunbar

**11:40 405.** Smectic A mesophases from luminescent sandic platinum(II) mesogens. **M. Krikorian**, C. Voll, M. Yoon, K. Venkatesan, T.M. Swager

**12:00 406.** Two synthetic systems of nonlinear optical crystals with disparate phase matchabilities. **M.D. Donakowski**, H. Lu, R. Gautier, K.R. Poeppelmeier

**12:20 407.** Addressing challenges in nanocrystal synthesis using substituted thiourea and selenourea precursors. **M.P. Campos**, M.P. Hendricks, L. Hamachi, I. Jen-La Plante, R. Swain, G. Cleveland, A. Graham, J.S. Owen

#### Section I

Boston Convention & Exhibition Center  
Room 158

### Organometallic Chemistry: Synthesis and Characterization



N. S. Radu, *Organizer*  
G. L. Powell, *Presiding*

**8:30 408.** Stabilizing unusual oxidation state of heterometallic complexes by coordination of low valent group 13 organyls ECp\* (E = Al, Ga, In). **J. Kim**, C. Gemel, R.A. Fischer

**8:50 409.** Bis-cyclometalated iridium complexes supported by  $\beta$ -ketiminate (acNac) and  $\beta$ -diketiminato (NacNac) ligands. **T.S. Teets**, A. Maity, Y. Radwan

**9:10 410.** Synthesis and reactivity of PBP-type pincer iridium and rhodium complexes. **W. Shih**, W. Gu, M.C. MacInnis, O. Ozerov

**9:30 411.** Aqueous hydride transfer thermodynamics of a bimetallic iridium ruthenium complex. **K.R. Breerton**, C.L. Pitman, A.J. Miller

**9:50** Intermission.

**9:55 412.** Synthesis, characterization, and reactivity of a novel Ru(0)-NHCP complex. T. Wang, L. Pan, E. Mosafari, D.W. Stephan

**10:15 413.** Multinuclear osmium carbonyl complexes with dicarboxylate ligands. **G.L. Powell**

**10:35 414.** Understanding electronic structure requirements for iron-catalyzed C-H bond hydroxylation. **C. Kleinlein**, T. Betley

**10:55 415.** Electronic effects of pincer-type N-heterocyclic carbene iron complexes and exploration of their catalytic applications. **J.L. Drake**, H.Z. Kaplan, M.J. Wilding, A. Vasilopoulos, C. Wolstenholme, S. Daifuku, B. Li, M.L. Neidig, J.A. Byers

**11:15 416.** New paramagnetic rhodium(II) dimers without Rh-Rh bonds. **D. Zhu**, P. Budzelaar

Section J

Boston Convention & Exhibition Center  
Room 157C

### Inorganic Spectroscopy

S. A. Koch, *Organizer*  
I. S. Butler, *Presiding*

**9:00 417.** Variable-temperature and high-pressure Raman spectra of the group 8 metallocenes  $(\eta^5\text{-C}_5\text{H}_5)_2\text{M}$  (M = Fe, Ru, Os). **I.S. Butler**, Y. Desjardins-Langlais

**9:20 418.** Two-photon absorption spectroscopy of inorganic compounds. **K. Takematsu**, S. Wehlin, W. Sattler, J.R. Winkler, H.B. Gray

**9:40 419.** Spectroscopic monitoring of proton transfer and proton-coupled electron transfer reactions. **T.T. Eisenhart**, W.C. Howland, J.C. Lennox, J.L. Dempsey

**10:00** Intermission.

**10:10 420.** Electronic coupling studies in quadruply bonded Mo<sub>2</sub> and W<sub>2</sub> complexes. **C. Ziehm**, M.H. Chisholm

**10:30 421.** Electronic and spectroscopic properties of avobenzene derivatives attached to M<sub>2</sub> quadruple

bonds (M = Mo and W). M.H. Chisholm, C.B. Durr, T.L. Gustafson, **W. Kender**, T. Spilker, P.J. Young

**10:50 422.** Probing molecular magnetism by inelastic neutron scattering. **S.E. Stavretis**, S. Hunter, A.A. Podlesnyak, L. Chen, X. Chen, **Z. Xue**

### 2015 ACS Catalysis Lectureship

Sponsored by CATL, Cosponsored by INOR

### International Entrepreneurship: How To Start a Business and Thrive in the Global Marketplace

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### Transition Metal Catalyzed Olefin Polymerization: Towards Structure Control

Sponsored by PMSE, Cosponsored by INOR<sup>2</sup>

### Technical Session

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### TUESDAY AFTERNOON

Section B

Boston Convention & Exhibition Center  
Room 159

### Organometallic Chemistry: Applications to Materials and Polymer Science

N. S. Radu, *Organizer*  
J. A. Byers, *Presiding*

**1:30 423.** On the mechanism of the regio- and stereoselective cyclopolymerization of 1,6-hepta- and 1,7-octadiynes by mo-imido alkylidene N-heterocyclic carbene catalyst. **M. Buchmeiser**, K. Herz, J. Haenle, W. Frey

**1:50 424.** Withdrawn.

**2:10 425.** Mechanistic insights into the stereoselective ring opening polymerization of poly(lactic acid) catalyzed by achiral iron(II) based complexes. **A. Kaur**, C.M. Manna, F. Haeffner, J.A. Byers

**2:30 426.** Controlling stereochemistry, architecture, and composition in ring opening polymerization reactions using a versatile iron-based catalyst. **J.A. Byers**, A.B. Biernesser, K.R. Delle Chiaie, A. Kaur, J.A. Kehl, J.B. Curley

**2:50 427.** Hysteretic adsorption of CO<sub>2</sub> onto a Cu<sub>2</sub>(pzdc)<sub>2</sub>(bpy) porous coordination polymer and concomitant framework distortion. **K. Riascos-Rodríguez**, A.J. Schroeder, M.R. Arend, P.G. Evans, A.J. Hernandez-Maldonado

**3:10 428.** General mechanism for the synthesis of group II-VI and IV-VI nanocrystals. **H. Liu**, R. García-Rodríguez

Section C

Boston Convention & Exhibition Center  
Room 162B

### High-Energy Organometallic Complexes: Reactivity Driving New Synthesis and Catalysis

C. C. Cummins, R. Waterman, *Organizers*

M. R. Smith, *Organizer, Presiding*

**1:30 429.** Self-assembled multinuclear palladium catalysts for olefin polymerization. **R.F. Jordan**, J. Wei

**1:50 430.** Secondary coordination sphere effects promote chlorine photoelimination from monomeric Ni(III) complexes. **D.G. Nocera**, B. Anderson, S. Hwang, D.C. Powers, A. Maher, R. Hadt

**2:10 431.** Importance of making molecules in catalysis. **M.R. Smith**

**2:30 432.** Gold diazomethyl and gold ketenylidene clusters: Reactive carbide precursors? **J.P. Sadighi**, N.T. Daugherty, J. Bacsa

**2:50 433.** Electronic and reactivity effects of N-heterocyclic carbene and functionalized diphosphine ligands on tungsten-benzylidyne complexes. **C. Hansen**, M.D. Hopkins

**3:10** Intermission.

**3:20 434.** Reactivity of nitrene/imido complexes of {bis-(1-N(DIPP),2-phenyl)diimine}M (1-M; M = Ti, Cr, Fe). **P.T. Wolczanski**, S.P. Heins, W.D. Morris, E.B. Lobkovsky, T. Cundari

**3:40 435.** New rhodium complexes for the activation and functionalization of strong bonds. **T.B. Gunnoe**, W.A. Goddard, T. Cundari, R.J. Nielsen, M.S. Webster-Gardiner, M.E. O'Reilly, B.A. Vaughan, R. Fu, D. Pahls, M. Sabat

**4:00 436.** Joys of nickel(0) chemistry: C–CN bond activation of aromatic nitriles, h<sup>2</sup>-arene intermediates, and the effect of Lewis acids. **W.D. Jones**, T. Li, J.J. Garcia, B.D. Swartz

**4:20 437.** High-energy organometallics featuring encumbering isocyanides. **J.S. Figueroa**, C.C. Mokhtarzadeh, A. Carpenter

**4:40 438.** Macrobicyclic hexacarboxamide cryptand coordination chemistry. J. Stauber, E.D. Bloch, **C.C. Cummins**, D.G. Nocera, K.D. Vogiatzis, L. Gagliardi

**5:00** Concluding Remarks.

Section D

Boston Convention & Exhibition Center  
Room 160C

### Coordination Chemistry Macrocycles and More

D. C. Crans, *Organizer*  
E. Rybak-Akimova, *Presiding*

**2:00** Introductory Remarks.

**2:05 439.** From reversible oxygen binding with synthetic macrocycles to oxygen activation and catalytic oxidations. **E. Rybak-Akimova**

**2:25 440.** Not so sticky side of sugars: Metal complexes interaction with monosaccharides in aqueous media.

**G.T. Musie**, C. Stewart, M.A. Pedraza, H. Arman

**2:45 441.** Rhenium chalcogenide clusters containing N-heterocyclic carbene ligands. **L.F. Szczepura**, W. Wilson, D. Huh

**3:05 442.** Imaging gene expression in mammals: A coordination chemistry solution. **T.J. Meade**, S.M. Kamper

**3:30 443.** Macrocyclic metal complexes designed for enhanced protein binding: Biological activity and molecular imaging. B. Burke, G. Clemente, C. Cawthorne, **S.J. Archibald**

**3:55 444.** Reprogramming EF-hands for design of catalytically amplified lanthanide sensors. **I.V. Korendovych**, K. Mack, O. Moroz, Y. Moroz, A. Olsen, J. McLaughlin

**4:15 445.** Heterobimetallic complexes: Structure and function. **A. Borovik**

**4:40 446.** Glimpses into the power of synthetic macrocycles in transition metal and supramolecular coordination chemistry. **K. Bowman-James**

Section E

Boston Convention & Exhibition Center  
Room 161

### Bioinorganic Chemistry: Proteins and Enzymes and Model Systems

S. A. Koch, *Organizer*

D. Rokhsana, D. K. Wicht, *Presiding*

**1:30 447.** Mimicking [FeFe] hydrogenase by covalent linkage of a synthetic diiron cluster to polymer scaffolds. **C.A. Tooley**, E.B. Berda, S. Pazicni

**1:50 448.** Lewis acid-induced valence tautomerism of a manganese(V)-oxo porphyrinoid complex results in dramatic inhibition of oxygen atom transfer reactivity. **J. Zaragoza**, R.A. Baglia, M. Siegler, D.P. Goldberg

**2:10 449.** Streptavidin artificial metalloproteins for asymmetric catalysis. **C. Chen**, C. Chang, C. Yang, S.C. Hsu, J. Carey

**2:30 450.** Porphyrin-containing polymer nanoparticles for modeling heme proteins iron coordination. **K. Rodríguez**, S. Pazicni

**2:50 451.** Constrained peptides: Investigating metal binding and catalytic activity. **A.R. Aldous**, K.P. Neupane, M.R. Eshelman, J. Kritzer

**3:10** Intermission.

**3:20 452.** Old cofactor in a new light: Adenosylcobalamin in light-dependent gene regulation. **M. Jost**, S. Padmanabhan, M. Elias-Arnanz, C.L. Drennan

**3:40 453.** Insights from QM and QM/MM models of carbon monoxide dehydrogenase containing a unique Mo-Cu center. **D. Rokhsana**, T. Large, M. Dienst, M. Retegan, F. Neese

**4:00 454.** Geometrical and electronic structure of the nitrosyl adduct of the non-heme iron active site in anthranilate 1,2-dioxygenase revealed through <sup>14,15</sup>N and <sup>1,2</sup>H ENDOR spectroscopy. **V. Hoeke**, D.M. Kurtz, B.M. Hoffman

**4:20 455.** Functional bioinorganic peptide assemblies. **H.C. Fry**, L.A. Solomon

**4:40 456.** Spontaneous carbon dioxide activation by bimetallic nickel complexes. **F. Möller**, **U. Apfel**

Section F

Boston Convention & Exhibition Center  
Room 160B

### Chemistry of Materials: Metal Organic Frameworks

C. G. Lugmair, *Organizer*  
J. A. Byers, C. R. Wade, *Presiding*

**1:30 457.** Variable-temperature in situ powder X-ray diffraction monitoring of mechanosynthesis of metal-organic frameworks. **K. Uzarevic**, I. Halasz, C. Mottillo, A. Puškarić, P. Julien, V. Štrukil, T. Friscic

**1:50 458.** Synthesis of nanoscale zirconium porphyrin MOFs for biomedical applications. **M. Kelty**, W. Morris, D. Harris

**2:10 459.** Molecular encapsulation beyond the aperture size limit in metal-organic framework crystals. **C. Tsung**

**2:30 460.** In situ monitoring of a mechanochemical reaction reveals a metastable polymorph of the archetypal framework ZIF-8. **A.D. Katsenik**, A. Puškarić, C. Mottillo, P. Julien, K. Uzarevic, S.A. Kimber, P. Lazić, R. Dinnebier, I. Halasz, T. Friscic

**2:50 461.** Mechanochemistry: An excellent approach to bulk, clean and high-yielding synthesis of metal-organic frameworks. **T. Friscic**

**3:10** Intermission.

**3:20 462.** Mechanistic features of linker exchange in ZIF-8 and UiO-66. **J.A. Byers**, C. Tsung, J.V. Morabito, Z. Li, R. Kyada, M. Nero

**3:40 463.** polyMOFs: A new class of interconvertible polymer-MOF hybrid materials. **Z. Zhang**, S. Cohen

**4:00 464.** Metal-organic framework supported pincer complexes: At the interface of homogeneous and heterogeneous catalysis. **C.R. Wade**, S.A. Burgess, S. Baranowski

**4:20 465.** Basic post-synthetic modification approach of Cr derived metal-organic frameworks (MIL-101) for the efficient promotion of Knoevenagel condensation reaction. **Y. Luan**

**4:40 466.** Metal-organic frameworks as platform to arrange and protect single-molecule magnets in multidimensional arrays. **M. Wriedt**, D. Aulakh, J.B. Pysier

Section G

Boston Convention & Exhibition Center  
Room 160A

### Organometallic Chemistry: Catalysis

N. S. Radu, *Organizer*  
M. Buchmeiser, *Presiding*

**1:30 467.** New methods for the construction of highly-encumbered C–C bonds using a simple cobalt catalyst. **M.R. Brennan**, A. Fout

**1:50 468.** New molecular ruthenium and iron electrocatalysts for the reduction of carbon dioxide. **C.W. Machan**, M.D. Sampson, C.P. Kubiak

**2:10 469.** Molybdenum and tungsten imido alkylidene N-heterocyclic carbene complexes: Activity, immobilization, and functional group tolerance in olefin metathesis. **M. Buchmeiser**, S. Sen, R. Schowner, D. Imbrich, W. Frey

**2:30 470.** Challenges in optimizing alkyne metathesis catalysts. **Ö. Arias i Burguera**, K. Brandhorst, M. Freytag, P.G. Jones, M. Tamm

**2:50 471.** Molecular iridium complexes for applied water oxidation electrocatalysis. **S.W. Sheehan**, U. Hintermair, J. Thomsen, G.W. Brudvig, R.H. Crabtree, C.A. Schmuttenmaer

**3:10** Intermission.

**3:20 472.** Insights into redox cooperativity between cocatalysts: Mechanistic studies of aerobic alcohol oxidation by Cu and redox-active organic cocatalysts. **S.D. McCann**, S.S. Stahl

**3:40 473.** Homogeneous catalysis for signal enhancement in NMR: From catalyst design to analytical applications. **B. van Weerdenburg**, N. Eshuis, N. Herkmens, S. Wijmenga, M. Tessari, M. Feiters, F.P. Rutjes

**4:00 474.** (NHC)<sub>2</sub>Pd(0)-catalyzed *cis*-bis-silylations of internal alkynes with unactivated disilanes. **O. Navarro**, J. Spencer, M.B. Ansell, G. Cloke, M. Roe

**4:20 475.** Hydrosilylation of internal C–C multiple bonds – insights on mechanism and kinetics. **T.K. Zimmermann**, K. Riemer, F.E. Kuehn

**4:40 476.** Metal-ligand multiple bonds in iron complexes competent for ppm-loading C–H amination. **M.J. Wilding**, T. Betley

**5:00 477.** Ring-opening polymerization of lactides and lactones by an indium alkoxide salen complex. **S. Quan**, P. Diaconescu

Section H

Boston Convention & Exhibition Center  
Room 157C

### Organometallic Chemistry: Applications to Organic Transformations

N. S. Radu, *Organizer*  
C. T. O'Hara, *Presiding*

**1:30 478.** Iron catalyzed  $\alpha$ -C–H oxidation of tertiary amines inspired by cytochrome P450. **C.J. Legacy**

**1:50 479.** Developing a complementary metalation strategy to directed *ortho*-metalation: Directed *meta-meta'*-dimetalations of polyaromatics. **C.T. O'Hara**, A. Martinez-Martinez, R.E. Mulvey

**2:10 480.** Template base directed metallations in arene and metallocene chemistry. **R.E. Mulvey**, C.T. O'Hara

**2:30 481.** Competitive C–N and C–O reductive elimination from an isolated Pd(IV) hydroxo alkyl amido complex. **E. Abada**, A.N. Vedernikov

**2:50** Intermission.

**3:00 482.** PCN pincer complexes of Pd<sup>II</sup>: Hydrogenolysis of mono- and dinuclear hydroxides. **W.D. Bailey**, L. Luconi, A. Rossin, S.E. Flowers, W. Kaminsky, R.A. Kemp, G. Giambastiani, K.I. Goldberg

**3:20 483.** Catalysis with low-valent cobalt bis(carbene) pincer complexes. **A. Ibrahim**, A. Fout

**3:40 484.** In the quest for new highly active and versatile catalysts for Pd-catalyzed allylic substitution reactions. **O. Pamies**, M. Diéguez

**4:00 485.** Photoredox catalytic trifluoromethylation of non-prefunctionalized alkenes and heterocycles using cyclometalated Pt(II) complexes. **Y. You**

**4:20 486.** Mechanistic details for the acceptorless dehydrogenation of primary amines to nitriles with Ru-[NNN] pincer complexes. **L. Hale**, N.K. Szymczak, T. Malakar, A. Paul

**4:40 487.** Mechanistic studies on the reductive elimination of C(sp<sup>3</sup>)-X bonds from Rh<sup>III</sup>. **T. Stevens**, K.I. Goldberg

Section I

Boston Convention & Exhibition Center  
Room 158

### Organometallic Chemistry: Synthesis and Characterization

N. S. Radu, *Organizer*  
C. R. Wade, *Presiding*

**1:30 488.** Intermetallic transition metal-group 13 clusters: A novel approach on molecular congeners of Hume-Rothery phases. **J. Wessing**, C. Ganesamoorthy, C. Gemel, R.A. Fischer

**1:50 489.** Nickel complexes supported by a monoanionic bis(carbene) ligand: Reactivity and accessibility of higher oxidation states. **G. Espinosa**

**Martinez**, A. Fout

**2:10** Intermission.

**2:15 490.** Characterization of iron imido species relevant to *N*-group transfer chemistry. **D. Iovan**, T. Betley

**2:35 491.** Development of binuclear gold complexes for reductive coupling. **B. Reiner**, C.R. Wade

**2:55 492.** Synthesis of group VI carbonyl species bearing bis-tetrazinyl

pyridine (btzp) ligand. **N.A. Maculis**, S.M. Curtis, C. Chen

**3:15 493.** Alkene and alkyne activation in a bisphosphine monoxide gold(I) complex. **C. Hahn**

**3:35 494.** Synthesis and characterization of heptacoordinate amidinate complexes. **T. Callaway**, Z. Xue

**3:55 495.** Actinide metal fluorides: Synthesis, characterization, and chemistry. **A.G. Lichtscheidl**, M.J. Monreal, K. Browne, D.E. Morris, B. Scott, A.T. Nelson, J.L. Kiplinger

### International Entrepreneurship: How To Start a Business and Thrive in the Global Marketplace

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### TUESDAY EVENING

Section A

Boston Convention & Exhibition Center  
Hall C

### Chemistry of Materials

C. G. Lugmair, *Organizer*

**6:00 - 8:00**

**496.** Synthetic approaches to iron selenide nanostructures. **S.E. Ingram**, S.L. Stoll

**497.** Effects of calcination on rutile white pigment via short sulfate process. **C. Tian**

**498.** Tryptophan as fluorescent guest in metal-organic framework. **N. Fedorka**, B. Yan

**499.** Precursor synthesis and atomic layer deposition of CoO<sub>x</sub> thin films. **J. Kim**, R.A. Fischer, A. Devi

**500.** Mechanochromic luminescence and mechanochromic luminescence quenching of iodine-substituted difluoroboron  $\beta$ -diketonate dyes with varying alkyl chain lengths. **W.A. Morris**

**501.** Superacidic mesoporous materials. **A. Vasiliev**, O. Adetola

**502.** Pattern formation observed during the flow-driven precipitation of calcium oxalate and calcium carbonate. **B. Bohner**, G. Schuszter, D. Horvath, A. Toth

**503.** Multicomponent metal-organic frameworks and their controlled defect structures. **S.J. Lee**, L. Liu, **J.J. Pak**, S.G. Telfer

**504.** Oxygen reduction reaction using MnO<sub>2</sub> and ordered mesoporous carbon composites as electrocatalysts for Li–O<sub>2</sub> battery applications. **J. Chen**, C. Chin, H. Yang

**505.** Synthesis of novel PEG-2000/Fe-MIL-101 composite phase change material and study of its thermal properties. **Y. Qi**, Y. Luan, M. Yang, G. Wang

**506.** Tuning non-covalent interactions between substituted

subphthalocyanines with C<sub>60</sub> and C<sub>70</sub> fullerenes. **H.M. Rhoda**, M. Kayser, Y. Wang, A.Y. Nazarenko, R. Belosludov, P. Kiprof, D.A. Blank, V. Nemykin

**507.** Carbonized metal organic frameworks for electrocatalysis and electrochemical energy storage. **M. Sheehan**, H. Cai, C. Tsung

**508.** Synthesis of functionalized of Co- and Zn-dipyrazolate metal-organic frameworks. **S.O. Gunther**, C.R. Wade

**509.** Synthesis of novel porous coordination polymer material for smart antenna application. **H. Wang**

**510.** Mechanical and thermal properties study of silica aerogel insulation material and its property prediction using big data. **H. Wang**

**511.** Magnetic behavior of conductive 2D metal-organic frameworks. **T. Soejima**, M.G. Campbell, M. Dinca

**512.** General approach to robust, freestanding MOF-polymer composite membranes. **M.S. Denny**

**513.** Palladium detection and sorption by sulfur-laced MOFs: Implications for heterogeneous catalysis and nuclear wastes. **Z. Xu**, M. Zha, J. Liu

**514.** Graphene-polypyrrole composite materials as counter electrodes in dye sensitised solar cells. **K. Devarepaly**

**515.** Size dependence of metal-insulator transition in stoichiometric Fe<sub>3</sub>O<sub>4</sub> nanocrystals. **J. Lee**, T. Hyeon

Section B

Boston Convention & Exhibition Center  
Hall C

### Coordination Chemistry: Characterization and Applications

D. C. Crans, *Organizer*

6:00 - 8:00

**516.** Calixarene compounds and their use as molecular materials. J.F. Ferreira, **I.A. Bagatin**

**517.** Terpyridine-based metal complexes incorporating secondary sphere hydrogen bonding. **E.W. Dahl**, N.K. Szymczak

**518.** Characterization of oxometalates interactions with interfaces. **I. Sanchez Lombardo**, S. Alvarez, K.R. Werst, N.A. Segaline, N.E. Levinger, D.C. Crans

**519.** Bipyridine-supported zinc flavonolate photoCORMs. **M. Popova**, S.A. Sorenson, A. Arif, L.M. Berreau

**520.** Further explorations in Cu-O<sub>2</sub> interactions with perfluorinated O-donor ligands. **S. Neville**, L. Doerren

**521.** Spontaneous thermal dispersion of LiCl in [Zn(bdc)(ted)<sub>0.5</sub>]: A study of structural changes and pure component equilibrium adsorption of carbon dioxide, methane, and hydrogen. **G. Mass-Gonzalez**, J. Guerrero-Medina, L. Pacheco-Londoño, S.P. Hernandez-Rivera, R. Fu, A.J. Hernandez-Maldonado

**522.** Single-ion magnetic properties in a new heterobimetallic complex. **M. Ding**, M. Pink, R. Clerac, Y. Lozovyy, J.M. Smith

**523.** Chemical tools for detecting Mn<sup>2+</sup> in live cells. **S. Bakthavatsalam**, A. Sarkar, A. Rakshit, A. Datta

**524.** Metalloporphyrin-based dual mode colorimetric sensors. **D.J. Miller**, M.J. Gunsch, K.A. Leamy, C.L. Bablin, L.J. Tucker, J.L. O'Donnell

**525.** Non-toxic and water-soluble CO-releasing molecule for medicinal applications. **R. Mede**, M. Klein, H. Görls, G. Gessner, R. Claus, M. Schmitt, M. Bauer, S. Heinemann, J. Popp, M. Westerhausen

**526.** Luminescent lanthanide complexes containing Schiff base ligands. C. Lau, **P.K. Yuen**

**527.** Synthesis and characterization of novel nickel complexes and their application in electrocatalysis. **S. Sobottka**, M. van der Meer, B. Sarkar

Section B

Boston Convention & Exhibition Center  
Hall C

### Coordination Chemistry: Synthesis and Characterization

D. C. Crans, *Organizer*

6:00 - 8:00

**528.** Fe(II), Co(II), and Ni(II) complexes of macrocycles with benzimidazole and imidazole pendants for ParaCEST MRI applications. **P.J. Burns**, P.B. Tsitovich, A. Olatunde, J.R. Morrow

**529.** Assignment of <sup>1</sup>H resonances in *cis*-(dichloro)ruthenium(II) complexes containing bidentate heterocyclic ligands based on 2,2'-bipyridine. **D. Rillema**, H. Nguyen

**530.** Varying binding mode and electronic structural aspects of ruthenium coordinated Nindigo ligand. **P. Mondal**

**531.** Coordination chemistry of sulfur and selenium oxidized derivatives of tris(2-pyridyl)phosphine with select lanthanide salts. **A.R. Bevan**, C. Fairfield, A.K. Frampton, D. Pericic, N.A. Piro, W.S. Kassel

**532.** Synthesis, characterization, and the coordination chemistry with select lanthanide nitrates of di(2-pyridinyl)phenylphosphonate and oxide derivatives. **C. Fairfield**, D. Pericic, A.K. Frampton, N.A. Piro, W.S. Kassel

**533.** Synthesis, characterization, and coordination chemistry of tris(3,5-dimethylpyrazolyl)phosphine oxide and bis(3,5-dimethylpyrazolyl)phenylphosphine oxide. **A.K. Frampton**, D. Pericic, C. Fairfield, W.G. Dougherty, N.A. Piro, W.S. Kassel

**534.** Synthesis and characterization of novel Cu(I) and Ag(I) azolate/phenanthroline and azolate/terpyridine complexes. **A.R.**

**Hinkle**, A. Siller, K. Reyes, T. Nguyen, M. Omary

**535.** Synthesis, characterization, and reactivity of Cl-Nb(<sup>i</sup>PrNPh<sub>2</sub>P)<sub>3</sub>M-Br complexes (M = Co, Fe). **G. Culcu**, C. Thomas

**536.** Novel ruthenium(II) complexes with polythiamacrocycles. **A.Y. Nazarenko**, E. Rybak-Akimova

**537.** Induction of E/Z azobenzene isomerization as a pendant moiety of Re(CO)<sub>3</sub> diimine complexes. **A. Hasheminasab**, L. Wang, M. Dawadi, R.S. Herrick, J. Rack, C.J. Ziegler

**538.** Intermolecular nucleophilic attack to coordinated 1,10-phenanthroline. **J.A. Perez**, R. Arevalo, L. Riera

**539.** Mid- to late- transition metal complexes with a new NNN pincer ligand. **H. Lin**, S. Nguyen, W. Lee

**540.** Mimicking the secondary coordination sphere of metalloproteins using a pyrrole-imine ligand scaffold. **M.J. Drummond**, Z. Gordon, A. Fout

**541.** Synthesis and self assembly of a bis-bidentate secondary [hosphine oxide metal complex for small molecule activation. **N.I. Rinehart**, A. Kendall, D. Tyler

**542.** Mixed ligand complexes of bis(2,2'-bipyridine)copper(II) perchlorate with selected pseudohalides: Synthesis, characterization, and X-ray structures. **O. Adekunle**, R. Butcher, O. Bakare, O.A. Odunola

**543.** Spectroscopic and solid state evaluation of tetra-aza macrocyclic cobalt complexes with solution behavior that parallels the classic cobalt(II) chloride equilibrium. **H.M. Johnston**, K.M. Lincoln, K.N. Green

**544.** Metal-metal bonding in heterobimetallic Ti/M complexes. **B. Wu**, C. Thomas

**545.** Reduction and hydrogenation processes on polynuclear titanium nitrido complexes. **M. Gonzalez-Moreiras**, M. Greño, M. Mena, A. Perez-Redondo, C. Yelamos

**546.** Toward the synthesis of metal-epoxide coordination complexes. **A.S. Braegelman**, N.L. Fackler

**547.** Towards structural-functional mimics of *Acetylene hydratase*: Reversible activation of acetylene with biomimetic tungsten alkyne-complexes. **L.M. Peschel**, F. Belaj, N.C. Mösch-Zanetti

**548.** Synthesis and structural characterization of zinc complexes with 1,3-bis(diphenylphosphinomethyl)benzene. **M. Young**, T. Siddiquee

Section C

Boston Convention & Exhibition Center  
Hall C

**Electrochemistry**

B. L. Lucht, *Organizer*

6:00 - 8:00

Boston Convention & Exhibition Center  
Hall C

**Electrochemistry**

B. L. Lucht, *Organizer*

6:00 - 8:00

**549.** Electrochemical rectification of molecular multilayered films towards redox mediators for dye-sensitized solar cells. **M.R. Civic**, P.H. Dinolfo

**550.** Direct and stable attachment of a molecular iridium catalyst for water oxidation to electrode surfaces. **S.W. Sheehan**, J. Thomsen, U. Hintermair, R.H. Crabtree, G.W. Brudvig, C.A. Schmuttenmaer

**551.** Linking protein folding, cofactor affinity and electrochemistry in heme proteins by determination of the formal reduction potential of heme. **B.R. Gibney**

**552.** AlCl<sub>3</sub> based ionic liquid with a neutral substituted pyridine ligand for electrochemical deposition of aluminum. **Y. Fang**, X. Jiang, X. Sun, S. Dai

**553.** Transition metal chalcogenide nanofilms: Oxygen reduction reaction catalysts prepared by E-ALD. **B. Yan**, J. Falkowski, Y. Surendranath

**554.** Metal-coordinating molecular catalyst grafted onto carbon electrodes. **R.S. Kim**, T. Fukushima, Y. Surendranath

**555.** Cyclic voltammetric studies of singly-bridged lanthanum, europium and gadolinium polyoxometalates in the presence of potassium. **J.F. Kirby**, D.K. Ampadu

Section D

Boston Convention & Exhibition Center  
Hall C

**Inorganic Spectroscopy**

S. A. Koch, *Organizer*

6:00 - 8:00

**556.** Effect of metal-remote amino-groups on metal center in ruthenium (II) complexes with terpyridine ligands. **H. Li**, Y.A. Jeilani, J. Melnyczuk, H. Lisa, J. Wu, T. Yerokun, C.W. Ingram, I. Harruna

**557.** Investigating the photophysical properties of dendrimeric fluorophore-labeled palladium catalysts using single-molecule fluorescence spectroscopy. **K. Lupo**, S. Upadhyay, A. Marquard, R.H. Goldsmith

Section E

Boston Convention & Exhibition Center  
Hall C

**Organometallic Chemistry: Catalysis**

N. S. Radu, *Organizer*

6:00 - 8:00

**558.** Insight into the active species and mechanism of alkyl-alkyl cross-coupling with iron. **V. Fleischauer**, M.L. Neidig

**559.** Iridium-catalyzed hydrogenation of electron-deficient carbonyls under acidic conditions. **T. Brewster**, N.M. Rezaee, Z. Culakova, A.J. Miller, D.M. Heinekey, M.S. Sanford, K.I. Goldberg

- 560.** New iridium pincer complexes for the aldehyde-water shift reaction. **J.M. Goldberg**, T. Brewster, G.W. Wong, T. Lekich, J.C. Tran, K.I. Goldberg, D.M. Heinekey
- 561.** Catalytic dehydroaromatization of alkanes via an iridium pincer complex: Toward a mechanistic understanding and control of product distribution. **A.M. Steffens**, A.S. Goldman
- 562.** Synthesis and reactivity of pincer-supported rhenium. **A.J. Kosanovich**, O. Ozerov
- 563.** CNN-pincer complexes of ruthenium for the catalytic hydrogenation of esters. **A.R. Chianese**, D. Kim, M. Barnard, L. Le, T. Cervarich, K. Bogdanovski, M.J. Drance, K.H. Jensen
- 564.** Methyl JohnPhos as a new ligand for cross-coupling catalysis. **A.J. Kendall**, D.T. Seidenkranz, D. Tyler
- 565.** Stoichiometric and catalytic reactivity of hexamethyldisilane at an (*N*-heterocyclic carbene)<sub>2</sub>-palladium centre. **M.B. Ansell**, G. Cloke, J. Spencer, O. Navarro
- 566.** Mechanistic study of catalyst initiation in Suzuki coupling using single-molecule and NMR spectroscopy. **A. Marquard**, K. Lupo, J. Ng, S. Upadhyay, D. Hinton, R.H. Goldsmith
- 567.** High yielding and selectivity in the solventless telomerisation of isoprene with alcohols using NHC-Pd catalysts at room temperature. **I. Maluenda**, M. Chen, D. Guest, M. Roe, M.L. Turner, O. Navarro
- 568.** Ambiphilic phosphine boronate esters by the iridium-catalyzed C-H borylation of phosphines. **S. Wright**, K.M. Crawford, N. Huynh, T.R. Ramseyer, E. Albitz, T.B. Clark
- 569.** Bimetallic hafnium pyridyl-amido olefin polymerization catalysts. Y. Gao, A.R. Mouat, A. Motta, **A. Macchioni**, C. Zuccaccia, M. Delferro, T.J. Marks
- 570.** Rapid, regioconvergent, solvent-free alkene hydrosilylation with a cobalt catalyst. **C. Chen**, M.B. Hecht, A. Kavara, W.W. Brennessel, B.Q. Mercado, D.J. Weix, P.L. Holland
- 571.** Activation of monohalogenated substrates using photo initiated copper catalyzed atom transfer radical addition (ATRA). **G.J. Pros**, T. Pintauer
- 572.** Boryl cyclopentadienyl transition metal complexes for C-H functionalization of pyridines. **A. Carl**, J.R. Andreatta
- 573.** Mechanistic investigations of the concerted-metalation deprotonation reaction with [Cp\*RhCl<sub>2</sub>]. **A.P. Walsh**, W.D. Jones
- 574.** Silica-supported tungsten-oxo alkylidene catalysts for use in phase-separated tandem alkane metathesis. **P.E. Sues**, V. Mougel, C. Coperet, R.R. Schrock
- 575.** Kinetic studies on the formation of alternating *trans*-AB copolymers through ring-opening metathesis polymerization using molybdenum alkylidene initiators. H. Jeong, **J.M. John**, R.R. Schrock, A.H. Hoveyda
- 576.** *Z*-to-*E* isomerization processes in reactions catalyzed by cyclometalated ruthenium alkylidenes. **T. Ahmed**, J.M. Grandner, M.B. Herbert, B.L. Taylor, K.N. Houk, R.H. Grubbs
- 577.** Homogeneous copper catalysts for the hydrogenation of carbonyl compounds at room temperature. **A. Chakraborty**, **M.E. Healey**, **J.A. Krause**, H. Guan
- 578.** Microwave assisted formation of binuclear rhodium paddlewheel complexes. **O. Serrano**, O.F. González-Belman, M. Flores-Alamo

Section F

Boston Convention & Exhibition Center  
Hall C

**Solid-State Inorganic Chemistry**

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

6:00 - 8:00

- 579.** Microporous titanates with band gaps in the visible range for photocatalytic splitting of water. **B.C. Hodges**, P. Moetakef, E.E. Rodriguez
- 580.** Large electric-field-induced strain in La-doped Bi-perovskite ceramics. **J. Lee**, J. Kang, T. Dinh
- 581.** Electrodeposition and nucleation studies of vanadium oxide polymorphs. **Z.M. Chan**, C.R. Cox, D.G. Nocera
- 582.** Synthesis and characterization of Mn<sup>2+</sup> doped Ni<sub>3</sub>(BO<sub>3</sub>)<sub>2</sub> nanopowder. **A.U. Morkan**, E. Gul
- 583.** Synthesis and characterization of rare earth metal doped magnesium borates. **A.U. Morkan**, **I.A. Morkan**, E. Gul, G.O. Kahveci
- 584.** Preparation and characterization of new borophosphates of PrB(PO<sub>4</sub>)<sub>2</sub> and TbB(PO<sub>4</sub>)<sub>2</sub>. **A.U. Morkan**, **I.A. Morkan**, G.O. Kahveci, E. Gul
- 585.** Structural and photoluminescent characterization of antiperovskite phosphors: Sr<sub>2</sub>AlO<sub>4</sub>F:P<sup>3+</sup> and Sr<sub>2-x</sub>Na<sub>x</sub>Al<sub>1-2x</sub>P<sub>x</sub>Zn<sub>x</sub>O<sub>4</sub>F (0 ≤ x ≤ 1). **S. Keil**, E.C. Sullivan

**WEDNESDAY MORNING**

Section A

Boston Convention & Exhibition Center  
Room 160A

**Coordination Chemistry Characterization and Applications**

D. C. Crans, *Organizer*  
N. Gerasimchuk, *Presiding*

- 8:00 586.** Extreme service lubrication: Synthesis and characterization of trimeric silver(I) 3,5-dimethyl-4-n-hexylpyrazolate complex and its tribological implementation. **A.M. Seyam**, B.A. Johnson, M. Desanker, D. Jin, H.S. Bazzi, Y. Chung, Q. Wang, M. Delferro, T.J. Marks

- 8:20 587.** Mechanistic studies of oxidative aliphatic carbon-carbon bond cleavage in Cu(II) chlorodiketonate complexes. **S. Saraf**, D. Tierney, C. James, T. Borowski, L.M. Berreau
- 8:40 588.** Reactivity and cation exchange of MOF-5. **C. Brozek**
- 9:00 589.** Flash photolysis of C<sub>3</sub> symmetric first-row transition metal azides: A photochemical investigation of the preparation of high-valent nitrido complexes. **A.S. Kinne**, K.G. Caulton, J.M. Smith, J.M. Zaleski
- 9:20 590.** Regulation of primary geometry in pincer complexes bearing secondary sphere hydrogen bonds. **E.W. Dahl**, N.K. Szymczak

- 9:40 591.** Design of a macrocyclic self-assembled secondary phosphine oxide metal complex for dinitrogen rejection from natural gas. **N.I. Rinehart**, A. Kendall, D. Tyler

10:00 Intermission.

- 10:10 592.** Heterobimetallic Ti-Co complex featuring a metal-metal multiple bond and its application to the reductive coupling of ketones to alkenes. **B. Wu**, C. Thomas
- 10:30 593.** Hydrogen activation by iridium(III) complexes bearing a bidentate protic NH<sub>2</sub>NR-NHC<sup>+</sup>phosphine ligand. **S. Cepa**, E.F. Hahn
- 10:50 594.** Vanadium(IV) complexes with nuclear spin-free ligands: Application of coordination chemistry principles to quantum information processing. **J. Zdrozny**, J. Niklas, O. Poluektov, D.E. Freedman
- 11:10 595.** New strategy for the NIR emitters beyond 900 nm: Preparation of self-assembled luminescent 1D Pt-cyanoximates. **N. Gerasimchuk**, M.Y. Berezin
- 11:30 596.** Fluorescent ratiometric Cu(II) sensor based on Poly(*N*-isopropylacrylamide). **L. Nyiranshuti**
- 11:50 597.** Modeling the ligand tuning effect over the transition temperature in spin-crossover systems using density functional methods. **J. Cirera Fernandez**

Section B

Boston Convention & Exhibition Center  
Room 159

**Organometallic Chemistry: Synthesis and Characterization**

- N. S. Radu, *Organizer*  
C. C. Cummins, *Presiding*
- 8:30 598.** Electrochemical and computational studies of (bisiminopyridine)ruthenium complexes. **M. Noss**, D.H. Berry
- 8:50 599.** Study of low-valent nickel chemistry supported by a series of PEP pincer-type ligands. **Y. Lee**
- 9:10 600.** Reversible P-S bond formation/cleavage reactions at a nickel center supported by an anionic PPP ligand: A mechanistic view of a

- new type of metal-ligand cooperation. **S. Oh**, Y. Lee
- 9:30 Intermission.**
- 9:35 601.** CO<sub>2</sub> activation with uncommon metal-ligand cooperation. **Y. Kim**, S. Oh, S. Kim, J. Kim, Y. Lee
- 9:55 602.** CO activation at a low-valent nickel center. **C. Yoo**, Y. Lee
- 10:15 603.** Silane-cobalt interaction in stepwise formation of a silyl cobalt(II) complex. **J. Kim**, S. Kim, Y. Lee
- 10:35 604.** Molybdenum hydride and dihydride complexes bearing diphosphine ligands with a pendant amine: Formation of complexes with bound amine. **S. Zhang**, M. Bullock

Section C

Boston Convention & Exhibition Center  
Room 158

**Solid-State Inorganic Chemistry**

C. G. Lugmair, V. Poltavets, *Organizers*  
B. M. Bartlett, A. J. Norquist, *Presiding*

- 8:30 605.** Solid state chemistry of AMX<sub>3</sub> halide perovskites (X = I, Br, Cl). **P. Woodward**, M. Linabug, E. McClure
- 9:10 606.** Sodium and terbium chlorobismuthate(III) salts: Synthesis, structure, and photocatalytic behavior. **J. Ahern**, A. Kelly, H.H. Patterson, R.D. Pike
- 9:30 607.** Electronic and steric factors guiding the synthesis of magnesium-based battery electrolytes. **B.M. Bartlett**, A.J. Crowe, E. Nelson
- 9:50 608.** Exfoliation of layered perovskites through microwave assisted grafting with *n*-alcohols. **J. Boykin**, L. Smith
- 10:10 609.** Electronic paramagnetic resonance spectroscopy of transition metal ions in Sr<sub>2</sub>TiO<sub>4</sub> and chemically reduced Sr<sub>2</sub>TiO<sub>4</sub> powders. K.A. Lehuta, A. Haldar, **K.R. Kittilstved**

10:30 Intermission.

- 10:45 610.** Materials discovery in templated metal oxides. **A.J. Norquist**
- 11:05 611.** {W<sub>2</sub>O<sub>7</sub>} building block: A route to gigantic isopolyoxotungstates with pentagonal and double-stranded motifs. **C. Zhan**, D. Long, L. Cronin
- 11:25 612.** Solid-state synthesis of bismuth-based metallodrugs. **D. Tan**, F. Qi, T. Friscic
- 11:45 613.** Synthesis of metal-organic architectures from metals by redox-promoted mechanochemical self-assembly. **M. Glavinovic**, F. Qi, A.D. Katsenis, T. Friscic, J. Lumb
- 12:05 Concluding Remarks.**

Section D

Boston Convention & Exhibition Center  
Room 160C

**Coordination Chemistry Macrocycles and More**

D. C. Crans, *Organizer*  
K. J. Takeuchi, *Presiding*

**9:00 614.** Direct synthesis of non-stoichiometric nanocrystalline metal oxides and their composites: Impact on battery-relevant electrochemistry. **K.J. Takeuchi**, A.C. Marschilok, E.S. Takeuchi

**9:25 615.** Probing life limiting parasitic reactions in electrochemical energy storage. **E.S. Takeuchi**, A.C. Marschilok, K.J. Takeuchi

**9:50 616.** Reactions of boronic acids with tetrafluoroborate. **J.J.**

**Grzybowski**, P. Smith, J. Korsan, D. Aleo

**10:15 617.** Science and technical arts collaborative teaching (STACT) project: Touching the third rail of chemical education. **K.A. Goldsby**, S.M. Ames

**10:40 618.** Hybrid active organic/inorganic materials: Impact of molecular ordering on charge transport performance. **E. Reichmanis**

**11:05 619.** Daryle Busch, supporter of inclusion and diversity. **E.A. Nalley**

**11:30 620.** Research-based strategies for enhancing student performance in introductory chemistry courses. **J.A. Heppert**, M. Barker, D. Pakhira, L. Myers

#### Section E

Boston Convention & Exhibition Center  
Room 161

#### Nanoscience: Applications

R. M. Richards, *Organizer*  
D. Yablon, *Presiding*

**8:30 621.** Enantiomeric separations of chiral pharmaceuticals using chiral tetrahedral Au nanoparticles. **N. Shukla**, D. Yang, A.J. Gellman

**8:50 622.** Engineering of nanoparticles to achieve macroscopic functionality. D. Ha, H. Zhang, B. Hu, T. Ly, O. Otelaja, M. Fayette, A. Nelson, M. Islam, L. Sun, R. Hovden, F. Wise, D. Muller, **R.D. Robinson**

**9:10 623.** Mechanisms and behavior of gas permeation through single layer graphene membranes. **L. Drahushuk**, M. Strano

**9:30 624.** Light or heat? The origin of cargo release from nanoimpeller particles containing upconversion nanocrystals under IR irradiation. **J. Dong**, J.I. Zink, M. Strano

**9:50** Intermission.

**10:00 625.** Advances in nanomechanical measurements with scanning probe microscopy based methods. **D. Yablon**

**10:20 626.** Cell uptake of boron-nitride nanotubes loaded with curcumin. **J. Niskanen**, Y. Wang, X. Zhang, I. Zhang, Y. Xue, D. Golberg, D. Maysinger, F.M. Winnik

**10:40 627.** Quantum dot luminescent concentrator cavity exhibiting thirty fold concentration. **N. Bronstein**, Y.

Yao, L. Xu, E. O'Brien, A.S. Powers, V.E. Ferry, P. Alivisatos, R.G. Nuzzo  
**11:00 628.** Absorption measurements of single plasmonic metal oxide nanocrystals reveal considerable peak heterogeneity hidden within ensemble spectra. **R.W. Johns**, D.J. Milliron, H. Bechtel

**11:20 629.** Understanding the effect of hydrogen passivation of impurities in solution processed metal oxide thin films. **J.C. Ramos**, Y. Huang, C. Perkins, D. Park, D.A. Keszler

**11:40 630.** Preparation and precise size control of metal oxide nanocrystals via a "living" growth synthesis. **A.W. Jansons**, B.M. Crockett, M.C. Sharps, L.K. Plummer, J.E. Hutchison

#### Section F

Boston Convention & Exhibition Center  
Room 160B

#### Chemistry of Materials: Nanomaterials

C. G. Lugmair, *Organizer*  
H. Liu, L. M. Wheeler, *Presiding*

**8:00 631.** Synthesis and structure of colloidal silica - polymethacryloxypropylsiloxane nanocomposite particles. H. Tu, M.J. Monello, R. Lewis, **D. Fomitchev**

**8:20 632.** Chemical transformations of semiconductor nanocrystals: Mechanism and role of defects and surfaces. **S.L. White**, P.K. Jain  
**8:40 633.** Inorganic ligand exchange on germanium nanocrystals. **L.M. Wheeler**, B. Chernomordik, M.C. Beard, N.R. Neale

**9:00 634.** Formation of endohedral mono-metallofullerenes. **P.W. Dunk**, A.G. Marshall, H.W. Kroto

**9:20 635.** DNA-based nanofabrication of inorganic materials. **H. Liu**, F. Zhou, H. Kim

**9:40 636.** Electrospinning SiO<sub>2</sub>-TiO<sub>2</sub> nanofibers using sol-gel chemistry. **F. Huang**, S. Das, M.T. Janish, P.G. Kotula, C. Carter, C.J. Cornelius

**10:00** Intermission.

**10:10 637.** Nonplasmonic nanoparticles as extremely stable photothermal sources. **R.J. Johnson**, B. Lear

**10:30 638.** Synthesis of hollow Ge nanoparticles via electroless deposition. **B. Nolan**, E. Muthuswamy, E. Chan, S. Kaulzarlich

**10:50 639.** Thermochemistry of reduced graphene oxide and its nitrogen-doped variants. **E. Muthuswamy**, J. Chen, A. Navrotsky

**11:10 640.** Iron(II) spin crossover nanoparticles in a block-copolymer matrix. O. Klimm, C. Stiegelmeier, S. Rosenfeldt, S. Foerster, **B. Weber**

**11:30 641.** Generating efficient and tunable white light using hybrid transparent metal oxide-based nanoconjugates. **P. Radovanovic**

**11:50 642.** Solid-solid phase transformations and 2D

heterostructures in copper sulfide nanoparticles. D. Ha, A.H. Caldwell, M. Ward, S. Honrao, K. Mathew, R. Hovden, M. Koker, D. Muller, R. Hennig, **R.D. Robinson**

#### Section G

Boston Convention & Exhibition Center  
Room 162A

#### Lanthanide and Actinide Chemistry

A. De Bettencourt Dias, *Organizer*  
D. T. de Lill, D. A. Penchoff, *Presiding*

**9:00 643.** Synthesis, structure, and electronic spectroscopy of actinide complexes and materials. **H.S. La Pierre**, E.R. Batista, E.D. Bauer, D.L. Clark, S.A. Kozimor, M. Loeble, R.L. Martin, S.G. Minasian, D.K. Shuh, P. Yang

**9:20 644.** Selective and sustainable separation of rare earth elements. **K.D. Field**, **M. Emmert**

**9:40 645.** Spector ion-directed synthesis of lanthanide-organic frameworks. **D.T. de Lill**

**10:00 646.** Actinide and lanthanide complexes: What the CSD and structural informatics can tell us about their complexation. K. Moyle, **S. Vyas**, S. Wiggan, P.C. Sanschagrin, J. Brennan

**10:20** Intermission.

**10:30 647.** Optimizing ligand design for extraction of low concentration uranyl from aqueous media: An integrated theoretical and experimental study. **D.A. Penchoff**, C. Peterson, J.P. Camden, D.M. Jenkins, A.K. Wilson

**10:50 648.** Generation of uranium(IV) bis(imido) intermediates in the synthesis of U(VI) bis(imido) complexes. **J.M. Boncella**, N.C. Tomson, A.M. Tondreau, B. Scott

**11:10 649.** Precision design of new multidentate ligands for f-elements. **I. Yakovlev**, R.J. Abergel

#### Section H

Boston Convention & Exhibition Center  
Room 157C

#### Main Group Chemistry

T. W. Hudnall, *Organizer*  
J. D. Protasiewicz, D. Vidovic, *Presiding*

**8:30 650.** Activation of robust bonds by aluminum(I). **T. Chu**, Y.D. Boyko, G.I. Nikonov

**8:50 651.** Complexation and activation of silanes with a strongly Lewis acidic alane: Isolation, structural characterization, and diverse catalysis. **J. Chen**, E.Y. Chen

**9:10 652.** Homo- and hetero-aryl Lewis acidic boranes: H<sub>2</sub> activation by an electrochemical-frustrated Lewis pair approach. **R.J. Blagg**, G. Wildgoose

**9:30 653.** Reactions between compounds contained protonic and

hydric hydrogens. **X. Chen**, H. Li, X. Chen, Q. Yang

**9:50** Intermission.

**10:00 654.** C-C coupling reactions catalyzed by a Pd(II) complex with the ambiphilic ligand 8-quinolyldimesitylborane. **S.R. Tamang**, J.D. Hoefelmeyer

**10:20 655.** Coordination of N-heterocyclic phosphonium cations to nickel using a chelating ligand framework. **M. Bezpalko**, C. Thomas

**10:40 656.** Coordination chemistry of Group 1 cations with soft donor macrocycles. M. Champion, M. Everett, A. Jolleys, W. Levason, **D. Pugh**, G. Reid

**11:00 657.** Competition between ligation and solvation in heavy alkaline earth metal tetraarylborates. **C.M. Lavin**, A.G. Goos, D.G. Allis, K. Ruhlandt-Senge

**11:20 658.** Calcium arylphosphonates for bone therapy. **V. Lopez**, M.D. Lijewski, V.N. Bampoh, K. Ruhlandt-Senge

#### Innovation in Chemical Synthesis

Sponsored by MPPG, Cosponsored by INOR, MEDI and ORGN

#### International Symposium on Mesoporous Zeolites

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

#### WEDNESDAY AFTERNOON

#### Section A

Boston Convention & Exhibition Center  
Room 160A

#### Nanoscience: Semiconductors

R. M. Richards, *Organizer*  
M. zamkov, *Presiding*

**1:30 659.** Quantitative theory of adsorptive separation for the electronic sorting of single-walled carbon nanotubes. **R. Jain**, K.C. Tvrdy, R. Han, Z. Ulissi, M. Strano

**1:50 660.** Titanium nitride etching in the semiconductor industry: Mechanistic considerations. **J. Hoogboom**, D. Yu, M. Shen, S. Braun, Y. Burk, A. Klipp

**2:10 661.** Liquid contacting of PbS quantum dot solids. **E. Johansson**, V. Dereviankin, V. Uzunov

**2:30 662.** Hole transfer from photoexcited quantum dots to molecular species: Understanding the relationship between driving force and rate. **J.H. Olshansky**, T. Ding, Y. Lee, P. Alivisatos

**2:50 663.** Quantum confined semiconductor nanoshells. **M. Zamkov**, N. Razgoniaeva, D. Burchfield

**3:10 664.** Insights on the solution syntheses of 0D and 2D tin chalcogenide semiconductors. **A.J. Biacchi**, A.R. Hight Walker

**3:30 665.** Heavily transition metal doped semiconductor nanocrystals using magnetic molecular clusters as single source precursors. **S. Pittala**, K.R. Kittilstved

**3:50 666.** Mastering the seed-mediated synthesis of gold nanorods. **N.D. Burrows**, S. Harvey, C.J. Murphy

**4:10 667.** Biaxially stretchable Ag NW-based transparent conductors. **J. Pyo**, B. Kim, T. Kim, H. Park, J. Park, J. Lee, S. Lee

**4:30 668.** Using conduction electron spin resonance to probe the degree of interfacial mixing between chemisorbed aromatic thiols and gold nanoparticles. **A. Cirri**, B. Lear

**4:50 669.** Temperature dependence of the nanocrystal nucleation revealed through plasmon resonance of bimetallic nanoparticles. **N. Razgoniaeva**, A. Acharya, N. Sharma, P. Adhikari, M. Zamkov

**5:10 670.** Assembly of well-defined nanomaterials from transition metal clusters: Emergence of new properties at the nano/small-molecule boundary. **A. Beecher**, J.S. Owen

#### Section B

Boston Convention & Exhibition Center  
Room 159

#### Organometallic Chemistry: Catalysis

N. S. Radu, *Organizer*  
T. Betley, L. Do, *Presiding*

**1:30 671.** Synthesis, characterization, and reactivity of a nonclassical dihydride cobalt bis(carbene) complex. **K. Tokmic**, M.R. Brennan, D. Kim, A. Fout

**1:50 672.** Carbodicarbene ruthenium complexes: Highly active catalysts for the chemoselective hydrogenation of olefins. **C. Prankeviccius**

**2:10 673.** Pd-catalyzed selective hydrosilylation of allylimines. **H. Tafazolian**, J.A. Schmidt

**2:30 674.** Reactivity of the low-coordinate bis(alkoxide) metal complexes in N-N and C-N bond formation reactions. **M. Yousif**, J. Bellow, R. Lord, S. Groysman

**2:50 675.** Phosphine-directed C–H borylation of arenes: Synthesis and utility of phosphine boronate esters. **T.B. Clark**, K.M. Crawford, N. Huynh, S. Wright, T.R. Ramseyer

**3:10** Intermission.

**3:15 676.** JohnPhos palladium catalysis: How structure affects kinetics. **A.J. Kendall**, D.T. Seidenkranz, D. Tyler

**3:35 677.** Synthesis of dimethylphosphino-Buchwald-type ligands: Ligands for the coupling of extremely bulky, deactivated aryl chlorides. **D.T. Seidenkranz**, A.J. Kendall, D. Tyler

**3:55 678.** Activation of chlorohydrocarbons by a

rhodiumtrispyrazolylborate complex.

**Y. Jiao**, W.D. Jones

**4:15 679.** Redox active ligand design on a surface: Synthesis and characterization of tetrazine complexes of Pt, V, and Nb from metal atoms. **D. Skomski**, C. Tempas, A.V. Polezhaev, B.J. Cook, J. Man, S.L. Tait, **K.G. Caulton**

**4:35 680.** Tuning nickel for catalytic olefin hydrogenation via dative bonds to Lewis acidic metalloligands. **R. Cammarota**, C. Lu, P.A. Rudd

**4:55 681.** Selective alcohol hydrogenation and dehydrogenation catalysis and their potential applications inside living systems. **L. Do**

**5:15 682.** Selective formation of n-butanol from ethanol with iridium-based homogeneous catalysts. **S. Chakraborty**, W.D. Jones

#### Section C

Boston Convention & Exhibition Center  
Room 162A

#### Inorganic Catalysts

S. A. Koch, *Organizer*  
A. M. Angeles Boza, S. C. Marinescu, *Presiding*

**1:30 683.** Ethylene addition to cobalt bis(thiooxolene): A DFT study. **D. Sredojevic**, E.N. Brothers

**1:50 684.** Synthesis and reactivity of peroxide and oxide bridged cofacial bimetallic complexes. **E.D. Bloch**, J. Stauber, C.C. Cummins, D.G. Nocera

**2:10 685.** H<sub>2</sub> oxidation by cobaloximes: Mechanistic insight into hydrogen evolution catalysis. **S.A. Del Ciello**, J.R. Winkler, J.C. Peters, H.B. Gray

**2:30 686.** Heavy atom isotope effects as probes of CO<sub>2</sub> activation. **A.M. Angeles Boza**

**2:50 687.** Rational design of photochemical super-reductants based on tungsten-alkylidyne chromophores. **H.B. Vibbert**, M.D. Hopkins

**3:10** Intermission.

**3:20 688.** Gas generation from simple carboxylic acids and diphosphine-supported first-row transition metals. **A.M. Tondreau**, J.M. Boncella, B. Scott

**3:40 689.** Synthesis, properties, and water oxidation activity of a novel dinuclear Ru(II) polypyridine complex. **N. Nair**, R. Zhou, R.P. Thummel

**4:00 690.** Efficient proton reduction from water by cobalt dithiolene metal-organic surfaces (MOS). **S.C. Marinescu**

**4:20 691.** DNA-hosted gold nanocluster enhances enzymatic electroreduction of oxygen by mediating efficient electron transfer. **S. Chakraborty**, S. Babanova, R.C. Rocha, A. Desireddy, K. Artyushkova, P.B. Atanassov, J.S. Martinez

**4:40 692.** Determination of the relative acidity of binary HCl/MCl<sub>m</sub> superacids

that involve Lewis acids from groups 13 & 15. **J. Stiel**, Z. Tun, **C. Tessier**

**5:00 693.** Metal complexes for fixation, electrocatalytic, photocatalytic and chemical CO<sub>2</sub> reduction. **I. Ivanovic-Burmazovic**

#### Section D

Boston Convention & Exhibition Center  
Room 160C

#### Coordination Chemistry: Synthesis and Characterization

D. C. Crans, *Organizer*  
T. Betley, R. C. Scarrow, *Presiding*

**1:30 694.** Vapochromic materials that don't incorporate vapors. **M. Karimi Abdolmaleki**, S. Chatterjee, M. Olen Bovee, J.A. Krause, W.B. Connick

**1:50 695.** Transition metal single-molecule magnet in a nuclear spin-free ligand field environment. **M. Fataftah**, J. Zadrozny, D. Rogers, D.E. Freedman

**2:10 696.** Synchrotron-based methods to study metal-metal bonded complexes of the first-row transition metals. **R.J. Eisenhart**, L.J. Clouston, Y. Chen, V.G. Young, C. Lu

**2:30 697.** Strong magnetic coupling in dinuclear transition-metal complexes bridged by a 2,5-diamino-1,4-benzoquinonediimine radical. **J. DeGayner**, I. Jeon, D. Harris

**2:50 698.** High-spin ground state and single-molecule magnet behavior in octahedral iron clusters [M<sub>6</sub>]. **R. Hernandez Sanchez**, T. Betley

**3:10 699.** Strong magnetic exchange in high-dimensional networks of transition metal ions bridged by benzosemiquinonoid ligands. **I. Jeon**, D. Harris

**3:30 700.** Emergent single molecule magnetism in highly symmetric clusters. **T. Betley**, R. Hernandez Sanchez

**3:50 701.** Synthesis and magnetic properties of 1,2,4,5-benzenetetrathiolate-bridged dinuclear complexes. **A. Banisafar**, I. Jeon, D. Harris

**4:10 702.** Synthesis, structural and spectroscopic characterization of thiocyanate ligated heterobimetallic lantern complexes. **J.L. Guillet**, C.J. Daley, J.A. Golen, A.L. Rheingold, L. Doerrer

**4:30 703.** Excited state charge distribution in Mo<sub>2</sub>L<sub>4</sub> paddlewheel compounds indicated by C≡C stretch. **C. Jiang**, P.J. Young, M.H. Chisholm

**4:50 704.** Influence of environmental factors on quantum decoherence in mononuclear transition metal complexes. **M. Graham**, J. Zadrozny, M. Shiddiq, J.S. Anderson, M. Fataftah, S. Hill, D.E. Freedman

#### Section E

Boston Convention & Exhibition Center  
Room 161

#### Bioinorganic Chemistry: Proteins and Enzymes and Model Systems

S. A. Koch, *Organizer*  
J. P. Caradonna, *Presiding*

**1:30 705.** H<sub>2</sub>S and metal mediated HNO generation as new signaling mechanisms. **I. Ivanovic-Burmazovic**

**1:50 706.** Diiron μ-thiolate complexes that bind N<sub>2</sub> across multiple oxidation states: Towards new structural/functional models of nitrogenase. **S. Creutz**, J. Peters

**2:10 707.** Stabilization of reactive species within a metal organic framework. **J.S. Anderson**, A. Gallagher, J. Park, D. Harris

**2:30 708.** Mechanistic insights into the N-N reductive coupling of NO by low coordinate Cu and Ni complexes. **S. Kundu**, T.H. Warren

**2:50 709.** Modeling halogen bonding and protein dynamics in iodothyronine deiodinase. **C.A. Bayse**

**3:10 710.** Activation of oxygen at an iron(II) center: Coupling α-ketoacid decarboxylation with alkane to alcohol conversion. **J.P. Caradonna**, L. Gregor, J. McNally, P. Tarves

**3:50** Intermission.

**3:30 711.** Novel thermodynamic cycle to determine the reduction potential and reduction enthalpy and entropy of azurin. **M.L. Croteau**, D. Wilcox

**4:10 712.** Delivery of active large proteins using mesoporous silica nanoparticles. **G. Deodhar**

**4:30 713.** Biomimetic corroles as heme protein cofactors. **M. Hoffmann**, K. Kleeberg, B. Wolfram, P. Schweyen, U. Papke, M. Bröring

**4:50 714.** Thermodynamics of Cu(I), Ag(I), and other d<sup>10</sup> metal ions binding to the metallochaperone HAH1, and the effect of glutathione on this binding. **M. Stevenson**, J. Schuster, D. Wilcox

**5:10 715.** Ruthenium dihydroxybipyridine complexes are tumor activated prodrugs due to low pH and blue light induced ligand release. **E.T. Papish**, M. Lockart, K. Jernigan, D.J. Charboneau, K.D. Hughes, S.E. Brown, F.S. Thowfeik, D. Dozier, E.J. Merino, Y. Kim, J.J. Paul

#### Section F

Boston Convention & Exhibition Center  
Room 160B

#### Chemistry of Materials: Metal Organic Frameworks

C. G. Lugmair, *Organizer*  
M. G. Campbell, *Presiding*

**1:30 716.** New rare-earth-free hybrid phosphor for efficient solid-state lighting. **Z. Hu**, G. Huang, W.P. Lustig, F. Wang, H. Wang, S.J. Teat, D. Banerjee, D. Zhang, J. Li

**1:50 717.** Functionalizing polymer fibers with UiO-66-NH<sub>2</sub> using ALD oxide nucleation layers. **J. Zhao**, P.S. Williams, W. Xie, D.T. Lee, G.W. Peterson, G.N. Parsons

**2:10 718.** Porphyrinic metal–organic frameworks for photodynamic therapy. **J. Park**, D. Feng, H. Zhou

**2:30 719.** Electrochemical investigations of conductive metal–organic frameworks. **E. Miner**, D. Sheberla, M. Dinca

**2:50 720.** Electrically conductive 2D metal–organic frameworks for chemiresistive sensing. **M.G. Campbell**, D. Sheberla, S. Liu, T.M. Swager, M. Dinca

**3:10 721.** Molecular-level characterization of the guest effect on the transition temperature in spin crossover metal–organic frameworks. **J. Cirera Fernandez**, F. Paesani

**3:30** Intermission.

**3:45 722.** Electrically conductive metal–organic frameworks based on through-bond charge transport design principle. **S. Lei**, T. Miyakai, C.H. Hendon, S. Seki, A. Walsh, M. Dinca

**4:05 723.** Cation-dependent intrinsic electrical conductivity in tetrathiafulvalene-based microporous metal–organic frameworks. **S.S. Park**, E. Hontz, L. Sun, C.H. Hendon, A. Walsh, T.A. Van Voorhis, M. Dinca

**4:25 724.** Thermochemistry of multiferroic organic–inorganic hybrid perovskites. **N. Gowdaiana pallya puttaiah**, A. Navrotsky

**4:45 725.** Leach-free catalysis and electroactive materials from metal–thiolate-enabled porous frameworks. **Z. Xu**, K. Yee, M. Zeller

**5:05 726.** Imparting functionality to biocatalysts via embedding enzymes into nanoporous materials by a de novo approach: Size-selective sheltering of catalase in metal–organic framework microcrystals. **W. Chang Cheng**

**5:25 727.** Lanthanide-based nano-MOFs as multimodal bioimaging agents. **D.T. de Lill**

Section G

Boston Convention & Exhibition Center  
Room 158

#### Coordination Chemistry: Synthesis and Characterization

D. C. Crans, *Organizer*

L. Doerrner, G. T. Musie, *Presiding*

**1:30 728.** Rational design: Programming small molecule reactivity in a multinuclear iron cluster. **B. Malbrecht**, T. Betley

**1:50 729.** Synthesis and structure of (dpp-BIAN)V( $\mu_2$ -Cl) $_3$ ( $\mu_3$ -Cl) $_2$ Mg $_2$ (thf) $_4$ : A trinuclear vanadium(II)-magnesium species with a radical anion dpp-BIAN ligand coordinated to the vanadium(II) center. **D.A. Nadelman**, R. V. Nadelman, S. Leed, J. Niklas, J.D. Gorden, C.D. Abernethy

**2:10 730.** Mononuclear and terminally bound titanium nitride complexes formed via reductive denitrogenation of a titanium azide. **M. Carroll**, P.J. Carroll, D.J. Mindiola

**2:30 731.** Structure correlation of square-planar metal complexes with pendant nucleophiles. **J. Ringo**, T. Green, J.A. Krause, W.B. Connick

**2:50 732.** Synthesis and crystallographic study of zinc and mercury complexes with a three-N-donor asymmetric pyridine–amine ligand 2,9-di(pyridin-2-yl)-1,3,6-triazabicyclo[4.2.1]nonane. **M. Hakimi**

**3:10** Intermission.

**3:20 733.** Biomimetic coordination chemistry of bi- and tridentate thioligands. **N.C. Möscher-Zanetti**, L.M. Peschel, S. Holler, M. Tüchler, F. Belaj

**3:40 734.** Multidentate pyrrole-based phosphine, polypyrazolyl, and Schiff base ligands for transition metal complexes: Catalysis and fluxional properties. **G. Mani**, S. Kumar, D. Ghorai, R. Kumar

**4:00 735.** Broadening the scope of luminescent Ru(II) diimine complexes of the type [(diimine) $_2$ Ru(L) $_2$ ] $^{2+}$  through control of the MLCT – LF state energy gap. **T. Feng**, R.H. Schmehl

**4:20 736.** Tunable spin equilibria in four-coordinate iron trisphosphine phosphiniminato complexes. **S. Creutz**, J. Peters

#### International Symposium on Mesoporous Zeolites

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

#### Polymer Concepts in Inorganic Chemistry Courses

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#### WEDNESDAY EVENING

Section A

Boston Convention & Exhibition Center  
Hall C

#### Bioinorganic Chemistry: Proteins and Enzymes and Model Systems

S. A. Koch, *Organizer*

**6:00 - 8:00**

**737.** Mössbauer studies of multimetallic assemblies of complexes with different spin states. **V.C. Popescu**, M. Cohara, P. Ghosh, M.Y. Darenbourg

**738.** Secondary coordination sphere effects in copper macrocyclic complexes. **B.D. Neisen**, W.B. Tolman

**739.** Magnetic circular dichroism studies of iron binding in wild-type and mutant calprotectin. **T.M. Woodruff**, T.G. Nakashige, E.M. Nolan, M.L. Neidig

**740.** Modeling reversible S–NO bond formation and S–S disulfide cleavage at copper and zinc sites. **A. Gee**, S. Zhang, T.H. Warren

**741.** Release of NO from nitrite at copper(I) via electrophilic activation. **Z. Sakhaei**, S. Kundu, T.H. Warren

**742.** Determination of the reactivity of Fe $^{3+}$ -1,2-dihydroxibenzenes complexes in the Fenton reaction. **D. Contreras**, Y. Duran, **D. Carmona**, H.D. Mansilla, L. Cornejo

**743.** (Bi)carbonate reactivity with synthetic FDH models. **E. Kim**, **L. Elrod**

**744.** Reaction pathway prediction and differentiation in the TBP geometries found in vanadium-phosphatase protein complexes using shape analysis. **I. Sanchez Lombardo**, S. Alvarez, C. McLaughlan, D.C. Crans

**745.** Discrimination of nitroxyl and biological thiols with modular, lysine-based fluorophores. **A. Loas**, R.J. Radford, A.D. Liang, S.J. Lippard

**746.** Reaction of bis-(1,4,7-triazacyclononane)nickel(III) with L-cysteinesulfenic acid. **D.M. Stanbury**, R. Chan, N. Payne

**747.** Synthetic modeling of the sMMO diiron active site with a preorganized macrocyclic ligand framework. **F. Wang**, M. Minier, A. Loas, S.J. Lippard

**748.** Interaction of the heme protein cytochrome *c* with negatively-charged lipid membranes. **X. Chen**, Y. Liu, E.V. Pletneva

**749.** Vanadium phosphatase inhibitors favor the trigonal bipyramidal transition state geometry. **D.C. Crans**, B. Peters, C.C. McLaughlan, G.R. Willsky

**750.** Preparation of metal-substituted myoglobin to promote new reactivities. **K.L. Stone**

**751.** Efforts toward the synthesis of catalytic antibiotics via attachment of a metal binding domain to Vancomycin. **J. Gray**, J.A. Lundeen, P.J. Loll, E.T. Papish

**752.** Degradation of aromatic hydrocarbons by functional and structural models of iron-containing dioxygenases. **M. Molenda**, J. Li, M. Panda, W.W. Brennessel, F.A. Chavez

Section C

Boston Convention & Exhibition Center  
Hall C

#### Inorganic Catalysts

S. A. Koch, *Organizer*

**6:00 - 8:00**

**753.** Low-temperature precursors for vanadium oxide nanomaterials for catalytic application. **A.A. Alothman**, A.W. Apblett

**754.** Terminal alkene isomerization using the bifunctional ruthenium catalysts: Stability study. **D. Vidovic**, A. Smarun

**755.** Mechanistic studies of O–O bond formation in cobalt-catalyzed water oxidation. **C. Brodsky**, A. Ullman, D.G. Nocera

**756.** Pyridine-aza macrocycles (PyMACs) with appended functionalities for hydrogen peroxide activation and oxidation catalysis. **T. Palluccio**, **S.G. McKenzie**, E. Rybak-Akimova

**757.** Biomimetic chemistry of Ttz relevant to copper nitrite reductase: The influence of protonated Ttz $^{R1, R2}$  in copper complexes toward electrochemical behavior and reactivity (Ttz=tris(1,2,4-triazolyl)hydroborate). **S. Siek**, N. Dixon, E.T. Papish

**758.** Mechanistic investigation of non-heme iron-aminopyridine oxidation catalysts. **M. Piquette**, O. Makhlynets, D. Bowen, E. Rybak-Akimova

**759.** Diastereoselective binding of bis(secondarily phosphines) in [Cu(*i*-Pr-DuPhos)(PhHP~PPh)][PF $_6$ ] complexes: Synthesis, structure, and dynamic processes. **S. Gibbons**, J.L. Peltier, C.R. Valleau, D.S. Glueck, J.A. Golen, A.L. Rheingold

**760.** Development of novel iron complexes for catalytic C–H bond activation and amination. **C. Giberson-Chen**, A. Mikhailine, T. Betley

**761.** Exfoliation of nitrogen and tetravalent niobium doped yellow and black [Ca $_2$ Nb $_3$ O $_{10}$ ] $^{-1}$  nanosheets for visible-light-driven hydrogen evolution. **Y. Wang**, Y. Zhou

**762.** Homogeneous hydrogenation of carbon dioxide to methanol through cascade catalysis. **N.M. Rezaee**, C.A. Huff, M.S. Sanford

Section D

Boston Convention & Exhibition Center  
Hall C

#### Organometallic Chemistry: Applications to Materials and Polymer Science

N. S. Radu, *Organizer*

**6:00 - 8:00**

**763.** Synthesis and radiation chemistry of phosphonium hexatungstate compounds for the precursor of metal oxide thin films. **S. Saha**, J.M. Amador, S.R. Decker, L.N. Zakharov, D.A. Kesziar

**764.** Application of achiral, sterically constrained bis(imino)pyridine iron complexes for the stereoregular polymerization of lactide, a mechanistic study. **J.A. Kehl**, J.A. Byers, C.M. Manna, L. Yablou

**765.** Synthetic avenues to high oxidation state group VI imidophosphorane complexes bearing metal–element multiple bonds. **C.J. Varjas**, R.K. Thomson

Section E

Boston Convention & Exhibition Center  
Hall C

#### Organometallic Chemistry: Synthesis and Characterization

N. S. Radu, *Organizer*

6:00 - 8:00

- 766.** Synthesis and reactivity of a new class of frustrated Lewis pairs. **A.C. McQuilken**, T.H. Warren
- 767.** One pot synthesis of arene-based PCP/PNP ligands and corresponding nickel complexes. **W. Shih**, O. Ozerov
- 768.** Water-soluble organogold(III) complex: Luminescence, self-assembly, and photochemistry in water. **F. Wang**, **C. Che**
- 769.** Low-valent, neutral, and isocarbonyl complexes of iron with multidentate carbene ligands. **A. Hickey**, C. Chen, J.M. Smith
- 770.** Synthesis, characterization, and photophysical properties of dendrimeric fluorophore-labeled palladium catalysts for single-molecule spectroscopy. **S.P. Upadhyay**, K. Lupo, A. Marquard, R.H. Goldsmith
- 771.** Reactivity of carbene transfer reagents with high-spin iron dipyrin complexes. **A. Wrobel**, M.J. Wilding, T. Betley
- 772.** Effects of a pyrene substituent on indium containing porphyrins. **C. Holstrom**, H.M. Rhoda, E. Maligaspe, V. Nemykin
- 773.** Rutheniumtetraphenylporphyrin axially coordinated with bisferrocenylisonitriles: A synthesis, spectroscopic, electrochemical, and theoretical study. **M. Fathi-Rasekh**, S. Dudkin, M.V. Barybin, V. Nemykin, A.D. Spaeth
- 774.** Conformational dynamics control selectivity for two-electron chemistry in three-coordinate Co(I) amide complexes. **M.R. Brennan**, H. Patel, A. Fout
- 775.** High-spin cobalt dipyrin complexes featuring metal-ligand multiple bonds. **Y. Baek**, M.J. Wilding, T. Betley
- 776.** Synthesis and reactivity of low-valent, low-coordinate Co(I) and Fe(I) complexes. **J.A. Killion**, M.R. Brennan, A.R. Fout
- 777.** Competition between the formation of seven-membered and five-membered cyclometalated platinacycles. **C.M. Anderson**, M.W. Greenberg, J. Tanski
- 778.** Synthesis and characterization of neutral bis-PTA pincer ligands for catalysis in water. **K. Zielinski**, J.R. Andreatta
- 779.** Insertion of transition metal carbonyls into the dimetallenes of germanium and tin. **M.L. McCrea-Hendrick**, P.P. Power
- 780.** Reversible transformation between a phosphinite-Ni(0) and a phosphide-Ni(II) alkoxide via unique metal-ligand cooperation. **S. Kim**, Y. Kim, S. Oh, Y. Lee
- 781.** C-C bond formation between CO and iodoalkanes at a nickel(I) center and its mechanistic study. **C. Yoo**, Y. Lee
- 782.** Syntheses of silyl cobalt(II) complexes via SiH-cobalt interaction. **J. Kim**, S. Kim, Y. Lee

- 783.** Photophysical properties of a series of copper complexes. **Y. Kim**, J. Kim, S. Kim, Y. Lee

- 784.** Reversible P-S bond formation/cleavage: PPP vs. PNP. **S. Oh**, Y. Lee

Section F

Boston Convention & Exhibition Center  
Hall C

### Organometallic Chemistry: Applications to Organic Transformations

N. S. Radu, *Organizer*

6:00 - 8:00

- 785.** Development of Ru(II) complexes for the activation of covalent bonds. **K.H. Taylor**, T.B. Gunnoe, M. Sabat
- 786.** New chemistry of high-valent nickel fluoroalkyl complexes. **S. Yu**, D. Vicio
- 787.** Stepwise conversion of a platinum dimethyl complex to a perfluorometallacyclobutane derivative. **L. Xu**, D. Solowey, D.A. Vicio
- 788.** High oxidation state molybdenum imido complexes for the catalytic preparation of haloalkenes. **J.K. Lam**, J. Hyvl, R.R. Schrock, A.H. Hoveyda
- 789.** Fast "Wittig-like" reactions as a consequence of the inorganic enamine effect. **S. A. Gonsales**, M. Pascualini, I. Ghiviriga, K. Abboud, A.S. Veige