

- 2:20 I&EC 160.** Optimizing high-pressure chemical vapor deposition processes for void-free filling of silica optical fiber microcapillaries with hydrogenated amorphous silicon. **S. Motevalian, S. Aro, H.Y. Cheng, J.V. Badding, A. Borhan**
- 2:40 I&EC 161.** High silica zeolite-Y membranes: Motivation, development, characterization, and application. **S. Chakraborty, P. Dutta, S.J. Singer**
- 3:00 I&EC 162.** Sustainable production of chemicals using continuous flow technology. **Y. Huang**
- 3:20 I&EC 163.** Assessment of advanced easy-clean durable coatings. **A. Wojdyła-Cieslak, G.G. Durand, A. Taylor, I. Boyd**
- 3:40 I&EC 164.** Isomerization and self-metathesis of raffinate butenes to propylene on a W/Si-Al catalyst. **F. Alshafei, N. Sulaim, M. Khokhar, R. Daadoush, R. Abudawoud, S. Shaikh**
- 4:00 I&EC 165.** Intensification of capture CO<sub>2</sub> from IGCC flue gas by hydrate formation under direct heat removal by phase change of n-tetradecane. **Y. Luo, X. Guo**
- 4:20 I&EC 166.** Encapsulated ferrate for air purification application. **W. Den, R. Wu, E. Kanchanatip**
- 4:40 I&EC 167.** Resistive response of carbon nanotube membrane for the detection of chlorophenols. **W. Den, N. Grisdanurak, E. Kanchanatip**
- 5:00 I&EC 168.** Synthesis of poly(vinyl butyral) based on a new micro-structured chemical system for process intensification. **X. Lin, K. Wang, J. Zhang, G. Luo**

## INOR

### Division of Inorganic Chemistry

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

#### OTHER SYMPOSIA OF INTEREST:

**Nobel Laureate Signature Award for Graduate Education in Chemistry: Symposium in honor of Matthew J. Polinski & Thomas E. Albrecht-Schmitt** (see NUCL, Sun)

**ACS Award for Creative Work in Fluorine Chemistry** (see FLUO, Sun, Mon)

**Heavy Element Inorganic Chemistry: A Tribute to Al Sattelberger** (see NUCL, Wed, Thu)

### SUNDAY MORNING

#### Section A

San Diego Convention Center  
Room 30B

#### Undergraduate Teaching at the Frontiers of Inorganic Chemistry

##### Framing the Future

*Cosponsored by CHED*

**B. A. Reisner, Organizer**

**J. L. Stewart, Organizer, Presiding**

**8:30** Introductory Remarks.

**8:35 INOR 1.** One eye on the past, one eye on the future: A reflection on the undergraduate inorganic chemistry curriculum. **B.A. Reisner**

**8:55 INOR 2.** Weaving the fundamentals of inorganic chemistry through upper level elective courses that touch on diverse topics such as nanoscale science and energy storage and conversion. **A.L. Prieto**

**9:15 INOR 3.** Beyond workshops: Partnering with R1-research groups to develop materials to post on VIPER. **M. Cass**

**9:35 INOR 4.** Development of a comprehensive multistep advanced laboratory experiment: Synthesis and characterization of Re(V)-oxo complexes with study of catalysis and reaction kinetics. **E.A. Ison, A. Ison**

**9:55** Intermission.

**10:10 INOR 5.** New teaching experiments for inorganic chemistry. **G. Lisensky**

**10:30 INOR 6.** Authoring an inorganic chemistry textbook in the 21st century. **P.J. Fischer**

**10:50 INOR 7.** Teaching inorganic materials chemistry and nanoscience at the undergraduate level. **T.E. Mallouk**

**11:10 INOR 8.** Teaching modern inorganic chemistry: A personal perspective. **G.S. Girolami**

**11:30** Panel Discussion.

#### Section B

San Diego Convention Center  
Room 30C

#### ACS Award for Distinguished Service in the Advancement of Inorganic Chemistry: Symposium in honor of Vincent L. Pecoraro

##### Early Years

**B. R. Gibney, A. F. Peacock, Organizers**

**C. M. Zaleski, Organizer, Presiding**

**J. Bodwin, Presiding**

**8:30 INOR 9.** Microbial iron transport: From coordination chemistry to human host competition. **K.N. Raymond**

**9:00 INOR 10.** Inorganic physiology: Distribution and speciation of metal ions in biological systems. **J.E. Penner-Hahn**

**9:30 INOR 11.** Ammonia binding to the manganese of the oxygen evolving complex (revisited). **R.D. Britt**

**10:00 INOR 12.** Bioinspired, alpha-hydroxy acid-containing chelates for tight binding and light-triggered release of metals. **M.J. Baldwin**

**10:30** Intermission.

**10:40 INOR 13.** Withdrawn.

**11:10 INOR 14.** Coordination chemistry of vanadium combined with ligand properties lead to effective phosphatase inhibitors with potential antidiabetic properties. **D.C. Crans, C.C. McClachlan**

**11:40 INOR 15.** Fabricated nano and micro-particles for non-oral delivery. **B. Farrer**

**12:10 INOR 16.** C-H bond cleavage by metalloenzymes and metalloporphyrins. **J.T. Groves**

#### Section C

San Diego Convention Center  
Room 30D

#### ACS Award in Inorganic Chemistry: Symposium in honor of Mercuri G. Kanatzidis

##### Synthesis & Applications of Solid State Materials

**J. A. Aitken, Organizer**

**K. Choi, Organizer, Presiding**

**S. E. Latturmer, Presiding**

**8:30** Introductory Remarks.

**8:35 INOR 17.** Early years/milestones in the career of Mercuri Kanatzidis in the University of Iowa and the University of Michigan. **D.N. Coucouvanis**

**8:50 INOR 18.** Semiquinoid radical-containing molecules and solids with strong magnetic exchange coupling. **D. Harris, I. Jeon, A. Gaudette, J. DeGayer**

**9:15 INOR 19.** Metal-organic frameworks as highly functional catalytic arrays. **S. Moon, Z. Li, S.S. Al-Juaid, P. Li, Y. Liu, A. Howarth, J.B. DeCoste, G.W. Peterson, C.J. Cramer, L. Gagliardi, J.T. Hupp, O.K. Farha**

**9:40 INOR 20.** Emerging biomedical applications of Prussian blue analogue compounds: From oral MRI contrast agents to catalytic anticancer drugs, and to tumorigenic angiogenesis inhibitors. **S. Huang**

**10:05** Intermission.

**10:20 INOR 21.** Design of noncentrosymmetric materials. **K.R. Poeppelmeier**

**10:45 INOR 22.** Quaternary diamond-like semiconductors with infrared nonlinear optical properties. **J.A. Aitken, J. Brant, D. Clarke, J. Jang, J. Zhang, K. Rosmus, S. Wisneski**

**11:10 INOR 23.** Templating of silica mesophases by sustainable oleyl amine surfactants. **T.J. Pinnavaia, C. Canlas**

**11:35 INOR 24.** Surfactants as promising media for the preparation of crystalline inorganic materials. **Q. Zhang**

#### Section D

San Diego Convention Center  
Room 30E

#### ACS Award in Organometallic Chemistry: Symposium in honor of Karen I. Goldberg

*Cosponsored by WCC*

**N. E. Gruhn, W. D. Jones, Organizers**

**M. S. Sanford, Organizer, Presiding**

**A. J. Miller, Presiding**

**9:00 INOR 25.** New Pd(II) and Ni(II) catalysts for olefin polymerizations. **Z. Chen, D. Bezier, K. Allen, O. Daugulis, M. Brookhart**

**9:20 INOR 26.** Synthesis of allenes via isomerization of internal alkynes. **N. Phadke, M. Findlater**

**9:40 INOR 27.** Tuning olefin isomerization and hydrogenation with cation-responsive catalysts. **A.J. Miller, M.R. Kita, J.B. Smith, S.H. Kerr, J. Grajeda, L.C. Gregor, A.H. Sullivan**

**10:00 INOR 28.** Materials for organic light-emitting diode displays. **N.S. Radu, N. Herron, G. Rossi, F. Gentry, T.N. Hoerter, Y. Wang, A. Fennimore, R. Chesterfield, W. Gao**

**10:20** Intermission.

**10:30 INOR 29.** Organometallic chemistry of nickel(III) and (IV). **M.S. Sanford**

**10:50 INOR 30.** Approaches to the synthesis of Fe(IV) alkylidenes. **P.T. Wolczanski, B.M. Lindley, B.P. Jacobs, R. Agarwal, S.N. MacMillan**

**11:10 INOR 31.** Two decades of lessons in controlling selectivity in Pt (IV) reductive elimination, and new attempts to increase activity in Pt (II) oxidative addition. **N. Williams, M. Van Vleet, A. Liberman-Martin, T. Mortvedt, L.A. Watson, R.J. Cave**

**11:30 INOR 32.** Platinum(IV) and palladium(IV) aryldiazenido complexes. **U.W. Fekl**

**11:50 INOR 33.** Base-free transfer hydrogenation of aldehydes and ketones using Cp\*Ir(pyridinesulfonamide)Cl precatalysts. **A.R. O'Connor**

#### Section E

San Diego Convention Center  
Room 31A

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

**S. A. Koch, Organizer**

**L. E. Cheruzel, Presiding**

**8:30 INOR 34.** Series of N5 ligands as functional mimics of the nickel superoxide dismutase active site. **V.G. Snider, A. Mukherjee**

**8:50 INOR 35.** Bioinspired heterometallic systems for the activation of small molecules. **V. Oswald, A. Borovik**

**9:10 INOR 36.** Reactive copper-oxygen species with mixed benzimidazole/thio- and selenoether platforms relevant to the active site of PHM. **I. Castillo, B. Sanchez-Eguia, M. Orio**

**9:30 INOR 37.** Site-selective characterization of plastocyanin with linear and multidimensional infrared spectroscopy. **A. Le Sueur, M.C. Thielges**

**9:50 INOR 38.** Structural and functional mimic of the NiFe hydrogenase with unprecedented Ni-centered chemistry. **D. Brazzolotto, M. Gennari, N. Queyriaux, F. Meyer, M. Orio, V. Artero, C. Duboc**

**10:10 INOR 39.** Activation of methyl-coenzyme M reductase, the enzyme involved in methane production or consumption in Archaea. **E.C. Duin, D. Prakash, R. Ghebreab, B. Cronin**

**10:30** Intermission.

**10:40 INOR 40.** Targetable, reaction-based small molecule-protein hybrid sensors for detecting mobile zinc. **M.L. Zastrow, Z. Huang, R.J. Radford, S.J. Lippard**

**11:00 INOR 41.** Selective substrate C-H functionalization using light-driven P450 biocatalysts. **L.E. Cheruzel**

**11:20 INOR 42.** Biomimetics of tri-iron arrangements involving cyanide as docking agent in maturases of the H cluster of the diiron hydrogenase. **A.M. Lunsford, C. Beto, S. Ding, N. Wang, M.B. Hall, M.Y. Darensbourg**

**11:40 INOR 43.** Improved method for the spectroscopic determination of inorganic phosphate to quantify nucleotide hydrolysis. **F.E. Katz, F.A. Tezcan**

**12:00 INOR 44.** Development of fatty acid derivatives to inhibit platelet aggregation and investigating their biochemical mechanism. **J. Roy, R. Adili, M. Holinstat, A. Das**

**12:20 INOR 45.** Artificial metalloproteins: Towards a blue copper center. **S.J. Mann, T. Heinisch, T.R. Ward, A. Borovik**

## Section F

San Diego Convention Center  
Room 31B

### Coordination Chemistry: Synthesis & Characterization

S. A. Koch, *Organizer*

A. Ghosh, C. H. Larsen, *Presiding*

**8:00 INOR 46.** Asymmetric ligand approach to design volatile molecular precursors for the Al-Fe intermetallic catalyst. **S. Mishra**, K. Soussi, E. Jeanneau, S. Daniele

**8:20 INOR 47.** Nitrile activation by intramolecular C-C bond coupling to a diimine ligand in group 7 metal tricarbonyl complexes. **V. Yempally**, W.Y. Fan, B. Arndtsen, A. Bengali

**8:40 INOR 48.** Unique highly connected / highly stable RE-MOF for moisture control in confined spaces: Introduction to moisture controlled swing adsorption. **R. Abdul Halim**, M. Eddaoudi, Y. Belmabkhout

**9:00 INOR 49.** Fundamental coordination chemistry for the recycle efforts of scandium. **J. Sears**, T.J. Boyle, L.J. Small, T.M. Alam

**9:20 INOR 50.** Reversible spin state changes in a 4-coordinate iron complex: Valence tautomerism involving redox-active formazanate ligands. **R. Travieso Puente**, E. Otten, M. Chang

**9:40 INOR 51.** Bulky N-heterocyclic thione (NHT) and seleno (NHSe) complexes of mercury(II) and copper(I). **M. Kocherga**, D. Rabinovich

**10:00 Intermission.**

**10:10 INOR 52.** 5d metallocorrolles: Bis(corrolato)tungsten(VI) sandwich complexes as novel, chiral members in a growing family. **A. Ghosh**, A. Alemayehu, H. Vazquez-Lima, K.J. Gagnon

**10:30 INOR 53.** Bifunctional Cu(II) and Zn(II) ligands for ratiometric metal ion sensing. **M. Abdalrahman**, W.S. Kassel, R. Seitz, **F. Abebe**, S. Burdette, R.P. Planalp

**10:50 INOR 54.** Reactivity of rhodium(I) ( $\beta$ -ketoaminate)(bipyridine) complexes with oxidants. **E. Seraya**, A.F. Heyduk

**11:10 INOR 55.** Toward the synthesis of tetrametallic terminal oxo complexes supported by aminopyrazole ligands. **Z. Han**, K. Horak, T. Agapie

**11:30 INOR 56.** One-step synthesis of substituted 2-(2'-pyridyl)quinoline ligands applied to study the solution and solid phase behavior of gold(III) complexes. **M. Sterling**, E.M. Laguna, P. Olsen, E. Roman, A.L. Rheingold, **C.H. Larsen**

**11:50 INOR 57.** Unraveling trends in metal-metal bonding: A comparison of Ti-M, V-M, and Cr-M heterobimetallics (M = Fe, Co, Ni). **L.J. Clouston**, S. Bernales Candia, L. Gagliardi, C. Lu

**12:10 INOR 58.** Computational study of propene polymerization promoted by postmetallocene octahedral systems: playing with steric and electronic factors. **G. Talarico**, P.H. Budzelaar

## Section G

San Diego Convention Center  
Room 31C

### Chemistry of Materials: Metal Organic Frameworks

C. G. Lugmair, *Organizer*

N. B. Shustova, *Presiding*

**8:30 INOR 59.** Structure dependent catalytic activity of bimetallic metal organic framework. **A. Pariyar**, A. Choudhury

**8:50 INOR 60.** Electrochemical investigation of MOFs as intercalation materials for batteries. **D.F. Sava Gallis**, H.D. Pratt, T.M. Anderson, J.S. Chavez, K.W. Chapman

**9:10 INOR 61.** Designing electrochromic MOFs. **K. AlKaabi**, M. Li, M. Dinca

**9:30 INOR 62.** Metal-organic frameworks as a versatile platform for renewable energy applications. **N.B. Shustova**, D.E. Williams, E.A. Dolgoplova, A.M. Rice

**9:50 INOR 63.** Development of engineered forms of metal-organic frameworks for chemical defense applications. **J.B. DeCoste**

**10:10 Intermission.**

**10:25 INOR 64.** Withdrawn.

**10:45 INOR 65.** Layer-by-layer coordinated thin films of metal-organic frameworks (MOFs): New artificial platforms for solar energy capture and directional electronic energy transfer. **M.C. So**, H. Park, D.J. Gosztola, G.P. Wiederrecht, J.D. Emery, A.B. Martinson, S. Er, C. Wilmer, N.A. Vermeulen, J.F. Stoddart, A. Aspuru-Guzik, O.K. Farha, J.T. Hupp

**11:05 INOR 66.** Catalytic hydrocarbon upgrading in metal-organic frameworks. **E. Metzger**, M. Dinca

**11:25 INOR 67.** Dual-ion battery cathode via oxidative insertion of anions in a metal-organic framework. **M.L. Aubrey**, J.R. Long

**11:45 INOR 68.** Electronic conductivity, ferrimagnetic ordering, and reductive insertion in semiquinoid metal-organic frameworks. **L.E. Darago**, M.L. Aubrey, C.J. Yu, M.I. Gonzalez, J.R. Long

## Section H

San Diego Convention Center  
Room 32A

### Harry Gray Award for Creative Work in Inorganic Chemistry by a Young Investigator: Symposium in honor of Eric J. Schelter

L. G. Sneddon, P. J. Walsh, *Organizers*

S. C. Bart, N. C. Tomson, *Presiding*

**8:30** Introductory Remarks.

**8:40 INOR 69.** Understanding the An=E bonds in  $[K(18\text{-crown-6})][An(E)(NR_2)_2]$  (An = Th, U; E = O, S, Se, Te; R = SiMe<sub>3</sub>). **T.W. Hayton**

**9:00 INOR 70.** Tris(pyrrolide) amine ligands as scaffolds for uranium chemistry. **J.M. Boncella**, M. Winston, B. Scott

**9:20 INOR 71.** Building uranium-nitrogen multiple bonds. **S.C. Bart**, N. Anderson, P.E. Fanwick

**9:40 INOR 72.** Covalency in pentavalent uranium. **S.A. Kozimor**, E.R. Batista, D.L. Clark, J. Cross, M.G. Ferrer, H. La Pierre, S.G. Minasian, A. Olson, B. Scott, D.K. Shuh, B. Stein, C. Stieber, P. Yang

**10:00 Intermission.**

**10:20 INOR 73.** Playing with plutonium. **D.L. Clark**, S.A. Kozimor, A. Mounce, E.D. Bauer, J.D. Thompson, H. Yasuoaka, G. Koutroulakis

**10:40 INOR 74.** Californium gleaming. **T.E. Albrecht-Schmitt**

**11:00 INOR 75.** Interesting, albeit brief, journey from Yb to Ac: Applications of f-elements. **K. John**

**11:20 INOR 76.** Characterizing temperature-independent paramagnetism in U(VI) bis-imido complexes. **N.C. Tomson**, B. Scott, J.M. Boncella

## Section I

San Diego Convention Center  
Room 32B

### Chemistry of Materials: Nanomaterials

C. G. Lugmair, *Organizer*

P. O. Adelani, T. J. Boyle, *Presiding*

**8:30 INOR 77.** Synthesis and characterization of PtNiCo nanoparticles with controllable size, shape, and composition. **H. Cronk**, S. Kim, Z. Skeete, S. Shan, D.M. Mott, J. Lou, C. Zhong

**8:50 INOR 78.** Loading gold-carbon nanoparticles on nanodiamonds and diamond platforms. **S. Orefuwa**, M. El Naggari, I. Shehadi, **A. Mohamed**

**9:10 INOR 79.** Magnetic isolation of single-domain FePt nanoparticles for controlled optimization. **P.O. Adelani**, J.D. Rinehart, A.N. Duke

**9:30 INOR 80.** Synthetic approaches to iron selenide nanostructures. **S.E. Ingram**, S.L. Stoll

**9:50 INOR 81.** Recent developments and new challenges in the design of EBID precursors. **J. Pedziwiatr**, Y. Wu, J.A. Brannaka, J. Spencer, H. Fairbrother, L. McElwee-White

**10:10 Intermission.**

**10:25 INOR 82.** Microscopic investigation of chemoselectivity in Ag-Pt-Fe<sub>3</sub>O<sub>4</sub> nanoparticle heterotrimer formation: Mechanistic insights and implications for controlling high-rdred hybrid nanoparticle morphology. **J. Morse**, R. Schaak

**10:45 INOR 83.** On the exploration of a general mechanism of precursor evolution at low temperature to colloidal semiconductor nanocrystals. **K. Yu**

**11:05 INOR 84.** Metal ion exchange in CdS-based molecular clusters. **K.R. Kittilstved**, S. Pittala, M. Mortelliti, F. Kato

**11:25 INOR 85.** Siloxide derivatives of early transition metal alkoxides for production of nanomaterials. **T.J. Boyle**, R.O. Chan, J.M. Sears, P. Lu

**11:45 INOR 86.** Filled tetrahedral semiconductors in the nano-regime: Synthesis and characterization of I-II-V Nowotny-Juza phases. **M.A. White**, M. Thompson, J. Vela-Becerra

**12:05 INOR 87.** DOPED calcium carbonate particles for decolorization of dyes. **H. Ramesh**, K. Radhakrishnan, S. Kumar, A. Raichur

## Section J

San Diego Convention Center  
Room 33A

### Coordination Chemistry: Characterization & Applications

S. A. Koch, *Organizer*

C. J. Daley, *Presiding*

**8:00 INOR 88.** Of triangles and squares: Hierarchical self-assembly of interlinked polyoxometalates. **S. Serapian**, G. Izzet, A. Proust, C. Bo

**8:20 INOR 89.** Synthesis and biological testing of cupric phenanthroline complexes: An alternative to cisplatin? **N. Angel**, J.F. Eichler

**8:40 INOR 90.** Structural and efficacy of some mixed antimalarial drugs-metal complexes. **J.A. Obaleye**, N. Simon, M.O. Bamigboye, A.O. Rajee, A.A. Ajibola

**9:00 INOR 91.** Production of carbon disulfide, a potentially relevant biological small molecule, from different vehicles, including photochemically via a cobalt(III) (1,1)-dithiooxalate-based complex. **A.W. DeMartino**, C. Sun, P.C. Ford

**9:20 INOR 92.** Synthetic inorganic chemistry approaches to the development of transition metal complexes as viable qubits. **J. Zadrozny**, J. Niklas, O. Poluektov, D.E. Freedman

**9:40 INOR 93.** Photoswitching in azobenzene-containing metal-organic framework thin films. **Z. Wang**

**10:00 Intermission.**

**10:10 INOR 94.** Redox-noninnocent and proton-responsive behavior of coordinated bispyrazolyl-pyridine type ligands. **A.V. Polezhaev**, C. Chen, B.J. Cook, K.G. Caulton

**10:30 INOR 95.** Exploring ligand-to-ligand charge-transfer (LL'CT) transitions of Ni(II) coordination complexes. **L.A. Cameron**, A.F. Heyduk

**10:50 INOR 96.** Electrochemical proton reduction using a redox-active W[SNS]<sub>2</sub> cofactor tethered to a Ni center. **K.E. Rosenkoetter**, A.F. Heyduk

**11:10 INOR 97.** Exploring the Mo[SNS]<sub>2</sub> complex as a redox-active cofactor in heterometallic systems. **M. Wojnar**

**11:30 INOR 98.** Cs<sub>2</sub>[H<sub>2</sub>NB<sub>2</sub>(C<sub>6</sub>F<sub>5</sub>)<sub>2</sub>], featuring the first unequivocal 16-coordinate cation. **K. Pörschke**, D. Pollak, R. Goddard

**11:50 INOR 99.** Spectroscopic characterization and application of iron(III) 1,4,7,10-tetra-aza-2,6-pyridinophane derivatives. **S.M. Brewer**, K. Lincoln, K.N. Green

**12:10 INOR 100.** Divergent reactivity of selenoethers with metal reagents: Formation of molecular complexes vs. metal selenide nanoparticles. **S. Mishra**

## Section K

San Diego Convention Center  
Room 33B

### Lanthanide & Actinide Chemistry

A. De Bettencourt Dias, *Organizer*

B. J. Holliday, E. J. Werner, *Presiding*

**8:30 INOR 101.** Excited-state metalloradicals: Luminescent cerium(III) complexes for photo-redox chemistry. **H. Yin**, P.J. Carroll, J.M. Anna, E.J. Schelter

**8:50 INOR 102.** Design and evaluation of selective CMPO-based extractants for f-element separations. **E.J. Werner**, S.M. Biros, M.G. Patterson, D.A. Hardy

**9:10 INOR 103.** Use of lanthanide-MOFs for the detection of VOCs derived from tire burning and crude oil emissions. **C.L. Crawford**

**9:30 Intermission.**

**9:40 INOR 104.** Towards bone-targeting using upconverting nanoparticles decorated with bisphosphonates. **S. Alonso de Castro**, L. Salassa

**10:00 INOR 105.** Excited-state dynamics in heteroleptic ligand environments that are efficient sensitizers of lanthanide ion luminescence. **J. Wilkerson**, A. King, D.J. Strohecker, J. Rack, **B.J. Holliday**

**10:20 INOR 106.** Synthetic routes to multi-metallic f-element complexes with redox-active ligands. **J.H. Farnaby**, J.R. Hickson, N.J. Long

**10:40 Intermission.**

**10:50 INOR 107.** Visible-emitting lanthanide complexes for multicolor imaging. **E. Borbas**

- 11:10 INOR 108.** Lanthanide complexes as potential luminescent markers and temperature probes. **J. Monteiro**, A. De Bettencourt Dias, F. Sigoli
- 11:30 INOR 109.** Photosensitized down-conversion in rare-earth fluoride nanocrystals. **P. Agbo**, T. Xu, R.J. Abergel

## Section L

San Diego Convention Center  
Room 33C

### Organometallic Chemistry: Catalysis

N. S. Radu, *Organizer*

T. Cantat, *Presiding*

- 8:30 INOR 110.** Depolymerization of wood lignin to isolated products using main group and organometallic catalysts. **T. Cantat**, E. Feghali, G. Carrot, C. Genre, P. Thuery
- 8:50 INOR 111.** Synthesis, reactivity, and catalytic applications of iridium pincer complexes. **J.M. Goldberg**, S. Tran, L.M. Guard, S. Bellows, F. Hornig, T.R. Cundari, K.I. Goldberg, D.M. Heinekey
- 9:10 INOR 112.** Directions in pincer chemistry: Progress towards the development of new methodology for catalytic isomerization of internal alkenes to allenenes via C-H bond activation. **N. Phadke**, F. De Jesus Martinez, S. Shafiei-Haghighi, M. Findlater
- 9:30 INOR 113.** Synthesis and reactivity of ruthenium ( $\eta^6$  PCP) complexes with perfluoroethylphosphine substituents. **S. Debnath**, D.M. Roddick
- 9:50 INOR 114.** Synthesis and catalytic activity of air-stable NHC Co(III) pincer complex in C-H borylation. **S.W. Reilly**, M. Zhang, H.U. Valle, C.E. Webster, T.K. Hollis
- 10:10 INOR 115.** Tuning product selectivity in catalytic ethylene tetramerization systems. **A. Lifschitz**, N. Hirscher, J.A. Buss, T. Agapie
- 10:30** Intermission.
- 10:40 INOR 116.** Potential hemi-labile (imino)pyridine palladium(II) complexes as selective ethylene dimerization catalysts: An experimental and theoretical approach. **S. Ojwach**, G. Nyamato, M. Akerman
- 11:00 INOR 117.** Withdrawn.
- 11:00 INOR 1225.** C<sup>+</sup> cyclometalated platinum(II) NHC complexes. **T. Strassner**, A. Tronnier, M. Tenne, J. Soellner
- 11:20 INOR 118.** Ethylene and  $\alpha$ -olefin copolymerization by bimetallic zirconium catalysts. **J. Sampson**, M.N. Akhtar, J. E.A., R. Theravalappil, H.A. Al-Muallem, M. Radlauer, T. Agapie
- 11:40 INOR 119.** Development of chromium compounds supported by chelating multi-aryl ligands for selective ethylene oligomerization. **N. Hirscher**, A. Lifschitz, A.M. Bryan, T. Agapie

### Alpha Olefin Catalysis: Production & Transformations

#### Catalytic Production

Sponsored by I&EC, Cosponsored by CATL and INOR $\ddagger$

### Nobel Laureate Signature Award for Graduate Education in Chemistry: Symposium in honor of Matthew J. Polinski & Thomas E. Albrecht-Schmitt

Sponsored by NUCL, Cosponsored by INOR

## SUNDAY AFTERNOON

### Section A

San Diego Convention Center  
Room 30B

### Undergraduate Research at the Frontiers of Inorganic Chemistry

#### Bioinorganic & Coordination Chemistry

Financially supported by IONIC (Interactive Online Network of Inorganic Chemists)

H. J. Eppley, C. Nataro, *Organizers*

S. K. Goforth, *Presiding*

**1:30** Introductory Remarks.

- 1:35 INOR 120.** Redox-induced ligand switching in mutants of cytochrome c. **K.R. Hoke**, M.R. Chandler, R.J. Quarles
- 1:55 INOR 121.** Sensitive colorimetric assay for light-driven P450 enzymes. **Q. Lam**, M. Kato, L.E. Cheruzel
- 2:15 INOR 122.** Application of molybdate complexes towards the oxidation and hydrolytic chemistry of organophosphate toxins. **L.Y. Kuo**
- 2:35 INOR 123.** Bis- and pendant armed tetraazamacrocyclic transition metal complex dual CXCR4/CCR5 antagonists. **D.J. Davilla**, O. Birdsong, D. Schols, S.J. Archibald, T.J. Hubin
- 2:55** Intermission.
- 3:10 INOR 124.** Multinuclear 51V NMR studies of aqueous vanadium-HEDTA complexes. **D.C. Crans**, X. Wu, B.J. Peters
- 3:30 INOR 125.** Synthetic, spectroscopic, and computational studies of tetraketimide complexes with an emphasis on Group 5. **J.A. Telsner**, P. Damon, C.J. Liss, R.A. Lewis, S. Morochnik, D.E. Szpunar, T.W. Hayton
- 3:50 INOR 126.** Synthesis and reactivity of new N-heterocyclic thione (NHT) and selenone (NHSe) ligands. **M. Styron**, L. Hernandez, M. Kocherga, **D. Rabinovich**
- 4:10 INOR 127.** Synthesis, structure, and catalytic activity of water soluble M-NHC complexes. **R.J. Swails**, S.K. Kariofillis, G.F. Riegel, N.F. Chaudary

### Section B

San Diego Convention Center  
Room 30C

### ACS Award for Distinguished Service in the Advancement of Inorganic Chemistry: Symposium in honor of Vincent L. Pecoraro

#### Metallacrowns

A. F. Peacock, C. M. Zaleski, *Organizers*

B. R. Gibney, *Organizer, Presiding*

G. Mezei, *Presiding*

- 1:30 INOR 128.** Controlling the magnetic anisotropy and the single molecule magnet behavior in trigonal bipyramidal mononuclear Co(II) complexes. **M. Talal**, V.E. Campbell, L. Batchelor, F. Shao, G. Zakhia, R. Guillot, R. Ruamps, N. Guihery, A. Barra, W. Wernsdorfer
- 2:00 INOR 129.** Carboxylate ligand modification of heterotrimetallic metallacrown. **C.M. Zaleski**
- 2:30 INOR 130.** Lanthanide/zinc metallacrowns as advanced near-infrared imaging agents for biological applications. **S. Petoud**, S. Eliseeva, I. Martinic, T.N. Nguyen, E.R. Trivedi, V.L. Pecoraro

- 3:00 INOR 131.** Visible and near-infrared luminescence of heterometallic metallacrowns incorporating Ga(III) and Ln(III) ions. **S. Eliseeva**, C. Chow, I. Martinic, V.L. Pecoraro, S. Petoud
- 3:30** Intermission.

- 3:40 INOR 132.** Molecular control of the magnetic exchange between self-assembled metal-complexes and ferromagnetic surfaces for molecular spintronic devices. **V.E. Campbell**

- 4:10 INOR 133.** Fluorescent pyrrolic macrocycles for tumor imaging. **M.A. Kaster**, N. Chaudhary, K.C. Nielsen, B.A. Corbin, J. Hovey, **E.R. Trivedi**

- 4:40 INOR 134.** Origin of ground state instability in new metallo-dichalcogenolenes. **M.L. Kirk**, J. Yang, P. Basu, D. Kersi, B. Mogesa

- 5:10 INOR 135.** Postsynthetic modifications of metal-organic frameworks. **M.S. Lah**

### Section C

San Diego Convention Center  
Room 30D

### ACS Award in Inorganic Chemistry: Symposium in honor of Mercouri G. Kanatzidis

#### Recent Advances in Inorganic Chemistry

J. A. Aitken, K. Choi, *Organizers*

D. Harris, A. L. Odom, *Presiding*

- 1:30 INOR 136.** Pluripotent nanoparticles with programmable and responsive DNA bonds. **C.A. Mirkin**
- 1:55 INOR 137.** Quantum dot-chemosensor conjugates for profiling metabolic states in tumor biology. **C. Lemon**, D.G. Nocera
- 2:20 INOR 138.** Functional molecular materials based on cobalt(II) spin-crossover building units. **X. Zhang**, H. Xie, Z. Wang, **K.R. Dunbar**
- 2:45 INOR 139.** Spin effects on the physical and photophysical properties of molecular systems. **J.K. McCusker**
- 3:10** Intermission.
- 3:25 INOR 140.** Seeing is believing: Coordination chemistry of molecular imaging probes. **T.J. Meade**
- 3:50 INOR 141.** Advances in the inorganic chemistry of biological nitrogen fixation. **B.M. Hoffman**
- 4:15 INOR 142.** Drawing inspiration from nature with a twist. **M.R. Smith**
- 4:40 INOR 143.** Alkanedithiolate  $\neq$  two alkanethiolates for nickel clusters: How and why. **T.B. Rauchfuss**, F. Arrigoni, G.M. Chambers, L. Yulong, G. Zampella
- 5:05 INOR 144.** New tools for high valent catalyst development. **A.L. Odom**, B. Billow, T. McDaniel

### Section D

San Diego Convention Center  
Room 30E

### ACS Award in Organometallic Chemistry: Symposium in honor of Karen I. Goldberg

Cosponsored by WCC

N. E. Gruhn, M. S. Sanford, *Organizers*

W. D. Jones, *Organizer, Presiding*

B. T. Donovan-Merkert, *Presiding*

- 2:00 INOR 145.** Catalytic, regioselective functionalization of alkyl C-H bonds. **J.F. Hartwig**

- 2:20 INOR 146.** Electrochemically-promoted catalytic asymmetric hydrogenation using C<sub>2</sub>-symmetric rhodium complexes. **B.T. Donovan-Merkert**

- 2:40 INOR 147.** High pressure NMR studies of catalytic alkene hydroformylation and metathesis. **C.R. Landis**, N.J. Beach, S.M. Knapp, A.C. Brezny

- 3:00 INOR 148.** Modeling the controlled burning of organometallics. **T.R. Cundari**

- 3:20 INOR 149.** Iron hydrogenation catalysts relying on ligand-assisted cleavage of dihydrogen. **L. Boisvert**

**3:40** Intermission.

- 3:50 INOR 150.** Homogeneous Ta/Ir tandem catalytic alkane/alkene coupling. **J.E. Bercaw**, J.A. Labinger, D. Leitch, K. Steelman

- 4:10 INOR 151.** New tandem catalytic route for conversion of ethanol to butanol. **S. Chakraborty**, C.E. Hayes, R.T. Baker, **W.D. Jones**

- 4:30 INOR 152.** Investigation of Pd catalysts for the selective methoxycarbonylation of ethylene. **T. Foskey**, L. Huffman, D. Arriola, J. Briggs, K. Frazier

- 4:50 INOR 153.** Catalysts for the decomposition of formic and oxalic acid. **J.M. Boncella**, A. Tondreau, B. Scott

- 5:10 INOR 154.** From fundamentals to catalysis. **D.M. Heinekey**

### Section E

San Diego Convention Center  
Room 31A

### ACS Award in Pure Chemistry: Symposium in honor of Jonathan S. Owen

G. Parkin, *Organizer*

B. Sadtler, *Presiding*

**1:30** Introductory Remarks.

- 1:35 INOR 155.** Size, dimensionality, and strong electron correlation in nanoscience. **L.E. Brus**

- 1:55 INOR 156.** Perovskite fever: Absorbing and emitting light. **H. Zhu**, D. Niesner, X. Zhu

- 2:15 INOR 157.** Electronic doping and redox potential tuning of colloidal semiconductor nanocrystals. **D.R. Gamelin**

- 2:35 INOR 158.** Solid-state chemistry of ternary metal halide nanocrystals. **B. Sadtler**

- 2:55 INOR 159.** Preparation and properties of strongly coupled nanocrystal superlattices: From artificial atoms to mesoscale quantum solids. **C.B. Murray**

**3:15** Intermission.

- 3:35 INOR 160.** Large exciton-energy shifts by reversible surface exchange in 2D II-VI nanocrystals. **Y. Zhou**, F. Wang, **W.E. Buhro**

- 3:55 INOR 161.** Intrinsic surface energy of graphite. **H. Liu**

- 4:15 INOR 162.** Materials complexity frontier: Nanostructure and heterogeneities. **S. Billinge**

- 4:35 INOR 163.** Role of magic-sized clusters in the growth of InP quantum dots. **B.M. Cossairt**, D. Gary, S. Flowers



## Section F

San Diego Convention Center  
Room 31B

**Alfred Bader Award in Bioinorganic or Bioorganic Chemistry: Symposium in honor of Edward I. Solomon**

**Bioinorganic Models**

K. D. Karlin, *Organizer*

P. Kennepohl, *Presiding*

**1:30 INOR 164.** Protein-like hydrogen exchange in a supramolecular structure. K.N. Raymond, W. Hart-Cooper, C. Sgarlata, C. Perrin, D. Toste, R.G. Bergman

**2:00 INOR 165.** Oxygen reduction reaction of a bio-inspired iron porphyrin with 2nd coordination sphere interaction. T. Ohta, P. Nagaraju, Y. Naruta

**2:30 INOR 166.** Bioinorganic nitrogen oxide chemistry with heme and/or copper complexes. S. Hematian, K.D. Karlin

**3:00 INOR 167.** From non-heme [FeNO]<sup>6</sup> to Fe(II)-HNO complexes: One ligand platform can do it all. N. Lehnert, A. Speelman

**3:30** Intermission.

**3:45 INOR 168.** Non-innocent ligands in bioinorganic chemistry: Detailed electronic structure and reactivity. K. Fujisawa

**4:15 INOR 169.** Tuning the relative stability of metastable Mn- and Fe-dioxygen intermediates. J. Kovacs, J. Rees, M.K. Coggins, A. Johansen, B. Leipzig

**4:45 INOR 170.** Amazing nonheme high-valent iron-oxo reactivity landscape. L. Que, M. Puri, A. Biswas

## Section G

San Diego Convention Center  
Room 31C

**F. Albert Cotton Award in Synthetic Inorganic Chemistry: Symposium in honor of Francois P. Gabbaï**

J. D. Hoefelmeyer, T. W. Hudnall, *Organizers*

F. N. Castellano, *Presiding*

**1:30** Introductory Remarks.

**1:35 INOR 171.** Endeavours in chemistry with Francois Gabbaï. H. Schmidbaur

**2:05 INOR 172.** Low-coordination numbers, unusual bonding, and dispersion force effects. P.P. Power

**2:25 INOR 173.** Reactive intermediates from molecular precursors: Intercepting them in solution and launching them into the gas phase. C.C. Cummins, R. Field, J. Jiang, M. Nava, W. Transue, A. Velian, C. Womack

**2:45 INOR 174.** Room temperature stable phosphinidenes and related species. G. Bertrand

**3:05** Intermission.

**3:15 INOR 175.** Carbene-stabilized main group oxides. G.H. Robinson, Y. Wang, H. Schaefer

**3:35 INOR 176.** Stabilizing low valent arsenic and boron using  $\pi$ -accepting carbene ligands. T.W. Hudnall

**Technical program information known at press time.**

The official technical program for the 251st ACS National Meeting is available at:  
[www.acs.org/sandiego2016](http://www.acs.org/sandiego2016)

**3:55 INOR 177.** Stabilization and "transition metal-like" reactivity of low oxidation state/low coordination s- and p-block metal complexes. C. Jones

**4:15 INOR 178.** Syntheses and reactivity studies of boron cations. C. Chiu

**4:35 INOR 179.** Phosphorus-boron and aluminum compounds: Highly reactive boron species & non-innocent ambiphilic ligands. D. Bourissou, B. Chenwa

## Section H

San Diego Convention Center  
Room 32A

**Harry Gray Award for Creative Work in Inorganic Chemistry by a Young Investigator: Symposium in honor of Eric J. Schelter**

L. G. Sneddon, P. J. Walsh, *Organizers*

R. K. Thomson, R. J. Trovitch, *Presiding*

**1:30** Introductory Remarks.

**1:35 INOR 180.** Group 1 and 2 metal alkyl and silyl compounds as precursors for molecular hydrides. J. Okuda

**1:55 INOR 181.** Synthesis of early-transition metals having methylidene and methylidyne ligands. D.J. Mindiola

**2:15 INOR 182.** Redox switchable polymerization processes. P. Diaconescu

**2:35 INOR 183.** Formation of epoxides from olefins via a radical mechanism using atmospheric oxygen in the presence of silver nanoparticles deposited on MCM-41. R.L. Luck, Z. Chen

**2:55 INOR 184.** Application of heterobimetallic catalysts to C-H functionalizations. P.J. Walsh

**3:15** Intermission.

**3:35 INOR 185.** Metalloradical reactivity patterns in even-electron ruthenium complexes: Intermediates and mechanistic insight into bimetallic activation of hydrogen by H-atom transfer. D.H. Berry, M. Noss

**3:55 INOR 186.** Mechanism of bis(imino)pyridine manganese-catalyzed carbonyl hydrosilylation. R.J. Trovitch

**4:15 INOR 187.** Ni(bpy)(cod)-catalyzed hydroboration of ketones, aldehydes, and imines. A.E. King, N. Henson, B. Scott, N.C. Smythe, A.D. Sutton, J.C. Gordon

**4:35 INOR 188.** Single electron transformations to enable cross-couplings via photoredox/Ni dual catalysis. G.A. Molander

## Section I

San Diego Convention Center  
Room 32B

**ExxonMobil Solid State Chemistry Faculty Fellow Award: Symposium in honor of Mircea Dinca**

S. L. Suib, *Organizer, Presiding*

**1:30** Introductory Remarks.

**1:35 INOR 189.** Simple interfaces for complex systems: A little oxide goes a long way. J. Schwartz

**2:00 INOR 190.** High-capacity methane storage in flexible metal-organic frameworks with internal thermal management. J.A. Mason, J. Oktawiec, M.K. Taylor, J. Bachman, J.R. Long

**2:25 INOR 191.** Designer interfaces for energy storage and recovery. Y. Surendranath

**2:50 INOR 192.** Lead free inorganic-organic hybrid perovskites: Chemistry and solar cells. M.G. Kanatzidis

**3:15 INOR 193.** High-temperature ion diffusion in colloidal semiconductor nanocrystals: Diffusion doping and cation exchange. D.R. Gamelin, C. Barrows, P. Chakraborty, L.M. Kornowski

**3:40** Intermission.

**3:50 INOR 194.** Energy transfer in metal-organic frameworks. N.B. Shustova

**4:15 INOR 195.** Proton coupled electron transfer mechanism of oxygen evolution and reduction reactions by molecular cobalt complexes. C. Brodsky, G. Passard, A.M. Ullman, D.G. Nocera

**4:40 INOR 196.** Metaphosphate acids. K. Chakarawet, C.C. Cummins, Y. Jiang, I. Knopf, M. Nava, J. Stauber

**5:05 INOR 197.** Conductive metal-organic frameworks: Fundamentals and applications. M. Dinca, K. Al-Kaabi, M. Campbell, E. Miner, S. Park, D. Sheberla, L. Sun, C.R. Wade

## Section J

San Diego Convention Center  
Room 33A

**Inorganic Catalysts**

S. A. Koch, *Organizer*

M. J. Rose, *Presiding*

**1:30 INOR 198.** Visible-light-driven hydrogen photoproduction with Rh(III) catalysts and platinum nanoparticles loaded on graphene oxides. J. Kim, S. Kim, H. Jang, J.H. Lee

**1:50 INOR 199.** Enhancing electrocatalytic hydrogen evolution by nickel molecular catalysts with the aid of Lewis acids in aqueous media. H. Shao, S. Muduli, P.D. Tran, H. Soo

**2:10 INOR 200.** Improving the efficiency of electrocatalysts for the reduction of CO<sub>2</sub> through supramolecular assembly with amino acid-modified ligands. C.W. Machan, S.A. Chabolla, C.P. Kubiak

**2:30 INOR 201.** Stability and reactivity of ligand capped platinum nanoparticles in the semihydrogenation of alkynes to alkenes. P. Wand, J.D. Bartl, U. Heiz, M. Tschurl, M. Cokoja

**2:50 INOR 202.** Ring-opening polymerization of cyclic esters by ferrocene-chelating heteroscorpionate zinc complexes. M. Abubekurov, P. Diaconescu

**3:10 INOR 203.** Heterobimetallic complexes for cooperative CO<sub>2</sub> reduction. A. Reath

**3:30** Intermission.

**3:40 INOR 204.** Cyclic (alkyl) (amino) carbene copper (I) catalyzed dehydrogenative borylation and  $\alpha$ -hydroboration of terminal alkynes. E.A. Romero, R. Jazzar, G. Bertrand

**4:00 INOR 205.** Lithium cobalt oxides as water oxidation catalysts: Correlating structure, electronic properties, and activity. H. Liu, Y. Zhou, R. More, R. Mueller, T. Fox, G.R. Patzke

**4:20 INOR 206.** Thermodynamic and electrochemical studies of [Ni(bis(diphosphine))]<sub>2</sub><sup>2+</sup> complex in water and organic solvents. B.M. Ceballos, C. Tsay, J. Yang

**4:40 INOR 207.** Attachment of molecular CO<sub>2</sub> reduction catalysts to gold electrodes. M.L. Clark, C.P. Kubiak

**5:00 INOR 208.** Light-driven homogeneous catalytic oxidation of hydrogen. M. Westwood, M.D. Hopkins

**5:20 INOR 209.** Photo-activation of hydrogen by an [FeFe]-hydrogenase model complex. A.E. Nelson, C.F. Works

## Section K

San Diego Convention Center  
Room 33B

**Nanoscience**

R. M. Richards, *Organizer*

J. L. Colon, N. Shukla, *Presiding*

**1:30 INOR 210.** Man-made microrobots in the mouse's stomach: An *in vivo* study. W. Gao, R. Dong, S. Thamphiwatana, L. Zhang, J. Wang

**1:50 INOR 211.** Renal clearance and degradation of glutathione-coated copper nanoparticles. S. Sun, S. Yang, C. Zhou, G. Hao, X. Sun, J. Zheng

**2:10 INOR 212.** Antibacterial activity and biocompatibility of nitrogen-doped titanium dioxide nanoparticles for use in dental resin formulations. A. Zane, R. Zuo, F.A. Villamena, A. Digeorge Foushee, S. Olsen, P. Dutta, A. Nagy

**2:30 INOR 213.** Enantiomeric separations of chiral pharmaceuticals using chiral tetrahedral Au nanoparticles. N. Shukla, D. Yang, Y. Zhao, A. J. Gellman

**2:50** Intermission.

**3:10 INOR 214.** Functionalized nanoparticles for SERS imaging and detection of biomolecular activities. Z. Skeete, J. Li, C. Salazar, C. Manahan, W. Sun, J. Luo, C. Zhong

**3:30 INOR 215.** Folic-acid functionalized polysilsesquioxane nanoparticles for targeted delivery of protoporphyrin-IX. Z. Lyles, B. Loftin, J.L. Vivero

**3:50 INOR 216.** Self-propelled nanomotors autonomously seek and repair cracks. J. Li, J. Wang

**4:10 INOR 217.** Drug delivery using zirconium phosphate layered structured nanomaterials. J.L. Colon, B. Casanas, A. Diaz

## Section L

San Diego Convention Center  
Room 33C

**Organometallic Chemistry: Synthesis & Characterization-Early Transition Metals**

N. S. Radu, *Organizer*

P. J. Fischer, T. P. Hanusa, *Presiding*

**1:30 INOR 218.** Titanium complexes of 2,6-dimesitylphenylisocyanide. P.J. Fischer, C.E. Moore, A.L. Rheingold, J.S. Figueroa

**1:50 INOR 219.** Reaction of group 4 metallacyclopentenes with isonitriles. T.N. Valadez, J.R. Norton

**2:10 INOR 220.** Exploring the reactivity of terminally bound nitriles of titanium. L. Grant, M. Carroll, G. Wu, P.J. Carroll, D.J. Mindiola

**2:30 INOR 221.** Hydroalkylation of internal alkynes via C(sp<sup>3</sup>)-H bond activation of 2,6-dimethyl-N-heterocycles by cationic alkylhafnium complexes supported by dianionic multidentate ligands. M. Lopez, A. Kondo, K. Yamamoto, H. Tsurugi, K. Mashima

**2:50 INOR 222.** Intermolecular zirconium-catalyzed double hydrophosphination of alkynes. C. Bange, R. Waterman

**3:10 INOR 223.** Routes to early transition metal corrole complexes: Synthesis, characterization, and reactivity. J. Ziegler, R.G. Bergman, J. Arnold

**3:30 INOR 224.** Formation of zwitterionic imido complexes upon activation of coordinated nitriles. D.V. Peryshkov, M. Rahman

**3:50 INOR 225.** Withdrawn.

**4:10 INOR 226.** Nitrene metathesis and catalytic nitrene transfer promoted by niobium bis(imido) complexes. **B.M. Kriegel**, L. Grant, R.G. Bergman, J. Arnold

**4:30 INOR 227.** Synthesis in nonpolar solvents: An unexpected mechanochemical parallel. N.C. Boyde, N.R. Rightmire, T.P. Hanusa

**4:50 INOR 228.** Regioselectivity of addition to the  $\pi$ -bond rich  $\text{Tp}^*\text{W}(\text{CO})(\text{HCCH})$  (NCHMe) molecule. **R. Beattie**, P. White, J.L. Templeton

**5:10 INOR 229.** Molybdenum (I) oxidation state: Preparation, characterization, and reactivity of bis(imino)pyridine Mo complexes. **R. Pal**, M. Flores, T.L. Groy, R.J. Trovitch

## Alpha Olefin Catalysis: Production & Transformations

### Alpha Olefin Transformations

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

### Discussions with the President's Task Force on Employment

Sponsored by PRES, Cosponsored by BIOL, BMGT, CARB, CELL, CHED, CINF, COLL, COMSCI, DAC, GEOC, I&EC, IAC, INOR, MEDI, ORGN, PHYS, PMSE, POLY, PROF, S&CB and WCC

### Industrial Research at the Interface of Inorganic Chemistry & Polymer Science

Sponsored by POLY, Cosponsored by BMGT and INOR†

## SUNDAY EVENING

### Section A

San Diego Convention Center  
Hall D

### ACS Award for Distinguished Service in the Advancement of Inorganic Chemistry: Symposium in honor of Vincent L. Pecoraro

B. R. Gibney, A. F. Peacock, C. M. Zaleski, Organizers

#### 6:00 - 8:00

**INOR 230.** Synthesis and crystal structure of a disodium metallacrown complex with bridging chloroacetate anions. **C. Daly**, M. Zeller, C.M. Zaleski

**INOR 231.** Understanding ligand complexation upon heavy metal binding into different geometries within *de novo* three-stranded coiled coil proteins. **L. Ruckthong**, M.L. Zastrow, J. Stuckey, V.L. Pecoraro

**INOR 232.** Withdrawn.

**INOR 233.** Exploration of single-molecule magnetism of a family of  $[\text{Ln}^{\text{III}}_4\text{Mn}^{\text{II}}_4]$  ( $\text{Ln}^{\text{III}} = \text{Y}^{\text{III}}, \text{Dy}^{\text{III}}, \text{Ho}^{\text{III}}, \text{Er}^{\text{III}}$ ) compound. **T.T. Boron**, A.H. Davis, J.W. Kamp, C.M. Zaleski, V.L. Pecoraro

**INOR 234.** Nitrite-nitro cobalt(III) compound as a carrier prototype for antitumor drugs. **B.M. Pires**, A.J. Bortoluzzi, **R.B. Faria**, M. Scarpellini

**INOR 235.** *De novo* designed metallopeptides: An unexpected binuclear Cu(I) site. **C. Mocny**, F. Yu, J.E. Penner-Hahn, V.L. Pecoraro

**INOR 236.** Fluorinated phthalocyanines as dual-mode fluorescent and MRI contrast agents. **M.A. Kaster**, N. Chaudhary, E.R. Trivedi

**INOR 237.** Combined spectroscopic and DFT investigations of Ni(II) complexes with tridentate ligands containing  $\text{NO}_2$ ,  $\text{N}_2\text{O}$ , and  $\text{N}_3$  donor spheres. **C.S. Mullins**, J.A. Berlanga, C.A. Grapperhaus, L. Bishop

**INOR 238.** Synthesis and crystal structure of a two-dimensional terbium-aluminum metallacrown-like compound. **G. Van Trieste**, M. Zeller, C.M. Zaleski

**INOR 239.** Consequences of methionine oxidation on the structural and functional properties of human calprotectin. **F. Yu**, E.M. Nolan

**INOR 240.** Many faces of designed metalloproteins: From heavy metal sequestration to nitric oxide reduction. **S. Chakraborty**, V.L. Pecoraro, Y. Lu

**INOR 241.** Synthesis and crystal structure of a two-dimensional network of aluminum metallacrowns. **J. Travis**, M. Zeller, C.M. Zaleski

**INOR 242.** Ring metal substitution of 12-metallacrown-4 compounds. **I. Kuhn**, C.M. Zaleski

**INOR 243.** Highly luminescent  $\text{Ga}_2\text{Ln}_2$  metallacrown complexes. **T.N. Nguyen**, S. Eliseeva, C. Chow, J.W. Kamp, S. Petoud, V.L. Pecoraro

**INOR 244.** Metallacrowns as novel near-infrared optical imaging probes for necrotic cells. **I. Martinic**, S. Eliseeva, T.N. Nguyen, V.L. Pecoraro, S. Petoud

**INOR 245.** Glutamate induced asymmetric binding of transition metals in *de novo* designed helical heterotrimers. **A. Tolbert**, C. Mocny, V.L. Pecoraro

**INOR 246.** Exploring metallacrowns: Novel  $\alpha$ -hydroxy hydroxamic acid ligands, platinum, and thermogravimetric analysis. **N.A. Law**, N. Duffy, K. Buxton

**INOR 247.** Designing an antiparallel, asymmetric three-stranded coiled coil. **K. Diffley**, C. Mocny, V.L. Pecoraro

**INOR 248.** Enhanced two-dimensional dispersion of supported group V metal oxides on silica. **J. Grant**, C. Carrero, A. Love, R. Verel, I. Hermans

**INOR 249.** Copper(II) complexes of pyridine and amide donor ligands as precursors to oxidation catalysts. **J. Bodwin**

**INOR 250.** Selective incarceration and extraction of oxoanion contaminants from aqueous media by self-assembled nanojars. **B.M. Ahmed**, B. Szymczyna, S. Jianrattanasawat, G. Mezei

**INOR 251.** Use of non-natural amino acids to bind metals in *de novo* designed 3-stranded coiled coils. **C. White**, K. Koebke, V.L. Pecoraro

**INOR 252.** Telescoping synthesis as an efficient, green method for preparing unsymmetrically derivatized pyrazole ligands. **B.M. Ahmed**, **G. Mezei**

**INOR 253.** Incorporation of electron transfer motifs in synthetic bacterial microcompartment shell proteins. **J.S. Plegaria**, C. Kerfeld

**INOR 254.** Structure and dynamics of the HNOX domain of the human soluble guanylate cyclase. **I.H. Saraiva**, M.C. Almeida, **M. Matzapetakis**

**INOR 255.** Utilization of copper-catalyzed alkyne-azide cycloaddition coupling in luminescent gallium based metallacrowns. **J.C. Lutter**, S. Eliseeva, J.W. Kamp, S. Petoud, V.L. Pecoraro

**INOR 256.** Novel non-chrome thin organic hybrid coatings for coil applications. **T.S. Smith**, B.D. Bammel, J. Comoford, G.T. Donaldson, J.D. McGee, J. Zimmerman

**INOR 257.** Analysis of physical properties of thiodiphenol epoxy resins cured with dicyandiamid. **C. Lim**, D. Kim, S. Kwon, S. Lee, B. Seo

### Section A

San Diego Convention Center  
Hall D

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

S. A. Koch, Organizer

#### 6:00 - 8:00

**INOR 258.** Withdrawn.

**INOR 259.** Assessing density functionals for simulations of structural, redox, and spectroscopic properties of [FeFe]-hydrogenases. **S. Niu**, H. Li, M.B. Hall

**INOR 260.** Novel optical trends in heme enzymes explained by density functional theory. **A. Graves**, M.D. Liptak

**INOR 261.** Biomimetic CFCs degradation: An insight into biotic halogen cycling. **M.A. Crick**, S.K. O'Shea

**INOR 262.** Identification of disulfide bonds by planned digestion and tandem mass spectrometry. **S. Park**, E. Jung, S. Lee

**INOR 263.** Redox non-innocent ligands on first row transition metals: Towards bio-inspired catalysts for C-H bond activation. **J. Bogart**, S.A. Cook, A. Borovik

**INOR 264.** Heme nitric oxide/oxygen binding protein and its role in regulating a bifunctional cyclic-di GMP-processing phosphodiesterase and cyclase in *Agrobacterium vitis*. **D.E. Williams**, N. Nesbitt, S. Muralidharan, L. Nisbett, E.M. Boon

**INOR 265.** NiSOD model complexes that probe the catalytic and electronic implications of a Ni-coordinated Cys-Thiol. **R.A. Steiner**, K.J. Martin, T.C. Harrop

**INOR 266.** Pterin reduction in chemical models of the molybdenum cofactor. **S. Zhu**, B.R. Williams, S.J. Nietzer Burgmayer

**INOR 267.** Comparison of S-H bond vs. S-Au bond beyond the isolobal relationship between proton and gold-phosphine anion. **S. Ding**, D. Crouthers, J. Denny, R.D. Bethel, C. Hsieh, M.B. Hall, M.Y. Darensbourg

**INOR 268.** One Fe(III) model complex for the active site of 2,4'-dihydroxyacetophenone dioxygenase (DAD). **J. Li**, M. Molenda, F.A. Chavez

**INOR 269.** Probing the structural difference between Ca(II) and Pb(II) bound syt1. **C.M. Dashnaw**, J.W. Karr

**INOR 270.** Investigation into the synthesis and characterization of derivatized electrochemical biosensors utilizing a biotin-ferrocene platform. **M. Burnett**, M. Goulet, K.N. Green

**INOR 271.** Using P450 BM3 as a model system to study stability as it relates to the catalytic cycle. **C.A. Denning**, D.K. Heidary, E.C. Glazer

**INOR 272.** Developing a novel dimetallic synthetic model complex for carbon monoxide oxidation. **J.J. O'Connor**, C. Williams, D. Rokhsana

**INOR 273.** Synthetic modeling of the organometallic active site of mono-iron hydrogenase: Fe-acyl complexes derived from CNS (S = thioether, thiophene) and CNP (P = PPh<sub>2</sub>) chelates. **Y. Cho**, M.J. Rose

**INOR 274.** Synthetic modeling of mono-iron hydrogenase: CNS Chelates supporting an iron-hydride species, substitution reactions, and C-H activation of TMAO. **Z. Xie**, M.J. Rose

**INOR 275.** Molybdenum pyranopterin dithiolene complexes: Investigating the steric effects on molybdenum cofactor models. **A. Nagelski**, D.R. Gisewhite, B.R. Williams, S.J. Nietzer Burgmayer

### Section A

San Diego Convention Center  
Hall D

### Chemistry of Materials

C. G. Lugmair, Organizer

#### 6:00 - 8:00

**INOR 276.** Time-resolved observation of reduction kinetics of iron oxides by *in situ* XAFS measurement. **K. Kimijima**, Y. Niwa, R. Muraio, M. Kimura

**INOR 277.** Stable blue phosphorescence Iridium(III) cyclometalated complexes prompted by intramolecular hydrogen bond in ancillary ligand. **S. Kim**, Y. Cho, J. Kim, S. Yi, W. Han, S.O. Kang

**INOR 278.** Synthetic design of cationic porous frameworks for anion immobilization and separation. **X. Bu**, X. Zhao

**INOR 279.** Synthesis and structural characterization of a unique ammonium borate containing a heptaborate anion. **D. Neiner**, Y. Sevryugina, D.M. Schubert

**INOR 280.** Development of lanthanide tagged nanoparticle (T-NP) system for tracking of underground fluid flow. **L.J. Treadwell**, T.J. Boyle, A.C. Cappuccilli, D.T. Yonemoto, P. Lu

**INOR 281.** Adsorption of amyloid beta peptide by metal-organic frameworks. **Z. Mensinger**, B. Cook, E. Wilson

**INOR 282.** Comparative study of *in situ* and pre-synthesized x-pillar ligand in self-assembly of homochiral porous frameworks. **E.T. Nguyen**, X. Zhao, X. Bu

**INOR 283.** CdSe/CdS core-shell nanocrystal sensitizers for molecule-nanocrystal photon upconversion. **Z. Huang**, M.L. Tang

**INOR 284.** Reductive sonochemical synthesis of superparamagnetic nanoparticles (SPMNs). **A.C. Miller**, D.J. Casadonte

**INOR 285.** Fabricating nanowires using site-specific attachment of gold nanoparticles and nanorods to DNA origami templates. **J.K. Jensen**, B. Upreti, K. Lee, J. Harb, R. Davis, A. Woolley

**INOR 286.** Lanthanide separation through size-selective crystallization of homochiral metal-organic frameworks. **X. Zhao**, C. Mao, P. Feng, X. Bu

**INOR 287.** Synthesis of metal-organic frameworks for carbon capture. **M. Cosio**, S.A. Fordham, H. Zhou

**INOR 288.** Postsynthetic cyclodehydrogenation of a large pore zirconium based metal-organic framework. **G. Pour**, F. Uribe-Romo

**INOR 289.** Electrografting organoboron compounds for applications in materials chemistry and catalysis. **S.E. Shaner**, F. Mujid, S. Doden

**INOR 290.** Soft-template synthesis of 3D porous graphene foams with tunable architectures for supercapacitors. **C. Ma**, S. Tong, J. Shen, D. Zhang, Y. Feng, Y. Yu, Y. Liu, Y. Min

**INOR 291.** Investigation of graphene oxide films. **J. Shen**, S. Mo, D. Zhang, Y. Liu, Y. Min

**INOR 292.** Hollow carbon nanospheres: Application and properties. **C. Zhang**

**INOR 293.** Investigating MOF mixed-matrix membranes with cellulose polymers. **J. Moreton**, M.S. Denny, S. Cohen

**INOR 294.** Metal-organic frameworks constructed from crown ether-based 1,4-benzenedicarboxylic acid derivatives. **T. Chen**, S. Cohen

**INOR 295.** Nanobowls: Creating silica-alumina interfaces to tune metal oxide behavior. **M.A. Ardagh**, Z. Bo, J.M. Notestine

**INOR 296.** Structural optical studies of copper sulphide nanocrystals by solvothermal synthesis from single molecule precursors. **P.A. Ajibade**, N.L. Botha

**INOR 297.** New approaches to the chemical syntheses of azamacrocyclic compounds. **E.J. Parish**, **H. Honda**, T. Wei, M. Hsiao

**INOR 298.** Highly connected rare-earth molecular building blocks: Assembly of iso-reticular porous metal-organic frameworks having novel topology. **A. PuthanPeedikakkal**, D. Alezi, L. Weselinski, V. Guillemin, Y. Belmabkhout, A. Cairns, Z. Chen, L. Wojtas, M. Eddaoudi

**INOR 299.** New approaches to the development of donor-sigma-acceptor materials for organic rectifiers. **Y. Lo**, **H. Shyu**, **W. Huang**, H. Honda, T. Wei

**INOR 300.** Production of anatase pigment by hydrolysis of low concentration TiOSO<sub>4</sub> solution via short sulfate process. **C. Tian**

**INOR 301.** Flow-driven precipitation in the magnesium and calcium carbonate systems. **B. Bohner**, T. Pivarscik, D. Horvath, A. Toth

**INOR 302.** Achiral routes to the synthesis of chiral inorganic open frameworks and their luminescence properties. **S.L. Wang**

**INOR 303.** Enhancing the visible-light absorption of TiO<sub>2</sub> with the use of key N, Co, and Na dopant concentrations. **Y. Han**, C. Yang

**INOR 304.** Synthesis of highly porous monolithic InNbO<sub>4</sub> aerogels. **R. Lord**, R. Baghi, L. Hope-Weeks

**INOR 305.** 3D DNA origami templated nanoscale device fabrication. **K. Lee**, J.K. Jensen, B. Uprety, R. Davis, J. Harb, A. Woolley

**INOR 306.** Towards the preparation of highly and functionalized porous covalent organic frameworks. **D.A. Vazquez-Molina**, F. Uribe-Romo, M. Lum

**INOR 307.** Preparation of CdTe quantum dots supported on modified silica gel. **K. Silva**, D.V. Freitas, J.M. Dias, M. Navarro

**INOR 308.** Synthesis of polyarylboranes: A new and diverse class of organic/inorganic hybrid materials. **M.W. Lee**

**INOR 309.** Increasing charge transport in metal-organic frameworks via generation of mixed-valency. **R.M. Torres-Gavosto**, L.E. Darago, J.R. Long

## Section A

San Diego Convention Center  
Hall D

### Coordination Chemistry: Characterization & Applications

S. A. Koch, *Organizer*

6:00 - 8:00

**INOR 310.** Withdrawn.

**INOR 311.** Squaramide metal-organic frameworks as catalysts. **X. Zhang**, Z. Zhang, J.A. Boissonnault, S. Cohen

**INOR 312.** Spectroelectrochemistry and reactivity of hexacoordinate polypyridylsilicon(IV) complexes. **D.M. Peloquin**, D.R. Dewitt, P. Tran, J. Pope, J. Merkert, B.T. Donovan-Merkert, T.A. Schmedake

**INOR 313.** Rhenium-manganese dinuclear carbonyl complexes as long wavelength absorbing photoCORMs. **Z. Li**, A. Pierri, P.C. Ford

**INOR 314.** Syntheses, spectroscopic characterization, and *in vitro* antibacterial activities of some metal (II) complexes of 2[(E)-(1H-indol-5ylimino)methyl]-6-methoxyphenol. **A.A. Osowole**, **A.O. Abiola**

**INOR 315.** Structure, electrochemistry, and photophysical properties of an Exocyclic di-ruthenium complex and its application as a photosensitizer. **S. Salpage**, B. Som, A. Paul, T. Banerjee, K. Hanson, M.D. Smith, A.K. Vannucci, L.S. Shimizu

**INOR 316.** Combined EPR and *ab initio* multiconfigurational studies of dirhodium(II,III) carboxylates and amidates and computational insight into dirhodium(II,III)-nitrene intermediates. **T. Yang**, K.P. Kornecki, J.F. Berry

**INOR 317.** Synthesis, structure, characterization, and photophysical properties of four copper(I) complexes containing polypyridyl ligands. **A. Báez**, V. Miranda Soto, M.P. Parra Hake, J.D. Campos-Gaxiola, H. Höpfl, A. Cruz-Enriquez

**INOR 318.** Phenylendiamine and phenazine-derived sulfonamides for fluorescent and optical sensing of toxic metals. **I. Lehman-Andino**, N. Bertolotti, G.G. Pena, K. Kavallieratos

**INOR 319.** Coordination chemistry of the rhodizonate anion: Towards understanding the Na-rhodizonate test for Pb. **J.A. Silverman**, E.V. Govor, K. Kavallieratos

**INOR 320.** Mn(II) complex of a new mixed pendant arm cyclen-based ligand: A correlation between chemical structure and relaxivity. **P. Brauchle**, S. Hensiek, T.D. Westmoreland

**INOR 321.** pH and temperature dependent <sup>17</sup>O NMR relaxivities of Mn(II) complexes as a probe of solution speciation and water coordination. **S. Briggs**, A. Lee, T.D. Westmoreland

**INOR 322.** Kinetic and mechanistic investigations on metal-assisted (Zn, Au) thiolate-disulfide exchange. **G.S. Garusinghe**, A.E. Bruce, M.R. Bruce

**INOR 323.** Development of chiral, tridentate, mer-coordinating, nitrogen-based ligands for use in enantioselective catalysis. **K. Zivkovic**, A. Villaseñor, F.F. Faucher, C. Alcocer, C.J. Daley

**INOR 324.** MOF-assisted organic synthesis of drug molecules from natural sources. **J. Garcia**

**INOR 325.** <sup>1</sup>H relaxation rate ratios as a probe of solution speciation for labile manganese (II) complexes. **D.W. Laurenza**, T.D. Westmoreland

**INOR 326.** Water stable metal-organic frameworks for gas separation. **X. Zhang**, **W. Shi**, P. Cheng

## Section A

San Diego Convention Center  
Hall D

### Main Group Chemistry

T. W. Hudnall, *Organizer*

6:00 - 8:00

**INOR 327.** Sodium borohydride amine complexes: A simple way to organic borohydride salts. **S. Schneider**, S.F. Deplazes, **C. Gibson**, Y. Ahmed

**INOR 328.** Bis-bipyridylsilicon(IV) diols as potential dual hydrogen bond donors for chiral catalysis. **C. Waters**, T.A. Schmedake

**INOR 329.** Synthesis of the frustrated Lewis pair dichloro(8-quinolyl)gallium(III) and its reaction with chloroform. **J.J. Fostvedt**, S.R. Tamang, J. Son, J.D. Hoefelmeyer

**INOR 330.** 5-(azido-alkyl)-1H-tetrazoles: Synthesis and characterization. **Y.O. Ahmed**, C. Gibson, S.F. Deplazes, S. Schneider

**INOR 331.** Lithium borohydride complexes of tetrazole derivatives. **S.F. Deplazes**, S. Schneider, Y.O. Ahmed, A.M. Beauchamp, C. Gibson

**INOR 332.** Selective defluorination of polyfluoroaromatics by alkyl-monophosphines. **A.R. Arevalo**, **J.J. Garcia**

**INOR 333.** Rapid synthesis of hypercloso-[B<sub>12</sub>(OR)<sub>12</sub>] dodecaalkoxy derivatives. **A.I. Wixtrom**, Y. Shao, S. Kevork, J.C. Axtell, S. Khan, A.M. Spokoyin

**INOR 334.** Synthesis and characterization of carbene-supported boron(II) radicals and radical cations. **A. Ledet**, T.W. Hudnall

**INOR 335.** Ligation of trialkyl antimony to open- and closed-shell first-row transition metals: Copper luminescence and complexes of cobalt and nickel. **M.J. Rose**

**INOR 336.** C-C coupling and sp<sup>2</sup> C-H bond activation catalyzed by transition metal complex (M = Pd<sup>II</sup> and Cu<sup>I</sup>) with the ambiphilic ligand 8-quinolyldimesitylborane. **S.R. Tamang**, J.D. Hoefelmeyer

## Section A

San Diego Convention Center  
Hall D

### Organometallic Chemistry: Catalysis

N. S. Radu, *Organizer*

6:00 - 8:00

**INOR 337.** Halogen exchange reactions on *o*-, *m*- & *p*-carborane cages for cancer imaging and therapy. **K. Ishita**, A. Khalil, R. Tiwari, W. Tjarks

**INOR 338.** Computational modeling of Hg-catalyzed methane oxidation in sulfuric acid. **S. Butler**, J.T. Fuller, D. Ess

**INOR 339.** Low-valent Ni catalyzed transfer hydrogenation of benzonitriles with diols as hydrogen source. **J.A. Garduño**, J.J. Garcia

**INOR 340.** From a DFT perspective, Milstein's chemistry can be related to a simple ion-pair formation and slippage metathesis mechanism. **F. Hasanayn**, L. Assi, R. Maousawi

**INOR 341.** Olefin metathesis with Ru-based catalysts containing N-heterocyclic carbenes attached to fullerenes. **A. Poater**, M. Solà, J. Martínez

**INOR 342.** Ruthenium complexes bearing metal-coordinated phosphonates for water oxidation. **J.M. Kamdar**, D.C. Marelius, C.E. Moore, A.L. Rheingold, D.K. Smith, D.B. Grotjahn

**INOR 343.** Stoichiometric reactivity of ruthenium-pincer complexes relevant to polar bond hydrogenation. **L. Le**, A.R. Chianese

**INOR 344.** Bifunctional ruthenium catalysts for the hydrogenation of polar bonds. **T.N. Cervarich**, A.R. Chianese

**INOR 345.** Highly active and (E)-selective bifunctional 16-electron ruthenium monoisomerization catalyst. **E.R. Paulson**, C.E. Moore, A.L. Rheingold, D.B. Grotjahn

**INOR 346.** Withdrawn.

**INOR 347.** Synthesis and water oxidation activity of sterically hindered [Ru(CI)(terpy)pyridyl(naphthyridine) Cl] analogs; an attempt at fluorinated oxidatively resilient ligands. **D.C. Marelius**, R. Shirey, F. Barnare, D.B. Grotjahn

**INOR 348.** Introducing a κ<sup>4</sup>-diazadiene Co(II) hydride catalyst for alkyne hydroboration. **H. Ben-Daat**, T.L. Groy, R.J. Trovitch

**INOR 349.** Comparative insights into the carbon-hydrogen activation of cycloalkanes by cyclopentadienylcarbonylrhodium and trispyrazolylborate-rhodium complexes. **G. Jia**, M.B. Hall

**INOR 350.** Redox control of an aluminum ring-opening polymerization catalyst. **J. Wei**, **P. Diaconescu**

**INOR 351.** Gold(I) catalyzed hydroamination of alkenes and alkynes using hemilabile phosphine ligand. **S. Immedi**, C. Hahn

**INOR 352.** Investigation and exploration of transition metal catalysis for site selective C-H bond functionalizations. **D. Kumar**, S. Vemula, R.C. Cook

**INOR 353.** Tuning five-coordinate trisboryl iridium catalyst reactivity through ligand modification. **B. Ghaffari**, B.A. Vanchura, G.A. Chotana, R.E. Maleczka, M.R. Smith

**INOR 354.** Development of new cyclometalated palladium complexes and their catalytic activity in carbon-carbon bond cross coupling reactions. **D. McAteer**, Y. Niyonzima, E. Javed, R. Mroz, **S. Huo**

**INOR 355.** Withdrawn.

**INOR 356.** Synthesis of nickel POCOP-pincer complexes for the catalytic hydrophosphination of unsaturated organic molecules. **A. Roering**, **J. Kraai**

**INOR 357.** Half-sandwich organometallic complexes incorporating a triazenido ligand functionalized with pyridine. **A.F. Velazquez Ham**, A. Aguilar, J.L. Gomez Lopez, M.P. Parra Hake, V. Miranda Soto

## Section A

San Diego Convention Center  
Hall D

### Organometallic Chemistry: New Ligand Platforms

N. S. Radu, *Organizer*

6:00 - 8:00

**INOR 358.** Ruthenium(II) coordination to pyridylidene remote N-heterocyclic carbenes: A complex story. **T. Cao**, D.C. Marelius, J.M. Kamdar, A.L. Rheingold, C.E. Moore, D.B. Grotjahn

**INOR 359.** Heteroatom polyaromatic hydrocarbon systems with nitrogen ligands. **W. Cross Lopez**, T. Haden, J. Herring, S.M. Kruse, S.K. Hurst

**INOR 360.** Design and synthesis of "para-pyridine-PCP" iridium complexes and their activity as catalysts for alkane dehydrogenation. **N. Lease**, A. Alape Seetharam, S. Martinez, T. Zhou, M. Blessent, A.S. Goldman, K. Krogh-Jespersen

**INOR 361.** Synthesizing redox-active ligand based first row transition metal complexes and studying their catalytic applications. **A. Saini**

**INOR 362.** Yttrium-alkyl complexes supported by a ferrocene-based phosphinimine ligand. **J.L. Brosmer**, P. Diaconescu

**INOR 363.** Synthesis of chiral ligands. **M. Talley**, **W. Walker**, **R. Stokes**, **D. Michaelis**

**INOR 364.** Synthesis and complexation of new multitopic non-chelating N-heterocyclic carbenes. **D. Tapu**, A. Carter, R. Justice

**INOR 365.** Rhodium and Iridium complexes derived from new annulated N-heterocyclic carbenes: Synthesis and catalytic studies. **D. Tapu**, O.J. Buckner, B. Norvell, C. Boudreaux

**INOR 366.** Cooperative reactivity of (PSIP)Rh pincer complexes. **T. Donnell**



**INOR 367.** Synthesis and characterization of iron half-sandwich complexes. J. Kephart, E.B. Hulley

**INOR 368.** Transition metal complexes of boron-containing heterocycles for multi-electron small molecule activation. L. Essex, W. Harman

## Section A

San Diego Convention Center  
Hall D

### Organometallic Chemistry: Synthesis & Characterization-Early Transition Metals

N. S. Radu, *Organizer*

6:00 - 8:00

**INOR 369.** Novel Cr(III)-HMC acetylides complexes: Preparation and emission properties. S. Tyler, E. Judkins, T. Ren

**INOR 370.** Novel reactivity in an anionic iron-nitride cluster. M.J. Drance, J.S. Figueroa

**INOR 371.** Reaction of  $WN(NR_2)_3$  complexes with alkyl halides. A.J. Touchton, M.M. Nolan, A. Koley, L. McElwee-White

## Section A

San Diego Convention Center  
Hall D

### Undergraduate Research at the Frontiers of Inorganic Chemistry Bioinorganic Chemistry

H. J. Eppley, C. Nataro, *Organizers*

6:00 - 8:00

**INOR 372.** Creation and characterization of rubrerythrin and symerythrin model proteins. J. Pellegrino, K.A. Bell, R. Polinski, S. Cimerol, A.B. Jacobs, E.I. Solomon, A.J. Reig

**INOR 373.** Structural and functional characterization of G4DFsc variants containing a 4-His/3-carboxylate active site. K. O'Shea, J. Dorsheimer, K. Biernat, A.B. Jacobs, E.I. Solomon, Y. Wu, W.F. Degrado, A.J. Reig

**INOR 374.** Modeling myo-inositol oxygenase (MIOX) using the *de novo* four-helix bundle protein G4DFsc. C. Philip, K. Drost, C.L. Kanya, A.J. Reig

**INOR 375.** Structural analysis of a novel group of biomimetic complexes for the active site of nickel acireductone dioxygenase (Ni-ARD). B.Z. Nabona, C.M. Gonzales, D.A. Ivan, S. Sanchez, S.A. Toledo

**INOR 376.** Characterization of copper(I) binding to the Sp1 zinc finger domains. A.M. Blumenreich, N.L. Mandel, M.D. Storlie, M.L. Stevens, K.E. Splan

**INOR 377.** Investigating the role of riboflavin binding protein in copper transport and storage in oviparous species. H. Masood, S.R. Smith, J.I. Matchynski

**INOR 378.** Cloning, expression, and characterization of novel hydroquinone ring-cleaving dioxygenases. E.R. Altman, T.E. Machonkin

**INOR 379.** Synthesis and characterization of  $V^O_2(3\text{-methoxysalicylaldehyde semicarbazone})$ . J. Hempfing, V.P. McCaffrey

**INOR 380.** Synthesis and characterization of Fe(II) coordination complexes and their reactivity with hydrogen peroxide. R.E. Coleman, K.N. Trotter, N. Arulsamy, E.B. Hulley

**INOR 381.** Thermodynamics of Zn(II) and surrogate metal ions binding to the glucocorticoid receptor DNA-binding domain. P. Luong, M.C. Carpenter, D. Wilcox

**INOR 382.** New octahedral cobalt(III) complex as a possible anti-cancer prodrug: Synthesis and characterization studies in solid state and solution. N. Joe, A. Morris

**INOR 383.** Sensing of biologically relevant anions with a luminescent europium(III) complex. K.H. Felix, K. Johnson, E.J. Werner

**INOR 384.** Synthesis and characterization of symmetric and asymmetric water soluble zinc(II) model complexes for liver alcohol dehydrogenase. N.A. Bernier, C.A. Van Akin, J.R. Miecznikowski

## Section A

San Diego Convention Center  
Hall D

### Undergraduate Research at the Frontiers of Inorganic Chemistry Computational Chemistry

H. J. Eppley, C. Nataro, *Organizers*

6:00 - 8:00

**INOR 385.** Redox potentials of ruthenium complexes to understand catalytic ability in water. A.A. Lopez, R.M. Adams, S. Bellows, T.R. Cundari

**INOR 386.** Oxidation states "naturally": A natural bond orbital study. F.P. Neil, M. Chelsea, J.S. D'Acchioli, A. Webster

**INOR 387.** Theoretical modeling of the asymmetric hydroamination-cyclization of aminoallenes by tantalum amide alkoxide complexes. G.S. Phun, R.J. Cave, A.R. Johnson

**INOR 388.** Mechanistic details of hydrogen evolution with  $[Cp^*Rh(phen)(MeCN)]^{2+}$  calculated by DFT. S.L. Corona, S.I. Johnson, L.M. Aguirre Quintana, H.B. Gray, J.R. Winkler, J.D. Blakemore, W.A. Goddard

## Section A

San Diego Convention Center  
Hall D

### Undergraduate Research at the Frontiers of Inorganic Chemistry

#### Coordination Chemistry

H. J. Eppley, C. Nataro, *Organizers*

6:00 - 8:00

**INOR 389.** Evaluating the physical and catalytic properties of complexes containing quinolyl arylsulfonamide ligands. M. Gole, B.C. Chan, A.R. O'Connor

**INOR 390.** Electrochemical investigation of tris(triphenylphosphine)rhodium(I) chloride and its analogues utilizing cyclic voltammetry. J. Turner, A. Weinick, B. Ross, A.J. Warhusen

**INOR 391.** Synthesis and characterization of TPAP. H.M. Bui, Z. Thammavongsy, J. Yang

**INOR 392.** Tripodal CMPO ligands as potential lanthanide extractants: A systematic study of ligand structure and selectivity in acidic aqueous media. M.G. Patterson, D.A. Hardy, S.M. Biros, E.J. Werner

**INOR 393.** Structure function relationships of multinuclear copper(II) carboxylate metal-omesogens. B. Musselman, K.A. Wheeler, T.W. Clayton

**INOR 394.** Reactivity of nitric oxide with  $[Fe(D(G_2tren)](triflate)_2$ . K. Gomez, A. Speelman, N. Lehnert, R.C. Scarrow

**INOR 395.** Reactivity of Rh and Ni silylamides. L. Qiu

**INOR 396.** Degrading organophosphate toxins: Fundamental studies of molybdate-mediated phosphonothioate hydrolysis. K.M. Dill, L.Y. Kuo

**INOR 397.** Aluminum alkoxide complexes prepared with tridentate  $\gamma$ -aminoalcohols. K.J. Goosherst, D.B. Green, J.M. Fritsch

**INOR 398.** Synthesis of early-late heterobimetallic compounds for fluorescence studies. C. Heaney, A. Hill

**INOR 399.** Design and characterization of bis(terpyridyl)chromium(III) complexes with enhanced visible absorption and emission. A.J. Kim, A.P. Grorud, B.M. Lovaasen

**INOR 400.** Structures of five-coordinate aluminum alkoxide complexes that polymerize  $\epsilon$ -caprolactone and L-lactide. A. Longo, A.L. Rheingold, J.M. Fritsch

**INOR 401.** Development of a biomimetic catalyst for dechlorination reactions. I. Lee, K.M. Van Heuvelen

**INOR 402.** Hydrosilylation activity of iron complexes supported by conjugated  $\alpha$ -diimine ligands. A. Volkov, G.N. Tran, M. Takemura, K.A. Wheeler, H.M. Hoyt

**INOR 403.** Carbon monoxide powered alkaline fuel cell operational at ambient condition. D. Shlian, J. Jiang

**INOR 404.** Structure function relationships of cobalt complexes with pendant bases in the secondary coordination sphere. R. Combs, J.F. Khosrowabadi, J. Yang

**INOR 405.** Synthesis of gold(III) complexes for chelation-assisted functionalization of strong,  $sp^2$ -hybridized C-H bonds. J.E. Thompson, K.M. Gilmore, R.L. Marley, A.R. McCormick, E.E. Heine, C.P. Owens, N.A. Curry, A. Brown, E. Robbins, M.K. Phillips, A.L. Rheingold, D.R. Weinberg

**INOR 406.** Mechanistic investigation of the molybdenum catalyzed oxidation of key phosphines and sulfides. C. Jamieson

**INOR 407.** Photochemical reactivity of a binuclear Fe(I)-Fe(I) hydrogenase model compound with cyano ligands. A. Hunt, J. Barrett, M. McCurry, C.F. Works

**INOR 408.** Zinc catalysts for the formation of bio-renewable polymers. E.G. Thalacker, J.F. Dunne

**INOR 409.** Exploration of the photochemical capabilities of cerium(IV) hexachloride. J. Hertzog, H. Yin, K.C. Mullane, P.J. Carroll, E.J. Schelter

**INOR 410.** Ionothermal synthesis and characterization of  $[EMIM]_4[CoS_4(Co(P_2S_6)_2)_2]$ ,  $[EMIM]_2[Cr(P_2S_6)_2]$ , and  $[EMIM]_2[Mn(P_2S_6)_2]$ . C. Juillerat, J.A. Cody

## Section A

San Diego Convention Center  
Hall D

### Undergraduate Research at the Frontiers of Inorganic Chemistry Environmental Chemistry

H. J. Eppley, C. Nataro, *Organizers*

6:00 - 8:00

**INOR 411.** Metallating ligands in catalyst development for carcinogens in groundwater. S. Kim, K.M. Van Heuvelen

**INOR 412.** Synthesis and characterization of ruthenium (II) complexes and their reactivity with  $ClO_2^-$ . K.N. Trotter, R.E. Coleman, N. Arulsamy, E.B. Hulley

**INOR 413.** Combatting organophosphate toxins with molybdenum-peroxo complexes. A. Bennett, L.Y. Kuo

**INOR 414.** Developing bio-inspired catalysts for dechlorination. K. Ariola, K.M. Van Heuvelen

**INOR 415.** Green metal binding for a brighter future. A. Russell, C. Butler, A.M. Schoffstall, R.M. Henry

**INOR 416.** Metal-organic frameworks with embedded basic sites for heavy metal capture from aquatic environments. C. Fast, T.A. Makal

**INOR 417.** Degradation of organophosphate pesticides using molybdenum (VI) oxides and ion exchange resin. G. Mehlhaff, L.Y. Kuo

## Section A

San Diego Convention Center  
Hall D

### Undergraduate Research at the Frontiers of Inorganic Chemistry

#### General

H. J. Eppley, C. Nataro, *Organizers*

6:00 - 8:00

**INOR 418.** Expanding the frontiers of inorganic chemistry. H.J. Eppley, C. Nataro, A.K. Bentley, E.R. Jamieson, A.R. Johnson, B.A. Reisner, J.L. Stewart, S.R. Smith, L.A. Watson, N. Williams

**INOR 419.** Incorporation of research in the undergraduate inorganic chemistry curriculum: IONIC VIPER workshops. S.K. Goforth, P.J. Fischer, C. Nataro

## Section A

San Diego Convention Center  
Hall D

### Undergraduate Research at the Frontiers of Inorganic Chemistry

#### Main Group Chemistry

H. J. Eppley, C. Nataro, *Organizers*

6:00 - 8:00

**INOR 420.** Aluminum complexes of redox-active ligands: Synthesis, characterization, and preliminary reaction studies. P.M. Wise, T.M. Herb, C. Koelner, A. Poitras, B.E. Cole, J. Bogart, N.A. Piro, P.J. Carroll, W.S. Kassel, E.J. Schelter, C.R. Graves

**INOR 421.** Redistribution reactions in organosiloxane complexes of 1-oxo-2-pyridinone. A.E. Ryan, W.W. Brennessel, J.G. Koch, B.M. Kraft

## Section A

San Diego Convention Center  
Hall D

### Undergraduate Research at the Frontiers of Inorganic Chemistry

#### Materials & Solid-State Chemistry

H. J. Eppley, C. Nataro, *Organizers*

6:00 - 8:00

**INOR 422.** Targeted synthesis of metal-organic frameworks for gas storage and hydrocarbon separations. J.F. Melville, M. Kapelewski, J.R. Long

**INOR 423.** Unique crystalline composite displaying three primary zoning events in the solid state and based upon self-assembled, helical coordination polymers. S. Cornell, S.R. Seidel

**INOR 424.** Coupling electrochemical and fluorescence investigations of failure modes in aerospace coating systems. K. Hull, E. Blidodeau, E. Sapper, C.E. Immoos

**INOR 425.** Synthesis of mixed metal metal-organic frameworks via ion-exchange in solution. S. Shaker, C. Malonzo, A. Stein

**INOR 426.** Synthesis, characterization, and growth kinetics of surface modified zinc oxide quantum dots. **A.D. Mena**, B. Colon, D. Francis, P.P. Vaughan, A. Schrock, K. Molek

**INOR 427.** Synthesis of photoactive gold nanoparticles for biomedical applications. **I. Musri**, **T. Lafferty**, **E. Park**

**INOR 428.** Potential nonlinear optical applications for high-temperature solid state and lithium polysulfide flux synthesized diamond-like semiconductors,  $\text{Li}_2\text{-II-IV-S}_4$ . **A. Weiland**, J. Brant, J. Zhang, J.A. Aitken

**INOR 429.** Cation exchange of copper iron sulfide nanoparticles. **A. Kim**, R.M. Kozloski, K. Plass

**INOR 430.** Gold nanoparticle aggregation: The role of capping agent and aqueous environment. **E.R. Carlson**, K. Roberts, A.K. Bentley

**INOR 431.** Energy storage by  $\text{MnO}_2$ -nanoparticle composite supercapacitors. **B.T. Hohman**, L.M. Santino, A.K. Bentley

**INOR 432.** Design and synthesis of cholesteric liquid crystalline porphyrin VOC sensors. **Z.R. Gregg**, M.E. Zick, M.E. Langton, E.L. Smith, J.C. Kranick, L.J. Tucker, J.L. O'Donnell

**INOR 433.** Improved synthetic methodologies for synthesizing polymeric subunits that incorporate extended aromatic acceptors and transition metal chromophores. **J. Callihan**, K.A. Walters

**INOR 434.** Stark absorption studies on supramolecular small molecules and polymers that connect fullerenes and transition metal chromophores. **S. Siemer**, K.A. Walters

**INOR 435.** Supramolecular organometallic sensitized solar cells: Advances in measurement procedures and refinement of cell preparation. **H. Hearn**, K.A. Walters

**INOR 436.** Temperature dependent phase behavior of pluronic F127 triblock copolymers in water. **J. Kim**, Y. Han, Z. Zhang, G. Smith, C. Do

**INOR 437.** Meso-structured styrene / butyl acrylate films containing  $\text{ZnO}$  quantum dots: Stability and fluorescence. **B. Colon**, A. Mena, K.S. Molek, A. Schrock

**INOR 438.** Developing a method to identify potential targets for zeolite encapsulation using computational techniques. **N. Robinson**, J. Burkett

**INOR 439.** Synthesis and characterization of titanium oxide nanopowders. **L. Barnes**, H. Hamilton, K.A. Reyes, C.J. Van Leeuwen, K. Molek

**INOR 440.** Synthesis and physicochemical characterization of quaternary, narrow-bandgap tellurides containing earth-abundant elements. **B. Hogan**, J.A. Aitken

**INOR 441.** Single-step electrodeposition of zinc oxide nanosheets on a compact layer for dye-sensitized solar cell photoanodes. **A. Lim**, H. Van Ryswyk

**INOR 442.** Surface passivation of copper sulfide nanoparticles with tetrathiomolybdate. **M.A. Tomat**, Z.N. Georgieva, C. Kim, K. Plass

**INOR 443.** Solvothermal synthesis of  $\text{Cu}_2(\text{Zn}_{1-x}\text{Co}_x)\text{SnS}_4$  solid solutions and kinetics of methylene blue adsorption. **A. Sharma**, A.H. Pinto, R. Penn

**INOR 444.** Synthesis and characterization of cobalt-zirconium heterobimetallic materials for photocatalysis. **N.G. Celia**, M.W. Bedford, I.R. Bogcaz, M.M. Gadzuk-Shea, C.L. Jahncke, A. Hill

**INOR 445.** Characterization liquid crystalline copper (II) m-toluate dimers. **D. Hong**, T.W. Clayton

## Section A

San Diego Convention Center  
Hall D

### Undergraduate Research at the Frontiers of Inorganic Chemistry Organometallic Chemistry

H. J. Eppley, C. Nataro, *Organizers*

6:00 - 8:00

**INOR 446.** Palladium(II) thiocrown and oxathiacrown complexes with cyclometalating ligands. **M.A. Bruening**, D.E. Janzen

**INOR 447.** Synthesis and reactivity of compounds containing 1,1'-bis(phosphino)metallocene ligands. **R.J. Dupuis**, E.P. Warnick, C. Nataro

**INOR 448.** Tetrahedral compounds with bis(phosphino)ferrocene ligands. **S.F. Hartlaub**, A.G. Furneaux, C. Nataro

**INOR 449.** Synthesis and reactivity of compounds with 1,1'-bis(phosphino)ferrocenediyl ligands. **V.A. Decker**, B.L. Blass, N.K. Lauricella, C. Nataro

**INOR 450.** Exploration of the catalytic reactivity of iron-NHC complexes. **L.G. Habgood**, C.E. Hedges

**INOR 451.** Synthesis of group VI pentacarbonyl complexes containing a bidentate phosphine ligand. **H. Drake**, B.J. Bellott

**INOR 452.** Electronic and steric properties of a modified proazaphosphatranes: Tri(pyridylmethyl)azaphosphatranes. **I. Kha**, Z. Thammavongsy, J. Yang

**INOR 453.** Norbornene polymerization initiated by cationic ( $\eta$ -allyl)nickel(II) complexes containing dialkylbiaryl phosphine ligands. **C. Lee**, A.R. O'Connor

**INOR 454.** Synthesis of molybdenum carbon dioxide complexes via oxidation of a carbonyl ligand. **G. Lorzing**, J. Vasta, M. Pogash, X. Duan, M.E. Graziani, R. Carden, J. Ohane, P.M. Graham

**INOR 455.** Mechanistic investigation of Tantalum amide-alkoxide catalyzed asymmetric hydroamination of aminoallenes. **M. Kosich**, A.R. Johnson

**INOR 456.** Synthesis and catalytic activity of water soluble *N*-heterocyclic carbene complexes. **S.K. Kariofillis**, R.J. Swails

**INOR 457.** Synthesis and application of a water soluble Pd-NHC catalyst toward Heck coupling in aqueous solvents. **G.F. Riegel**, R.J. Swails

**INOR 458.** Synthesis and reactivity of nickel silylamides. **M. Schaff**, M. Whited

**INOR 459.** Withdrawn.

## Section A

San Diego Convention Center  
Hall D

### Undergraduate Teaching at the Frontiers of Inorganic Chemistry

*Cosponsored by CHED*

B. A. Reisner, J. L. Stewart, *Organizers*

6:00 - 8:00

**INOR 460.** Writing research proposals across the undergraduate curriculum: Adapting a VIPeR Learning Object for use in multiple courses. **J.L. O'Donnell**, J.W. Karr

**INOR 461.** Exploring scientific communication using infographics. **R.M. Jones**

**INOR 462.** Teaching at the frontiers: Creating an appropriate scaffold the primary literature in a sophomore level inorganic course. **S.R. Smith**

**INOR 463.** Leveraging collegiate consortia to develop literature-based inorganic laboratory experiments. **L.G. Habgood**, K.J. Young

**INOR 464.** Development of synthetic teaching labs for crystallographic analysis. **O. Phillips**, L.Y. Kuo

**INOR 465.** Creating correspondence between teaching and research by "converting" the teaching laboratory to a research laboratory. **R.E. Bachman**

**INOR 466.** Online homework for foundations of inorganic chemistry: A new frontier! **S.G. Sobel**

### My Comments to the President's Task Force on Employment

*Sponsored by PRES, Cosponsored by BIOL, BMGT, CARB, CELL, CHED, CINF, COLL, COMSCI, DAC, GEOC, I&EC, IAC, INOR, MEDI, ORGN, PHYS, PMSE, POLY, PROF, SCHB and WCC*

### My Experience with & Advice for Improving Diversity in Chemistry

*Sponsored by PRES, Cosponsored by BIOL, CELL, CHED, CINF, COLL, COMSCI, DAC, GEOC, I&EC, INOR, MEDI, ORGN, PHYS, POLY, PROF and WCC*

### My Experiences in & Advice for Organic Chemistry Courses

*Sponsored by PRES, Cosponsored by BIOL, CELL, CHED, CINF, DAC, GEOC, I&EC, INOR, MEDI, ORGN, POLY and PROF*

## MONDAY MORNING

### Section A

San Diego Convention Center  
Room 20A-C

### ACS Awards in Inorganic Chemistry: Plenary Session

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

C. Turro, *Presiding*

**8:15 INOR 467. Award Address (ACS Award in Inorganic Chemistry sponsored by Aldrich Chemical Company, LLC).** New inorganic solids from synthesis in molten chalcogenide salts: Structural diversity to applications. **M.G. Kanatzidis**

**8:45 INOR 468. Award Address (ACS Award for Distinguished Service in the Advancement of Inorganic Chemistry sponsored by Strem Chemicals, Inc.).** Metallacrowns: From fundamental supramolecular chemistry to SMMs and near IR optical imaging agents. **V.L. Pecoraro**

**9:15 INOR 469. Award Address (Harry Gray Award for Creative Work in Inorganic Chemistry by a Young Investigator sponsored by the Gray Award Endowment).** Advances in coordination chemistry to improve the sustainability of the rare earth elements. **E.J. Schelter**

**9:45 INOR 470. Award Address (Earle B. Barnes Award for Leadership in Chemical Research Management sponsored by the Dow Chemical Company Foundation).** Development of sustainable alternatives for the next generation of chemicals and materials: Leadership in development of renewably-sourced materials. **H.E. Bryndza**

10:15 Intermission.

**10:25 INOR 471. Award Address (ACS Award in Organometallic Chemistry sponsored by the Dow Chemical Company Foundation).** Mechanistic understanding of fundamental organometallic reactions for catalyst development. **K.I. Goldberg**

**10:55 INOR 472. Award Address (F. Albert Cotton Award in Synthetic Inorganic Chemistry sponsored by the F. Albert Cotton Endowment Fund).** Lewis acidic and redox properties of organoantimony compounds: From anion sensing to catalysis. **F.P. Gabbai**

**11:25 INOR 473. Award Address (ACS Award in Pure Chemistry sponsored by the Alpha Chi Sigma Fraternity and the Alpha Chi Sigma Educational Foundation).** Synthesis and coordination chemistry of colloidal quantum dots. **J.S. Owen**

**11:55 INOR 474. Award Address (Alfred Bader Award in Bioinorganic or Bioorganic Chemistry sponsored by the Alfred R. Bader Fund).** Dioxigen binding, activation, and reduction to  $\text{H}_2\text{O}$  by Cu enzymes. **E.I. Solomon**

### Frontiers in Inorganic Chemistry

*Sponsored by SOCED, Cosponsored by INOR*

### Is There a Crisis in Organic Chemistry Education?

*Sponsored by PRES, Cosponsored by BIOL, CELL, CHED, CINF, DAC, GEOC, I&EC, INOR, MEDI, ORGN, POLY and PROF*

## MONDAY AFTERNOON

### Section A

San Diego Convention Center  
Room 30B

### Undergraduate Teaching at the Frontiers of Inorganic Chemistry

#### Innovations in the Classroom

*Cosponsored by CHED*

J. L. Stewart, *Organizer*

B. A. Reisner, *Organizer, Presiding*

**1:30 INOR 475.** New frontier: Foundations of inorganic chemistry to include non-inorganic chemists. **G.P. Wulfsberg**

**1:50 INOR 476.** Chemical philately and education: Teaching inorganic chemistry with postage stamps. **D. Rabinovich**

**2:10 INOR 477.** Apps to aid teaching inorganic chemistry. **C.C. Raymond**

**2:30 INOR 478.** Designing an undergraduate course in organometallic chemistry based on IONiC VIPeR learning objects. **D.A. Laviska**

**2:50 INOR 479.** Using and adapting VIPeR learning objects at Albion College. **V.P. McCaffrey**

Technical program information known at press time.

The official technical program for the 251st ACS National Meeting is available at:

[www.acs.org/sandiego2016](http://www.acs.org/sandiego2016)



**3:10 INOR 480.** Refreshing your local inorganic chemistry course with VIPER learning objects: Adventures in adaptation. **K.A. Marek**

**3:30 INOR 481.** Teaching molecular orbital theory and computational chemistry at the frontiers of inorganic chemistry. **J.L. Stewart**

## Section B

San Diego Convention Center  
Room 30C

### ACS Award for Distinguished Service in the Advancement of Inorganic Chemistry: Symposium in honor of Vincent L. Pecoraro Metallopeptides

B. R. Gibney, C. M. Zaleski, *Organizers*

A. F. Peacock, *Organizer, Presiding*

M. Matzapetakis, *Presiding*

**1:30 INOR 482.** De novo design of metalloproteins. **W.F. Degrado**

**2:00 INOR 483.** Coordination chemistry of designed metalloproteins: Insight into the biological function of natural metalloproteins. **B.R. Gibney**

**2:30 INOR 484.** Coiled coils as ligands for "non-biological" metal ions: New applications for metalloproteins. **A.F. Peacock**, M.R. Benwick, L.N. Slope, S.L. Newton, M. Britton

**3:00 INOR 485.** Protein-based radical (Trp<sup>•</sup> and Tyr<sup>•</sup>) intermediates and intramolecular electron transfer in mono- and bi-functional heme peroxidases. **T. Kuhl, A. Ivancich**

**3:30** Intermission.

**3:40 INOR 486.** Molecular factors that drive mitochondrial Fe-S cluster biosynthesis. **T.L. Stemmler**

**4:10 INOR 487.** Environmental nitrogen oxide abatement by single-site microporous catalysts. **M. Caudle**

**4:40 INOR 488.** Designing metalloenzyme inhibitors to be in-VINCE-able. **S. Cohen**, Y. Chen, C.V. Credille, C. Perez

**5:10 INOR 489.** Bionanotechnology-based enabling technologies. **S. Daunert**

## Section C

San Diego Convention Center  
Room 30D

### ACS Award in Inorganic Chemistry: Symposium in honor of Mercurio G. Kanatzidis

#### Synthesis & Applications of Solid State Materials

J. A. Aitken, K. Choi, *Organizers*

D. E. Freedman, P. F. Poudeu Poudeu, *Presiding*

**1:30 INOR 490.** How do we design materials for flexible hybrid electronic circuitry? **T.J. Marks**

**1:55 INOR 491.** Graphene-based supercapacitor. **R.B. Kaner**, M.F. El-Kady, Y. Shao, J. Hwang, L.J. Wang, K. Marsh, M. Li, H. Wang, M. Kowal, S. Dubin, W. Sun, R. Li, L. Chaney, S. Cho, R. Rizvi

**2:20 INOR 492.** Layered metal oxide nanosheets as model surfaces for understanding nanoparticle-support interactions. **M. Strayer**, T.P. Sentfle, J.P. Winterstein, N.M. Vargas-Barbosa, R. Sharma, R.M. Rioux, M.J. Janik, **T.E. Mallouk**

**2:45 INOR 493.** 2D inorganic nanosheets as efficient building blocks for exploring new functional nanohybrids. **S. Hwang**

**3:10** Intermission.

**3:25 INOR 494.** Multiscale heterostructured materials. **G.D. Stucky**

**3:50 INOR 495.** Ordered Pd based nanoparticles as low cost, highly efficient, and robust catalysts alternative to Pt in fuel cell applications. **S. Peter**

**4:15 INOR 496.** Sulfur chemistry in electrochemical energy storage. **K.A. See**, M.M. Butala, V. Doan-Nguyen, **R. Seshadri**

**4:40 INOR 497.** Energy and innovation in the chemical industry. **S.S. Dhingra**

**5:05 INOR 498.** Synthesis, modification, and utilization of BiVO<sub>4</sub> photoanodes. **K. Choi**

## Section D

San Diego Convention Center  
Room 30E

### ACS Award in Organometallic Chemistry: Symposium in honor of Karen I. Goldberg

*Cosponsored by WCC*

N. E. Gruhn, W. D. Jones, M. S. Sanford, *Organizers*

A. S. Goldman, J. M. Mayer, *Presiding*

**2:00 INOR 499.** Bonding in organometallic compounds of the actinide elements: Coordination and novel complexes. **B.E. Bursten**

**2:20 INOR 500.** Chemical surprises at the frontier of the periodic table. **J.L. Kiplinger**

**2:40 INOR 501.** Toward the development of high oxidation state iridium catalysts for alkane dehydrogenation. Lewis-acid catalyzed olefin insertion/ $\beta$ -hydrogen elimination. **Y. Gao**, C. Guan, Z.H. Syed, A.M. Wright, K. Allen, D.M. Heinekey, K. Krogh-Jespersen, K.I. Goldberg, **A.S. Goldman**

**3:00 INOR 502.** Platinum(II) complexes for C-H activation ligated by phosphite ligands. **K.A. Grice**, J. Kostarut, A.E. Lawando, E.J. Crespo, R. Sommer

**3:20 INOR 503.** New taggants for monitoring underground fluid flows. **L.J. Treadwell**, J.M. Sears, T.J. Boyle, B.A. Hernandez-Sanchez, R.F. Hess, J.E. Miller, A.C. Cappuccilli, C.D. Cannan, T.M. Roper, M. Spilde, **R.A. Kemp**

**3:40** Intermission.

**3:50 INOR 504.** Thermal and photochemical reactions mediated by water-soluble host-guest supramolecular systems. **R.G. Bergman**

**4:10 INOR 505.** Metal and non-metal catalyzed reactions with sulfenate anions. **P.J. Walsh**

**4:30 INOR 506.** Synthesis and reactivity of mono- and bimetallic complexes of a novel bisimidazole phosphine ligand. **B.M. Cossairt**, M. Norris, S. Flowers

**4:50 INOR 507.** CpCo(III) fluoride and fluoroalkyl complexes: Selective C-F bond abstraction, C-C bond formation and catalyzed fluorination of acyl chlorides. **M. Leclerc**, G.M. Lee, J.M. Bayne, S. Gorelsky, D.J. Harrison, M. Vasiliu, D.A. Dixon, **R. Baker**

**5:10 INOR 508.** Understanding the reactivity of reduced ZnO and TiO<sub>2</sub> nanocrystal. **J.M. Mayer**, C. Valdez, J. Peper, R. Mitsuhashi, T. Porter

## Section E

San Diego Convention Center  
Room 31A

### ACS Award in Pure Chemistry: Symposium in honor of Jonathan S. Owen

G. Parkin, *Organizer*

J. E. Bercaw, *Presiding*

**1:30 INOR 509.** Catalysis at Dow: Vignettes in olefin production & polymerization. **P.N. Nickias**

**1:50 INOR 510.** Diazaphospholanes and enantioselective catalysis. **C.R. Landis**, F. Foarta, B.R. Jones

**2:10 INOR 511.** Pentanuclear and heptanuclear copper hydrides. **J.R. Norton**, M.S. Eberhart, S. Liu, M.C. Neary

**2:30 INOR 512.** Applications of tetradentate and tridentate tripodal ligands for catalytic and stoichiometric transformations involving zinc and magnesium. **S. Ruccolo**, M. Rauch, W.I. Sattler, M. Rostami Chajjan, **G. Parkin**

**2:50** Intermission.

**3:10 INOR 513.** Oligo or poly? A mechanistic interpretation of a switchable catalyst. **J.A. Labinger**, J.E. Bercaw, E. Despagne-Ayoub

**3:30 INOR 514.** High spin electronic structures in cluster design. **T. Betley**

**3:50 INOR 515.** Carbon dioxide hydrogenation catalysts encapsulated in the metal organic framework UiO-66. **J.A. Byers**, C. Tsung, Z. Li, J.V. Morabito, K.F. Beal, L. Chou

**4:10 INOR 516.** Small molecule activation with metal complexes supported by ligands with pendant arene moieties. **T. Agapie**

## Section F

San Diego Convention Center  
Room 31B

### Alfred Bader Award in Bioinorganic or Bioorganic Chemistry: Symposium in honor of Edward I. Solomon

#### Bioinorganic Enzymology

K. D. Karlin, *Organizer*

T. E. Machonkin, *Presiding*

**1:30 INOR 517.** Electron flow through metalloproteins. **H.B. Gray**

**2:00 INOR 518.** Genetically encoded sensors to monitor the spatial distribution of zinc in cells. **A.E. Palmer**

**2:30 INOR 519.** Thermodynamic contributions to the metalloprotein reduction potential. **M. Creteau**, **D. Wilcox**

**3:00 INOR 520.** Metal-induced aggregation of human gamma-D crystallin: Insights into the bioinorganic chemistry of cataracts disease. **L. Quintanar**, J. Dominguez-Calva, E. Serebryany, C. Haasse-Pettingell, J. King

**3:30** Intermission.

**3:45 INOR 521.** Distance, conjugation, and torsional dependence of molecular electronic coupling. **M.L. Kirk**, D. Shultz, B. Stein, D. Habel-Rodriguez, D.E. Stasiw, C. Tichnell

**4:15 INOR 522.** Cuprous oxidase motifs in multi-copper oxidases: Structural identification and cladistic analysis. **D. Kosman**, P. Hart, S. Hardies

**4:45 INOR 523.** Oxygenase chemistry of the versatile diiron cluster. **J.D. Lipscomb**, R. Banerjee, C.J. Knoot, B.S. Rivard, A.J. Komor

## Section G

San Diego Convention Center  
Room 31C

### F. Albert Cotton Award in Synthetic Inorganic Chemistry: Symposium in honor of Francois P. Gabbaï

J. D. Hoefelmeyer, T. W. Hudnall, *Organizers*

C. R. Wade, *Presiding*

**1:30** Introductory Remarks.

**1:35 INOR 524.** My secret life as a main group chemist. **J.A. Gladysz**

**1:55 INOR 525.** New BN isosteres of polycyclic aromatic hydrocarbons. **W.E. Piers**, M. Morgan, E. Patrick, D. Spasyuk

**2:15 INOR 526.** Boracycles in Lewis acid chemistry and conjugated materials development. **F. Jaekle**

**2:35 INOR 527.** Studies of the coupling reactions of carbonyl sulfide (COS) and epoxides. Formation of cyclic- and poly(thiocarbonates). **D.J. Darensbourg**

**2:55** Intermission.

**3:05 INOR 528.** Experimental and computational approaches to understanding and implementing weak forces involving anions and aromatic  $\pi$ -systems. **J.F. Ellenberger**, S. Gomez-Coca, I.D. Giles, H.T. Chifitides, **K.R. Dunbar**

**3:25 INOR 529.** New single-molecule magnets with high blocking temperatures. **S. Demir**, P.C. Bunting, K.R. Meihaus, J. Zadrozny, **J.R. Long**

**3:45 INOR 530.** Sustainable manufacturing of functional materials. **C.J. Carmalt**

**4:05 INOR 531.** Kinetically controlled synthesis of stable metal-organic frameworks. **H. Zhou**

**4:25 INOR 532.** Energy storing photochemistry with first row transition metal complexes. **B.L. Anderson**, S. Hwang, A.G. Maher, D.C. Powers, **D.G. Nocera**

## Section H

San Diego Convention Center  
Room 32A

### Harry Gray Award for Creative Work in Inorganic Chemistry by a Young Investigator: Symposium in honor of Eric J. Schelter

L. G. Sneddon, P. J. Walsh, *Organizers*

C. R. Graves, J. R. Walensky, *Presiding*

**1:30** Introductory Remarks.

**1:35 INOR 533.** Xenon: New applications in materials chemistry and biosensing. **Y. Wang**, B.W. Roose, B.A. Riggie, I.J. Dmochowski

**1:55 INOR 534.** Competitive heavy atom kinetic isotope effects expose bond forming steps in carbon dioxide reduction catalysis by transition metal complexes. **A.M. Angeles Boza**

**2:15 INOR 535.** Synthesis and characterization of aluminum complexes of redox-active nitroxide-based ligands. **C.R. Graves**

**2:35 INOR 536.** Boron formates as surrogates for hydroboranes: Metal free dehydrogenation and disproportionation of formic acid. **T. Cantat**, C. Chaiver

**2:55 INOR 537.** Group 13 and 15 systems stabilized by electron rich ligands. **J.D. Masuda**

**3:15** Intermission.

**3:35 INOR 538.** Coordination chemistry and reactivity of polynuclear group 11 amidinate and carboxylate complexes. **J.R. Walensky**, P. Rungthanaphathophon, A. Lane

- 3:55 INOR 539.** Organosilane reactivity in solvent-borne epoxy coatings. **J.R. Robinson**, N. Caggiano, S.C. Korf, K. Adamsons, B.E. Priore
- 4:15 INOR 540.** Synthesis and coordination chemistry of chelating guanidinylligands. **N.A. Piro**, W.S. Kassel
- 4:35 INOR 541.** New approaches to the synthesis of group 6 metal-element multiple bonds. **R.K. Thomson**

## Section I

San Diego Convention Center  
Room 32B

### Earle B. Barnes Award for Leadership in Chemical Research Management: Symposium in honor of Henry E. Bryndza

*Cosponsored by ENVR, ORGN and POLY*

M. Harmer, N. S. Radu, *Organizers, Presiding*

#### 1:30 Introductory Remarks.

**1:35 INOR 542.** 20 years of the presidential green chemistry challenge awards: A perspective on chemistry innovation. **D.J. Constable**

**2:05 INOR 543.** Safety by design: Integration of safety / toxicology considerations into the early research process. **J.R. Damewood**

**2:35 INOR 544.** Only the best is good enough: The LEGO group's journey to leave a positive impact. **N. van der Pui**

#### 3:05 Intermission.

**3:15 INOR 545.** Framework to guide selection of chemical alternatives. **T. Fryberger**

**3:45 INOR 546.** Role of the EPA in deploying safer chemicals in both products and manufacturing processes. **J. Jones**

## Section J

San Diego Convention Center  
Room 33A

### Frontiers in Heavy Element Inorganic Chemistry

*Cosponsored by NUCL*

D. K. Shuh, L. Soderholm, *Organizers*

D. L. Clark, *Organizer, Presiding*

#### 1:30 Introductory Remarks.

**1:40 INOR 547.** Early metal chemistry featuring redox non-innocent (RNI) ligands. **P.T. Wolczanski**, S.P. Heins, N. Livezey, S.N. MacMillan, E.B. Lobkovsky

**2:00 INOR 548.** Bis-arene complexes of technetium and rhenium; with and without metal-metal bonds. **R.A. Alberto**, H. Braband, M. Bachmann, G. Meola, P. Schmutz

**2:20 INOR 549.** Metalloporphyrin monolayers as platforms for 3D organization of functional materials. **M.D. Hopkins**, W. Lau, J. Kamm

**2:40 INOR 550.** Mid-valent, early transition metal mononuclear and dinuclear chemistry (as inspired by Al Sattelberger), and novel  $\pi$ -donor ligand clusters as kinetic products. **L. Messerle**

**3:00 INOR 551.** Sustainable acetylde chemistry: 3d metals and tetraazamacrocycles. **T. Ren**, S.F. Tyler, T. Cook, S.N. Natoli, S.D. Banziger

#### 3:20 Intermission.

**3:40 INOR 552.** Adventures with stronger and weaker metal-metal bonds. **A.W. Maverick**, L.G. Butler

**4:00 INOR 553.** Coordination chemistry of 2,2'-biphenylenedithiophosphinate and diphenyldithiophosphinate with U, Np, Pu, and Am. **J. Macor**, S.R. Daly, A. Gaunt, S.A. Kozimor, **G.S. Girolami**

**4:20 INOR 554.** Mechanistic insights into carbon-carbon reductive elimination from tetrabenzyluranium. **S.C. Bart**, S.A. Johnson

**4:40 INOR 555.** Super electron-rich diiron dithiolate analogues of the active site of the [FeFe]-hydrogenases. **T.B. Rauchfuss**, X. Zhou, F. Arrigoni, G. Zampella

## Section K

San Diego Convention Center  
Room 33B

### Organometallic Compounds & Catalysts: Influence on Polymer Science & Synthesis

T. Y. Meyer, *Organizer*

D. E. Bowen, *Organizer, Presiding*

L. Rosenberg, *Presiding*

#### 1:30 Introductory Remarks.

**1:35 INOR 556.** Palladium and nickel catalysts for olefin polymerization and copolymerization with polar monomers. **C. Chen**, S. Dai, M. Chen

**1:55 INOR 557.** Synthesis of polyarylphosphonates and metallopolymers based upon a spirocyclic bisphosphite. **R.A. Stockland**

**2:15 INOR 558.** Phosphine-sulfonate palladium(II) catalysts with rigid, aliphatic backbones for copolymerization of ethylene and polar monomers. **R.E. Black**

**2:35 INOR 559.** Critical role of polymerization catalysis in the production advanced tire elastomers. **S. Rodewald**

**2:55 INOR 560.** Stereocontrol in *rac*-lactide polymerization with copper complexes. **F. Schaper**, P. Daneshmand, S. Fortun

**3:15 INOR 561.** Pd-initiated controlled polymerization of diazoacetates. **E. Ihara**

#### 3:35 Intermission.

**3:50 INOR 562.** Understanding the activity of half-sandwich ruthenium phosphido complexes in P-C bond formation. **R.G. Belli**, J. Yang, D. Pantazis, R. McDonald, **L. Rosenberg**

**4:10 INOR 563.** Reductive functionalization of CO<sub>2</sub>. **S. Bontemps**

**4:30 INOR 564.** Synthesis of biorenewable C5 compounds utilizing D-xylose obtained from agricultural biomass. **C.T. Burns**, M.H. Nantz, J. Satyavolu

**4:50 INOR 565.** From Hyde Park to Ames: An organometallic- and polyolefins-inspired approach to colloidal nanocrystal quantum dots. **J. Vela-Becerra**

**5:10 INOR 566.** From group 4 metal mono-dicarbollide complexes to nanocomposites containing boron cage compounds. **D.E. Bowen**, S.M. Wells, E.A. Eastwood, S. Sarkar, J.M. Messman, N. Bowler

**5:30 INOR 567.** Synthesis and applications of styrenic copolymers by metal catalyzed polymerization processes. **A. Grassi**, A. Buonerba, C. Capacchione, S. Milione

## Section L

San Diego Convention Center  
Room 33C

### Chemistry of Materials: Synthesis & Properties

C. G. Lugmair, *Organizer*

A. Beecher, G. Mezei, *Presiding*

**1:30 INOR 568.** Influence of metal vacancy of undoped anatase TiO<sub>2</sub> on p-type conductivity, room-temperature ferromagnetism, and remarkable photocatalytic performance. **S. Wang**, L. Pan, J. Zou, L. Wang, X. Zhang

#### 1:50 INOR 569. Withdrawn.

**2:10 INOR 570.** Magnetic study of Fe(III)-loaded synthetic melanin nanoparticles and their implications for MRI contrast agents. **Y. Xie**, Y. Li, N. Zang, Z. Wang, C.M. Andolina, L. Parent, N.C. Gianneschi, J.D. Rinehart

**2:30 INOR 571.** Mechanism of formation, structure, and reactivity of anion-incarcerating nanojars. **G. Mezei**

**2:50 INOR 572.** Assembling oligomers of transition metal clusters with single-atom linkers. **A. Beecher**, J.S. Owen

#### 3:10 Intermission.

**3:25 INOR 573.** Versatile access to polyphosphides by solution- and flow-chemistry activation of red phosphorus. **A. Dragulescu-Andrasi**, L. Miller, D.T. McQuade, M. Shatruk

**3:45 INOR 574.** Formation and reaction mechanisms of molybdenum complex species in acid solutions as precursors of hexagonal molybdenum trioxide. **C. Vargas Consuelos**, M.A. Camacho-Lopez, O. Graeve

**4:05 INOR 575.** Bimetallic molecular precursors for nanocrystalline functional oxides: The relationships between the crystal structure of the precursor and the phase of the metal oxide. **A.M. Moneeb**, A. Alabdulrahman, A. Bagabas, A.W. Appleb

**4:25 INOR 576.** Direct synthesis of polycarbonates from carbon dioxide and diols over a ceria catalyst. **S. Bian**, G. Du

**4:45 INOR 577.** New radical cation hybrid iodoplumbates: Functionalized organics and their impact on structure, stability, and performance. **H. Evans**, A. Lehner, J. Labram

### Diversity-Quantification-Success?

*Sponsored by PRES, Cosponsored by BIOL, CELL, CHED, CINF, COLL, COMSCI, DAC, GEOC, I&EC, INOR, MEDI, ORGN, PHYS, POLY, PROF and WCC*

### Undergraduate Research Posters

#### Inorganic Chemistry

*Sponsored by CHED, Cosponsored by INOR and SOCED*

## MONDAY EVENING

### Section A

San Diego Convention Center  
Halls D/E

#### Sci-Mix

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

#### 8:00 - 10:00

329, 334, 373, 385-386, 400-401, 414, 418-420, 442, 446, 450, 454, 456, 458, 461, 463-464. See previous listings.

910, 912, 915, 917, 1090, 1411. See subsequent listings.

## TUESDAY MORNING

### Section A

San Diego Convention Center  
Room 30B

### Undergraduate Research at the Frontiers of Inorganic Chemistry

#### Coordination Chemistry & Materials/Solid-State

*Financially supported by IONIC (Interactive Online Network of Inorganic Chemists)*

H. J. Eppley, C. Nataro, *Organizers*

R. J. Swails, *Presiding*

**8:30 INOR 578.** Structure and properties of coordination polymers containing hydrogen-bonding capable and conformationally flexible dipyriddy ligands: An introductory undergraduate research program at Lyman Briggs College at Michigan State University. **R.L. Laduca**, C. White, A. Sample

**8:50 INOR 579.** Layer-by-layer assembly of metal-organic coordinated thin films: Fundamentals of formation and sensing. **M.L. Ohnsorg**, M.E. Anderson

**9:10 INOR 580.** Understanding aluminum corrosion at the molecular level: Low-tech and high-tech approaches. **S.G. Sobel**

**9:30 INOR 581.** Surmounting the roadblocks to rechargeable zinc-air batteries by 3D architectural redesign of the air-breathing cathode and Zn anode. **E. Nelson**, J.F. Parker, P. DeSario, J. Long, D.R. Follison, C.N. Chervin

#### 9:50 Intermission.

**10:05 INOR 582.** Aryl-substituted BIAN complexes of iron dibromide: Synthesis, electronic structure, and catalytic hydrosilylation activity. **H.M. Hoyt**, M.J. Supej, A. Volkov, L. Darko, J. Darmon, C. Schultz, K.A. Wheeler

**10:25 INOR 583.** Novel metal alkoxide precursors for the production of high dielectric nanoinks for direct write applications. **D.T. Yonemoto**, T.J. Boyle, A. Cook, N.S. Bell, L.J. Treadwell, J.R. Farrell

**10:45 INOR 584.** Fluxional five-coordinate palladium(II) complexes with sulfur donor macrocycles: Reversible Pd<sup>II/IV</sup> electrochemistry, DFT calculations, and X-ray structure. **D.E. Janzen**

**11:05 INOR 585.** Withdrawn.

### Section B

San Diego Convention Center  
Room 30C

### Transition Metal Chemistry in DNA & RNA Regulation

S. L. Michel, *Organizer*

P. Chen, *Organizer, Presiding*

T. V. O'Halloran, *Presiding*

**8:30 INOR 586.** Exploring protein allostery and dynamics in metalloregulatory proteins. **D.P. Giedroc**, J.J. Braymer, D.A. Capdevila

**9:00 INOR 587.** Loz1, a zinc-responsive transcription factor from fission yeast. **A.J. Bird**

**9:30 INOR 588.** Biliverdin dependent regulation of extracellular heme uptake in *Pseudomonas aeruginosa*. **A. Wilks**

#### 10:00 Intermission.

**10:20 INOR 589.** Siderophore-mediated iron acquisition during nickel stress is controlled by the metalloregulatory protein YqjI in *E. coli*. **F. Outten**

**10:50 INOR 590.** Regulation of zinc homeostasis in *Bacillus subtilis*. P. Chandrangsu, J. Shin, J.D. Helmann

**11:20 INOR 591.** Controlling gene expression through DNA distortion: Structure and mechanism of metalloregulatory proteins. T.V. O'Halloran

## Section C

San Diego Convention Center  
Room 30D

### ACS Award in Inorganic Chemistry: Symposium in honor of Mercuri G. Kanatzidis

#### Synthesis & Applications of Solid State Materials

K. Choi, *Organizer*

J. A. Aitken, *Organizer, Presiding*

P. Trikalitis, *Presiding*

**8:30 INOR 592.** Metal chalcogenides as promising candidate semiconductors for g-ray detection. D. Chung

**8:55 INOR 593.** Synthesis of bismuth sulfide iodides in sulfur/iodine flux mixtures. R. Groom, S.E. Lattner

**9:20 INOR 594.** Magnetic anisotropy arising from main group elements: Bismuth-based molecules and materials. D.E. Freedman, S. Clarke, M. Fataftah

**9:45 INOR 595.**  $\text{FeM}_2\text{Se}_4$ : A fascinating family of high- $T_c$  ferromagnetic semiconductors. P.F. Poudeu Poudeu

**10:10** Intermission.

**10:25 INOR 596.** Enhancement of thermoelectric power factor in type I clathrate  $\text{K}_x\text{Ba}_y\text{Al}_z\text{Si}_{13}$  through charge carrier tuning. F. Sui, S. Kazuichir

**10:50 INOR 597.** Materials modules and systems for thermoelectric based waste heat recovery in passenger vehicles. J.R. Salvador

**11:15 INOR 598.** Thermoelectric properties of polycrystalline Pb-free metal chalcogenide compounds. J. Cha, K. Ahn, I. Chung

**11:40 INOR 599.** Efficient thermoelectric energy conversion in SnTe and GeTe. K. Biswas

## Section D

San Diego Convention Center  
Room 30E

### Memorial Symposium Honoring Karen J. Brewer

*Cosponsored by HIST†  
Financially supported by  
Washington State University*

S. C. Rasmussen, *Organizers*

M. T. Mongelli, *Organizer, Presiding*

**8:30** Introductory Remarks.

**8:40 INOR 600.** Karen J. Brewer (1961 - 2014). S.C. Rasmussen

**9:10 INOR 601.** Tribute to 22 years of collaboration and friendship across the chemistry/biology interface. B.S. Winkel

**9:40 INOR 602.** Ru,Rh,Ru supramolecular photocatalysts in Nafion® membranes. E.M. Naughton, K.S. Brewer, R.B. Moore

**10:10** Intermission.

**10:25 INOR 603.** Enhancing coreactant electrogenerated chemiluminescence. M. Richter

**10:55 INOR 604.** Photochemistry of metal organic frameworks: Ruthenium polypyridyl excited state chemistry in a new type of supramolecular material. W. Maza, A.J. Morris

**11:25 INOR 605.** Monitoring the excited state properties of dirhodium(II,II) complexes following visible light photoexcitation with potential applications in solar energy conversion. T.A. White, T.J. Whitemore, R.P. Thummel, K.R. Dunbar, C. Turro

**11:55 INOR 606.** Photo-uncaging and delivery of small molecule bioeffectors. P.C. Ford

## Section E

San Diego Convention Center  
Room 31A

### Organometallic Chemistry: Synthesis & Characterization-Late Transition Metals

N. S. Radu, *Organizer*

T. B. Clark, C. J. Daley, *Presiding*

**8:30 INOR 607.** Influencing excited states of iridium(III) cyclometalates by various aryl isocyanides and cyclometalating ligands. A. Maity, T.S. Teets

**8:50 INOR 608.** Mechanistic insights into the reactivity of (Phebox)Ir(H)(OAc) and molecular oxygen. A.M. Wright, D. Pahls, K.I. Goldberg, T.R. Cundari

**9:10 INOR 609.** Withdrawn.

**9:30 INOR 610.** Synthesis and reactivity of methyl-substituted PCP ligands and corresponding iridium complexes. T. Lekich, J.M. Goldberg, G.W. Wong, D.M. Heinekey

**9:50 INOR 611.** Redox-active heterobimetallic complexes with mesoionic carbenes: Electronic structures and catalytic properties. L. Hettmanczyk, S. Manck, C. Hoyer, S. Hohloch, B. Sarkar

**10:10 INOR 612.** Metal complexes with triazoles and triazolylidenes and a ferrocene backbone. S. Manck, T. Bens, M. van der Meer, L. Suntrup, B. Sarkar

**10:30 INOR 613.** Mechanistic studies of carboxylation of isostructural iron methyl complexes with different charge state. K. Lau, R.F. Jordan

**10:50 INOR 614.** Synthesis, structure, and reactivity of hydridosilylene complexes of iron. P. Smith, T. Tilley

**11:10 INOR 615.** Synthesis and characterization of chiral, highly water-soluble pyridyl phosphines derived from 1,3,5-triaza-7-phosphaadamantane (PTA). W.L. Ounkham, W. Lee, B.J. Frost

**11:30 INOR 616.** Effects of ligand modification on accessing various oxidation states in palladium pyridinophane complexes. A. Wessel, L.M. Mirica

## Section F

San Diego Convention Center  
Room 31B

### Alfred Bader Award in Bioinorganic or Bioorganic Chemistry: Symposium in honor of Edward I. Solomon

#### Bioinorganic Methods

K. D. Karlin, *Organizer*

D. R. Gamelin, *Presiding*

**8:30 INOR 617.** Understanding and controlling electrochemistry for fuel cells and electrolyzers. A.A. Gewirth

**9:00 INOR 618.** Nuclear resonance vibrational spectroscopic elucidation of binuclear non-heme iron enzyme intermediates. K. Park, E.I. Solomon

**9:30 INOR 619.** From electronic properties of non-heme iron active sites to biocatalysis. M. Srnc, E.I. Solomon

**10:00 INOR 620.** Vibrational stark effect spectroscopy on the blue light photosensor photoactive yellow protein. M.T. Kieber-Emmons, K.M. Light, V. Cheng

**10:30 INOR 621.** Catalytic cycle of multi-copper oxidases studied by theoretical methods. L. Rulisek, E.I. Solomon, U. Ryde

**11:00 INOR 622.** N2ase & H2ase vibrational spectroscopy with NRVs & FT-IR: The merits of big photons & little ones. S.P. Cramer

**11:30 INOR 623.** Novel mechanisms of transcription regulation in living cells: A lesson from metalloregulators. P. Chen

**12:00 INOR 624.** Synchrotrons and X-ray free electron lasers in structural biology: From "slow" to "ultrafast". B.G. Hedman, K.O. Hodgson

## Section G

San Diego Convention Center  
Room 31C

### F. Albert Cotton Award in Synthetic Inorganic Chemistry: Symposium in honor of Francois P. Gabbaï

J. D. Hoefelmeyer, T. W. Hudnall, *Organizers*

W. E. Piers, *Presiding*

**8:30** Introductory Remarks.

**8:35 INOR 625.** Main group strategy for fluorescent dyes. S. Yamaguchi

**8:55 INOR 626.** Organometallic photonics: Pt<sup>II</sup> dimer photochemistry and photophysics. F.N. Castellano

**9:15 INOR 627.** Functionalized triarylborane Lewis acids for anion sensing. M. Lee

**9:35 INOR 628.** Intramolecular frustrated Lewis pair dichloro-8-quinolylgallium(III) activates chloroform. J.D. Hoefelmeyer, S.R. Tamang, J.I. Fostvedt, J. Son

**9:55 INOR 629.** Synthesis of fluoromethyl-substituted organoboranes and their application in frustrated Lewis pair chemistry. H. Wang, Z. Lu, H. Ye, J. Zheng

**10:15** Intermission.

**10:25 INOR 630.** Designing and exploiting reversible small molecule capture by single component frustrated Lewis pairs. S. Aldridge, Z. Mo

**10:45 INOR 631.** Nitrogen fixation with iron complexes. J.C. Peters, T.J. Del Castillo, J. Rittle, N.B. Thompson

**11:05 INOR 632.** (Boryl)iminomethanes: Coordination chemistry and FLP behavior. J.S. Figueroa, B.R. Barnett

**11:25 INOR 633.** Evolving the coordination chemistry of p-block element Lewis acceptors. N. Burford

**11:45 INOR 634.** Electrophilic phosphonium cations in catalysis: New strategies for reactivity. D.W. Stephan

## Section H

San Diego Convention Center  
Room 32A

### Harry Gray Award for Creative Work in Inorganic Chemistry by a Young Investigator: Symposium in honor of Eric J. Schelter

L. G. Sneddon, P. J. Walsh, *Organizers*

J. R. Robinson, U. J. Williams, *Presiding*

**8:30** Introductory Remarks.

**8:35 INOR 635.** Designing new energetic chromophores for optical initiation of explosives: Tuning charge transfer in nitrogen-rich Fe(II) tetrazine complexes. J.M. Veauthier, T.W. Myers, D.E. Chavez, J. Ejorgaard, S. Tretiak, S.K. Hanson, R.J. Scharrf

**8:55 INOR 636.** Dye-sensitized solar cell as a tool to resolve intermolecular interactions. C.P. Berlinguette, G.J. Meyer, F.G. Parlane, S.J. Simon, K. Hu, W.B. Swords

**9:15 INOR 637.** Formal Ce(IV) coordination complexes and the role of configuration interactions: Closed-shell singlet ground states and temperature-independent paramagnetism. C. Booth, R.L. Halbach, G. Nocton, L. Maron, R.A. Andersen

**9:35 INOR 638.** Electronic structures and reactions of metal-oxos. H.B. Gray

**9:55** Intermission.

**10:15 INOR 639.** Spin crossover in mono- and multinuclear Fe(II) complexes with N<sub>4</sub>S<sub>2</sub> coordination environment. A. Dragulescu-Andrasi, A. Arroyave, V. Stubbs, S. Yergeshbayeva, M. Shatrak

**10:35 INOR 640.** New advances in lanthanide magnetism. M. Murugesu

**10:55 INOR 641.** Enhanced processing features in the family of lanthanide double-decker single molecule magnets. J. Galan-Mascaros, N. Gimenez, C. Saenz de Pipaon, P. Ballester, D. Ecija

**11:15 INOR 642.** Recent advances in the chemistry of the rare earth metals in the formal +2 oxidation state. W.J. Evans

**11:35 INOR 643.** Paramagnetic dinuclear complexes with radical diimine ligands. T.J. Woods, M.B. Rivas, K.R. Dunbar

**11:55** Concluding Remarks.

## Section I

San Diego Convention Center  
Room 32B

### Earle B. Barnes Award for Leadership in Chemical Research Management: Symposium in honor of Henry E. Bryndza

*Cosponsored by ENVR, ORGN and POLY*

M. Harmer, N. S. Radu, *Organizers, Presiding*

**9:00 INOR 644.** Catalysis, mechanistic understanding, and collaboration as tools to sustainable production of chemicals and fuels. K.I. Goldberg

**9:30 INOR 645.** Bridging the gap between homogeneous and heterogeneous catalysis at Argonne National Laboratory. E. Bunel

**10:00** Intermission.

**10:10 INOR 646.** Technology greenhouse: Ideas through commercialization. J.C. Warner

**10:40 INOR 647.** Building a robust biomaterials portfolio: An overview of DuPont's strategy and programs. M.A. Saltzberg

**11:10** Concluding Remarks.

Technical program information known at press time. The official technical program for the 251st ACS National Meeting is available at: [www.acs.org/sandiego2016](http://www.acs.org/sandiego2016)



## Section J

San Diego Convention Center  
Room 33A

Frontiers in Heavy Element  
Inorganic Chemistry

Cosponsored by NUCL

D. L. Clark, D. K. Shuh, L. Soderholm,  
Organizers

S. A. Kozimor, Presiding

8:30 Introductory Remarks.

8:35 INOR 648. Multinuclear metal complexes for challenging chemical transformations. T. Tilley

8:55 INOR 649. New ligand platforms for actinide chemistry. J. Arnold, C. Camp, N. Settineri, M. Garner, S. Hohlock

9:15 INOR 650. Heavier the better: Something old, something new, nothing radioactive. G.G. Stanley

9:35 INOR 651. Exploring redox noninnocence of pincer ligands for delivery to refractory substrates. K.G. Caulton, B.J. Cook, A.V. Polezhaev, N. Maciulis, S. Curtis, N. Labrum, M. Pink, C. Chen

9:55 INOR 652. Impact of Al Sattelberger on actinide chemistry at Los Alamos. C. Burns

10:15 INOR 653. Recent advances in the chemistry of thorium and uranium in the formal +2 oxidation state. W.J. Evans

10:35 Intermission.

10:55 INOR 654. Functional materials by design for energy conversion through integrated theory and experiment. W. Tumas, D.S. Ginley, A. Zakutayev, S. Lany, L. Garten, v. stevanovic, M. Toney

11:15 INOR 655. N vs. S: Bifunctional reactivity of Fe complexes bearing svelte thiolato- and amido-SNS ligands. U.K. Das, K. Ghoshine, R. Baker

11:35 INOR 656. New ligands and metal complexes for efficient outer sphere hydrogenation of ketonic substrates. P.A. Dub, B. Scott, J.C. Gordon

11:55 INOR 657. Redox processes of rare-earth metal complexes supported by ferrocene diamide ligands. P. Diaconescu

12:15 INOR 658. Proton-coupled electron transfer reactivity of ceria and samarium diiodide. J.M. Mayer, D. Damatov, S. Kolmar, O. Jung, J. Peng

## Section K

San Diego Convention Center  
Room 33B

Organometallic Compounds &  
Catalysts: Influence on Polymer  
Science & Synthesis

D. E. Bowen, Organizer

T. Y. Meyer, Organizer, Presiding

G. M. Diamond, Presiding

8:30 Introductory Remarks.

8:35 INOR 659. Application of chiral terpenyl groups in imine-type ligand design for olefin polymerization catalysis. F. Zhai, R.F. Jordan

8:55 INOR 660. Selectivity-enhanced entropy-driven ring-opening polymerization for the preparation of sequenced copolymers. T.Y. Meyer, R.M. Weiss, A.L. Short, M.A. Washington, D.J. Swiner

9:15 INOR 661. Combining N-heterocyclic carbenes with oxophilic and high-oxidation-state metal centers state (group 4, 12 and 13): Fundamental reactivity and use in polymerization and CO<sub>2</sub> functionalization catalysis. C. Fiedel, J. Bruyere, D. Specklin, S. Dagorne

9:35 INOR 662. Nature of secondary interactions in molecular and silica-supported organolanthanum complexes from solid-state NMR spectroscopy. M.P. Conley, C. Coperet, R.A. Andersen

9:55 Intermission.

10:15 INOR 663. Termination routes in alpha-olefin oligomerization with group IV metallocenes; evidence for beta-alkyl elimination where alkyl is greater than methyl. D.J. Crowther

10:35 INOR 664. Synthesis of metal phosphonate cage compounds for tetranuclear Pd polymerization catalysts. Q. Liu, R.F. Jordan

10:55 INOR 665. Development of novel D<sub>2h</sub>-symmetric aromatic tetraaza macrocyclic ligands. T. Gardner

11:15 INOR 666. Dithiobiuret ligands for the simultaneous leaching and extraction of gold from ore and secondary sources. S.R. Foley

11:35 INOR 667. Ethylene oligomerization promoted by chromium complexes bearing imine tridentate ligands. A. Pinheiro, A. Bergamo, A. Casagrande, E. Kirilov, J. Carpentier, O.L. Casagrande

## Section L

San Diego Convention Center  
Room 33C

Supramolecular Chemistry: A  
Crown & Anchor Approach

Cosponsored by ORGN

Financially supported by Elsevier,  
Supramolecular Chemistry, RSC

A. E. Gorden, Organizer

D. W. Johnson, Presiding

8:30 Introductory Remarks.

8:40 INOR 668. Enzyme-like catalysis in a chiral supramolecular cluster. K.N. Raymond, D. Kaphan, D. Toste, R.G. Bergman

9:10 INOR 669. Supramolecular catalyst with cyclic tetrapyrrole compound. Y. Hisaeda

9:30 INOR 670. Bioconjugated metallocorroles for medicine and catalysis. Z. Gross

9:50 INOR 671. Dynamic covalent self-assembly for determination of enantiomeric excess. P. Anzenbacher

10:10 INOR 672. Small pyrrole-based pigments as redox-active ligands. E. Tomat

10:30 Intermission.

10:50 INOR 673. Computer-aided molecular design in supramolecular chemistry. B.P. Hay

11:10 INOR 674. Exploring reactivity in self-assembled main group coordination clusters: A new route to cyclophanes? D.W. Johnson

11:30 INOR 675. Steric and electrostatic effects on the dynamic processes of rotaxane-like complexes. J. Tiburcio

11:50 INOR 676. New class of energetic chromophores for optical initiation of explosives: Transition metal complexes of explosive tetrazines. J.M. Vauthier, T.W. Myers, D.E. Chavez, S.K. Hanson, R.J. Scharff

12:10 INOR 677. Structured materials from a supramolecular approach. A. Try, M. Hashemi Karouei

## TUESDAY AFTERNOON

## Section A

San Diego Convention Center  
Room 30B

Undergraduate Research at the  
Frontiers of Inorganic Chemistry

## Organometallic Chemistry

Financially supported by IONiC (Interactive  
Online Network of Inorganic Chemists)

H. J. Eppley, C. Nataro, Organizers

J. P. Lee, Presiding

1:30 INOR 678. Catalytic interconversion of primary amines and nitriles by an iridium pincer complex. D.A. Laviska

1:50 INOR 679. Alkane dehydrogenation with (supercritical)Phebox)Ir(OAc)(X) complexes. Z.H. Syed, Y. Gao, C. Guan, A.S. Goldman, K.I. Goldberg

2:10 INOR 680. Carbon monoxide activation by metal cyano carbonyls. D. Shlian, J. Alboucaï, M. Stock, M. Khaloo, J. Jiang

2:30 INOR 681. Structural characterization and electrochemical properties of nickel(II) complexes bearing sterically bulky hydrotris(3-phenyl)- and hydrotris(3-tert-butylpyrazol-1-yl)borato ligands. A.K. Frampton, K. Gartland, N.A. Piro, W.S. Kassel, W.G. Dougherty

2:50 Intermission.

3:05 INOR 682. Synthesis and characterization of cyclopentadienyl- and pentamethylcyclopentadienyl-Co(II) mixed sandwich compounds containing either tridentate nitrogen or sulfur donor macrocycles. J.P. Lee, P.A. Dean, K.R. Henson, T.P. Latendresse

3:25 INOR 683. Structure, bonding, and reactivity of d<sup>9</sup> dioxolene and iminoxolene molybdenum and titanium complexes. T. Marshall-Roth, S.N. Brown

3:45 INOR 684. Sudo make me a sandwich complex: Terrifying true tales of organometallic palladium chemistry with undergraduates. S.K. Hurst

4:05 INOR 685. Oxidation of a coordinated bis(phosphino)ferrocene ligand. C. Nataro

4:25 INOR 686. 4-pyridonate ligands: A pi-basic approach to cleaving C-H bonds with platinum group metals. N. Williams, T. Mortvedt, E. Nesbitt, A. Sullivan, L.A. Watson

4:45 Concluding Remarks.

## Section B

San Diego Convention Center  
Room 30C

Transition Metal Chemistry in  
DNA & RNA Regulation

P. Chen, Organizer

S. L. Michel, Organizer, Presiding

D. Wilcox, Presiding

1:30 INOR 687. What determines metal specificity and metal affinity of a DNA binding transcriptional de-repressor? N. Robinson

2:00 INOR 688. Electron paramagnetic resonance spectroscopy characterizes structural and dynamics features of CueR-DNA-Cu(I) complex. S. Ruthstein

2:30 INOR 689. Disruption of zinc finger structure and function upon substitution with copper(I). K.E. Splan, B.T. Buse, A.M. Blumenreich, M.D. Storlie

3:00 Intermission.

3:20 INOR 690. Metal coordination and DNA interaction studies of classical and non-classical zinc fingers. S. Lee, S.L. Michel

3:50 INOR 691. Thermodynamics of metal ions binding to DNA-binding protein domains. D. Wilcox

4:20 INOR 692. Persulfidation of tristetraprolin by hydrogen sulphide. M. Lange, G.D. Shimberg, L. Marko, S.L. Michel, M. Filipovic

## Section C

San Diego Convention Center  
Room 30D

Metal-Oxygen Oxidants in Synthesis &  
Biology: Beyond Metal-Oxo Species

M. T. Kieber-Emmons, Organizer

T. A. Jackson, Organizer, Presiding

1:30 INOR 693. Kinetic and spectroscopic interrogation of a promiscuous thiol dioxygenase: 3-mercaptopropionic acid dioxygenase. B. Subedi, J. Crowell, S. Sardar, B.S. Pierce

1:55 INOR 694. Intermediates in hydrocarbon oxidations catalyzed by bio-inspired nonheme iron catalysts. L. Que, W. Oloo

2:20 INOR 695. Electrochemistry to probe the reactivity of metal-(hydro)peroxy species derived from reductive activation of O<sub>2</sub>. E. Anxolabehere, F. Banse, H. Ching, C. Costentin, H.E. Colmer, P. Dorlet, T.A. Jackson, C. Policar, M. Robert, N. Segaud, K. Senechal

2:45 INOR 696. Tuning the metal-dioxygen, -oxo, -hydroxo, and ligand reactivity landscape in heme-type complexes. D.P. Goldberg, H.M. Neu, G. Baglia, J. Zaragoza

3:10 INOR 697. Correlation between the structural, spectroscopic, and kinetic parameters of reactive Mn-peroxy complexes. J. Kovacs, J. Rees, M.K. Coggins, A. Johansen

3:35 Intermission.

3:45 INOR 698. Superoxonickel complexes as oxidants. C.G. Riordan, W. Green

4:10 INOR 699. Modeling catalytic intermediates of the thiol dioxygenases. A.T. Fiedler, A. Fischer

4:35 INOR 700. Involvement of metal-superoxo species in iron and copper C-H activating enzymes. J. Klinman, H. Zhu, S. Peck, F. Bonnot, W. van der Donk

5:00 INOR 701. Progress in the generation and characterization of primary copper(I)-dioxygen adducts. K.D. Karlin

Technical program information  
known at press time.

The official technical program  
for the 251st ACS National  
Meeting is available at:  
[www.acs.org/sandiego2016](http://www.acs.org/sandiego2016)

**5:25 INOR 702.** Differential oxidase and oxygenase reactivities in *de novo* Due Ferri proteins. **A.J. Reig**, R. Snyder, S.C. Butch, W.F. Degrado, E.I. Solomon

## Section D

San Diego Convention Center  
Room 30E

### Memorial Symposium Honoring Karen J. Brewer

*Cosponsored by HIST†  
Financially supported by  
Washington State University*

M. T. Mongelli, *Organizer*

S. C. Rasmussen, *Organizer, Presiding*

**1:30 INOR 703.** Asymmetric bimetallic ruthenium complexes as potential photodynamic therapy agents. **M.T. Mongelli**, K. Thomas, A. Abdulkarim, M. LaCorte, J. Osei-Fosu

**2:00 INOR 704.** Ultrafast photophysics of mixed-metal polyazine supramolecules: Os(II) or Ru(II) with Rh(III). **D.F. Zigler**, Z.A. Morseth, T. Canterbury, J.A. Rodriguez Corrales, K.S. Brewer, J.M. Papanikolas

**2:30 INOR 705.** Ru, Rh, Ru water reduction photocatalysts in ion containing polymers. E.M. Naughton, T. Canterbury, **R.B. Moore**

**3:00 INOR 706.** Emission study of Ir<sup>III</sup>Cp\* compounds and synthesis of Ru<sup>II</sup>-Ir<sup>III</sup>Cp\* bimetallic complex designed for anticancer activity. **S. Molnar**, J.S. Merola, A. Smith

**3:30** Intermission.

**3:45 INOR 707.** Ruthenium and rhodium based anticancer compounds with diimine ligands. **S. Saha**, B. Pena, A. David, C. Turro, **K.R. Dunbar**

**4:15 INOR 708.** Photocatalyst design with consideration for ligand sigma-donating ability and substrate accessibility to catalytically active site. **H.J. Sayre**, K.S. Brewer, C. Turro

**4:45 INOR 709.** Synthesis and characterization of a novel Ru(II)-polypyridyl complex with carboxylate functional groups for supramolecular water reduction photocatalyst-polymer assemblies. **K.M. Felice**, K.S. Brewer, R.B. Moore

**5:15 INOR 710.** Dipyrromethenes bridging ruthenium(II) polypyridyl complexes: Photophysical and electrochemical properties, and DNA photo-induced reactions. **S. Swavey**

## Section E

San Diego Convention Center  
Room 31A

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

S. A. Koch, *Organizer*

I. Garcia-Bosch, *Presiding*

**1:30 INOR 711.** Withdrawn.

**1:50 INOR 712.** Synthesis and structural characterization of a  $\beta$ -lactam adduct of a synthetic analogue of a metallo- $\beta$ -lactamase. **S. Ruccolo**, G. Parkin

**2:10 INOR 713.** Synthetic modeling of mono-iron hydrogenase (Hmd): Utility of an anthracene scaffold for the facial display of biomimetic donors. **M.J. Rose**, J. Seo, T.A. Manes

**2:30 INOR 714.** Comparison of Mn<sup>IV</sup>(O) and Cr<sup>VI</sup>(O) complexes in HAT and PCET reactivity. **R.A. Baglia**, K. Prokop-Prigge, H.M. Neu, M. Siegler, D.P. Goldberg

**2:50 INOR 715.** Macrocyclic rebellion: TMC Cu(I) conformations lead to dicopper peroxo species with unique spectroscopic, structural, and chemical properties. **I. Garcia-Bosch**, D.E. Diaz, K.D. Karlin

**3:10** Intermission.

**3:20 INOR 716.** Surprise comes twice: Coordinating a thioether-cholesterol ligand to the non-toxic [Ru(tpy)(bpy)(H<sub>2</sub>O)]<sup>2+</sup> complex leads to a highly cytotoxic compound with an unexpected mode-of-action. **B. Siewert**, V.H. van Rixel, E.J. van Rooden, M.J. Moester, S.L. Hopkins, F. Ariese, S. Bonnet

**3:40 INOR 717.** Termolecular proton-coupled electron transfer reactions: Separating proton and electron transfer effects. **W.D. Morris**, J.M. Mayer

**4:00 INOR 718.** Factors influencing acid plus reductant O-O cleavage in low-spin heme-peroxo-copper complexes. **S.M. Adam**, K.D. Karlin

**4:20 INOR 719.** Artificial metalloenzymes with metal-binding motifs made from canonical amino acids. **J. Eppinger**, J. Fischer, M. Groll

**4:40 INOR 720.** Recent advances into mechanistic insights gained from structural and spectroscopic studies of biosynthetic models of nitric oxide reductases. **S. Chakraborty**, J. Reed, M. Ross, H. Matsumura, P. Moenne Loccoz, T. Sage, C. Schultz, Y. Lu

## Section F

San Diego Convention Center  
Room 31B

### Organometallic Chemistry: New Ligand Platforms

N. S. Radu, *Organizer*

L. M. Mirica, D. V. Peryshkov, *Presiding*

**1:30 INOR 721.** Remote multi-proton storage within a pyrrolide-pincer type ligand. **S. Nadif**, M.E. O'Reilly, I. Ghiviriga, K.A. Abboud, A.S. Veige

**1:50 INOR 722.** Metal- and ligand-centered reactivity of *B*-metalated carbonyl pincer complexes of rhodium. **D.V. Peryshkov**, B.J. Eleazer

**2:10 INOR 723.** Variable binding modes of pyridine in molybdenum complexes supported by novel P-pyridine-P ligands. **R. Wan**, K. Horak, J.A. Buss, T. Agapie

**2:30 INOR 724.** Heavy metal for organometallic reactions: Palladium-phosphonium systems and their catalytic potential. **S.M. Kruse**, T. Haden, W. Cross Lopez, J. Herring, S.K. Hurst

**2:50 INOR 725.** Controlling the reactivity of high-valent Pd and Ni complexes with flexible multidentate ligands. **L.M. Mirica**

**3:10 INOR 726.** Extending the  $\pi$ -system: Modulation of arene and phosphine donor lability in polyarene diphosphine-supported molybdenum complexes and its application to small molecule reactivity. **C. Low**, J.A. Buss, T. Agapie

**3:30 INOR 727.** Donor-functionalized cyclic (alkyl)(amino)carbenes (CAACs): Synthesis, coordination, and catalysis. **J. Chu**, D. Munz, M. Melaimi, R. Jazzar, G. Bertrand

**3:50 INOR 728.** 6-membered Cyclic (alkyl)(amino)carbenes as strong donor ligands for transition-metals in catalysis. **C. Weinstein**, G. Junor, M. Melaimi, G. Bertrand

**4:10 INOR 729.** Bimetallic scaffolds for CO<sub>2</sub> reduction. **C.T. Saouma**, L. Mueller

**4:30 INOR 730.** Outer coordination sphere effect on Rh(diphosphine)<sup>+</sup> complexes catalyzed CO<sub>2</sub> hydrogenation. **S. Ni**, **L. Dang**

**4:50 INOR 731.** Role of the chemically non-innocent ligand in the catalytic formation of hydrogen and carbon dioxide from methanol and water with the metal as the spectator: A mechanism study. **H. Li**, M.B. Hall

## Section G

San Diego Convention Center  
Room 31C

### F. Albert Cotton Award in Synthetic Inorganic Chemistry: Symposium in honor of Francois P. Gabbai

J. D. Hoefelmeyer, T. W. Hudnall, *Organizers*

H. Wang, *Presiding*

**1:30** Introductory Remarks.

**1:35 INOR 732.** New bond activations, transformations, and catalysis in transition metal-silicon chemistry. **T. Tilley**

**1:55 INOR 733.** Dinuclear gold ylide complexes as catalysts for C—C bond forming reactions. **C.R. Wade**, B. Reiner

**2:15 INOR 734.** Pyrrole-based flexidentate phosphine, polypyrazolyl, and Schiff base ligands for transition and alkali metal complexes. **G. Mani**

**2:35 INOR 735.** N,O-chelates becoming unhinged. New perspectives in metal-ligand cooperativity. **M.W. Drover**, J. Love, **L. Schafer**

**2:55** Intermission.

**3:05 INOR 736.** Magnetization dynamics in heterometallic lanthanide: Transition metal complexes. **M. Nippe**

**3:25 INOR 737.** Sulfur directed acid-base pairs as guiding principle for adjudicating guilt vs. innocence in heterobimetallic complexes derived from metalodithiolate ligands. **M.Y. Darensbourg**, P. Ghosh, N. Wang, S. Ding

**3:45 INOR 738.** Molecular titanium nitrides: Synthesis, characterization, and reactivity studies. **D.J. Mindiola**

**4:05 INOR 739.** New boryl-centered pincer ligands and their complexes. **O. Ozerov**, W. Shih, W. Gu, N. Bhuvanesh, S.D. Timpa, M.C. MacInnis

## Section H

San Diego Convention Center  
Room 32A

### Solid-State Inorganic Chemistry

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

A. Choudhury, *Presiding*

**1:30 INOR 740.** Systematical study of chemical compositions in open framework chalcogenides. **X. Chen**, X. Bu, P. Feng

**1:50 INOR 741.** New insights into the structure, properties, and chemistry of Cu<sub>4</sub>SnS<sub>8</sub>. **A. Choudhury**, S. Mohapatra, H. Yaghoobnejad Asl

**2:20 INOR 742.** Structural variability and thermoelectric properties of transition metal-pnicogen clathrates. **J. Dolyuniuk**, J. Wang, K. Kovnir

**2:40 INOR 743.** Phase formation in mixed divalent hexaborides. **J.T. Cahill**, M. Alberga, S. Misture, D. Edwards, V.R. Vasquez, O. Graeve

**3:00 INOR 744.** Using computer generated decision trees to understand structural adaptivity in [V<sub>2</sub>O<sub>7</sub>(SeO<sub>3</sub>)<sub>3</sub>]<sup>2n-</sup> layered compounds. **P. Adler**, A.J. Norquist, R. Xu

**3:20** Intermission.

**3:35 INOR 745.** Hybrid main-group halide perovskites: Local structure and disorder. **D.H. Fabiani**, H. Evans, G. Laurita, C. Stoumpos, M.G. Kanatzidis, R. Seshadri

**3:55 INOR 746.** Exploring degradation of Van Gogh yellow from the inside: A computational study on the PbCr<sub>1-x</sub>S<sub>2</sub>O<sub>6</sub> solid solution. **A.B. Muñoz-García**, A. Massaro, M. Pavone

**4:15 INOR 747.** Structural analysis of the mixed sorosilicate phosphor, Ba<sub>4</sub>Si<sub>6</sub>O<sub>17</sub>·Eu<sup>2+</sup>. **C. Cozzan**, G. Laurita, R. Seshadri

**4:35 INOR 748.** Optical and scintillation properties of metal oxide nanoparticles. **Y. Mao**, M. Pokhrel

**4:55 INOR 749.** Supersaturation of complex ions in crystal growth of ZnO, CaCO<sub>3</sub> and Ca<sub>2</sub>H(PO<sub>3</sub>)<sub>3</sub>. **M.C. Gelabert**, D. Thibault, J. Zinna

## Section I

San Diego Convention Center  
Room 32B

### Environmental & Energy- Related Inorganic Chemistry

S. A. Koch, *Organizer*

S. R. Foley, L. J. Lyons, *Presiding*

**1:30 INOR 750.** Acetic acid process: A viable alternative to cyanide and aqua regia for leaching gold from primary and secondary sources. **S.R. Foley**, H. Salimi, L. Moradi

**1:50 INOR 751.** Homogeneous catalysis of the electrochemical reduction of CO<sub>2</sub> by Re(I) complexes. Role of the pyridine ligands. **J. Nganga**

**2:10 INOR 752.** Withdrawn.

**2:30 INOR 753.** Evidence of a through-bond mechanism for photo-initiated interfacial electron transfer at dye-sensitized titanium dioxide. **G.J. Meyer**, K. Hu, W.B. Swords, E. Piechota, R. Sampaio, C.P. Berlinguette

**2:50 INOR 754.** CO<sub>2</sub> reduction using cobalt aminopyridine complexes. **A. Chapovetsky**, S.C. Marinescu

**3:10 INOR 755.** Design principles for selective CO<sub>2</sub> reduction catalysis. **A. Hall**, A. Wuttig, Y. Yoon, **Y. Surendranath**

**3:30** Intermission.

**3:40 INOR 756.** Promoting interfacial photoinduced iodide oxidation: Halogen bonding at the interface. **W.B. Swords**, S.J. Simon, F.G. Parlani, K. Hu, G.J. Meyer, C.P. Berlinguette

**4:00 INOR 757.** Withdrawn.

**4:20 INOR 758.** Improved ion transport using silyl electrolytes for lithium-ion battery applications. **L.J. Lyons**

**4:40 INOR 759.** DFT study of an unusual proton-relay role for Cp\* in hydrogen evolution catalysis. **S.I. Johnson**, S.L. Corona, J.D. Blakemore, J.R. Winkler, H.B. Gray, W.A. Goddard

**5:00 INOR 760.** Immobilization of molecular electrocatalysts in a coordinating membrane to enhance their activity and selectivity for CO<sub>2</sub> reduction. **W.W. Kramer**, **C.C. McCrory**

**5:20 INOR 761.** High-pressure hydrogen evolution by the decomposition of formic acid in the presence of IR catalyst. **H. Kawanami**, M. Iguchi, Y. Himeda, Y. Manaka, K. Matsuoka

**5:40 INOR 762.** Conversion of cellulosic biomass to fuels and chemicals. **C.L. Marshall**

## Section J

San Diego Convention Center  
Room 33A

### Frontiers in Heavy Element Inorganic Chemistry

*Cosponsored by NUCL*

D. L. Clark, D. K. Shuh, L. Soderholm,  
*Organizers*

J. E. Bercaw, *Presiding*

**1:30 INOR 763.** Thorium, uranium, f-orbitals, and multiple bonds: These are just a few of Al's favorite things. J.L. Kiplinger

**1:50 INOR 764.** Heavy element molecular magnetism: Exploiting spin-orbit effects and anisotropic coupling. K.R. Dunbar, F.J. Birk, D. Kempe, K. Schulte

**2:10 INOR 765.** Unusual case where plutonium is simpler than cerium. T.E. Albrecht-Schmitt

**2:30 INOR 766.** Mercury-selenium interactions and the protolytic cleavage of Hg-C bonds induced by 1-methyl-1,3-dihydro-2H-benzimidazole-2-selone. J. Palmer, P. Quinlivan, K. Yurkerwicz, G. Parkin

**2:50 INOR 767.** Early transition metal complexes with bicyclic guanidinate ligands: Syntheses, structures, and LMCT spectrofluorimetry. J.R. Olson, C.J. Jensen, D.C. Swenson, L. Messerle

**3:10** Intermission.

**3:30 INOR 768.** Aqueous solution route to actinide thin films. T.M. McCleskey, B. Scott, E. Bauer, S.A. Kozimor, R.L. Martin, A. Burrell, Q. Jia

**3:50 INOR 769.** Uranium imido complexes: A window into uranium bonding and reactivity. J.M. Boncella, N.C. Tomson, A. Tondreau, M. Winston, B. Scott

**4:10 INOR 770.** Spectroscopic studies of metal-metal bonding. W.H. Woodruff

**4:30 INOR 771.** Multiple bonds: Some sojourns in heavy-metal chemistry with Al Sattelberger. B.E. Bursten

**4:50 INOR 772.** Solar-to-fuels conversion by the artificial leaf. D.G. Nocera, M. Huynh, D.K. Bediako, N. Li, C. Liu

## Section K

San Diego Convention Center  
Room 33B

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

N. S. Radu, *Organizer*

G. Du, A. M. Spokoyny, *Presiding*

**1:30 INOR 773.** Metal-free, boron-rich cluster cationic styrene polymerization photocatalysts. A.M. Spokoyny

**1:50 INOR 774.** Synthesis of novel luminescent PAHs featuring a boron ring junction. K.A. Schickedanz, M. Wagner

**2:10 INOR 775.** Zipping up alkynes with zirconocene: Toward a general route to functionalized expanded helicenes and cycloarenes. G.R. Kiel, T. Tilley

**2:30 INOR 776.** Copolymerization of cyclic esters and epoxides via redox-switchable Zr catalyst. S. Quan, P. Diaconescu

**2:50 INOR 777.** Ligand electronic effect in late transition metal catalyzed olefin polymerization and copolymerization. C. Chen, M. Chen, S. Dai

**3:10 INOR 778.** Insight into the mechanism and reactivity of ruthenium ROMP catalysts at the single-molecule and single-particle levels. Q. Easter, V. Trauschke, S.A. Blum

**3:30 INOR 779.** Withdrawn.

**3:50 INOR 780.** Stereoselective synthesis of biodegradable polyesters catalyzed by chiral zinc amido-oxazolinate complexes. G. Du, S. Abbina, V. Chidara, S. Bian

**4:10 INOR 781.** Tuning solid-state emission of push-pull chromophores via embedding into metal-organic materials. L.M. Lifshits, M. Zeller, J.K. Klosterman

**4:30 INOR 782.** Using bulky terphenyl thiolates as capping ligands for gold thiolate nanoclusters. N. Mendelson, J.S. Figueroa

**4:50 INOR 783.** Carboxylic acid functionalized polycarbonates from CO<sub>2</sub>: A versatile platform for the synthesis of functional polycarbonates. Y. Wang, F. Tsai, D.J. Darensbourg

**5:10 INOR 784.** From molecules to materials: The effect of precursor design on functional device synthesis. C.E. Knapp, C.J. Carmalt

## Section L

San Diego Convention Center  
Room 33C

### Supramolecular Chemistry: A Crown & Anchor Approach

*Cosponsored by ORGN*

*Financially supported by Elsevier,  
Supramolecular Chemistry, RSC*

A. E. Gorden, *Organizer*

P. A. Gale, *Presiding*

**1:30 INOR 785.** Cation-dependent gold recovery with  $\alpha$ -cyclodextrin facilitated by second-sphere coordination. Z. Liu, J.F. Stoddart

**2:00 INOR 786.** Water-soluble porphyrinoids as G-quadruplex binders and telomerase inhibitors. H. Furuta, Y. Ikawa, S. Katsumata

**2:20 INOR 787.** Imine donor ligands for actinide selective coordination and sensing materials. A.E. Gorden

**2:40 INOR 788.** Metal directed formation of self-assembly supramolecular structures and materials from acyclic ligands. T. Gunlaugsson

**3:00 INOR 789.** Supramolecular behaviors in metal-macrocyclic frameworks. M. Shionoya

**3:20** Intermission.

**3:40 INOR 790.** Mathematical control in the self-assembly of giant M<sub>n</sub>, L<sub>2n</sub> polyhedral complexes. M. Fujita

**4:10 INOR 791.** Synthesis and coordination chemistry of molecular and polymeric Wurster-type receptors: Redox-active hosts for cations and anions. J.W. Sibert

**4:30 INOR 792.** Organizing mechanically interlocked molecules to function inside metal-organic frameworks. K. Zhu, N. Vukotic, S.J. Loebe

**4:50 INOR 793.** Calix[4]pyrroles: From ion pair receptors to molecular switches and self-assembled materials. J.L. Sessler

**5:10** Concluding Remarks.

## TUESDAY EVENING

## Section A

San Diego Convention Center  
Hall D

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

S. A. Koch, *Organizer*

**6:00 - 8:00**

**INOR 794.** Synthesis, characterization, and anticancer activity of gold(III) complexes with (1*R*,2*R*)-(–)-1,2-diaminocyclohexane. A.A. Isab

**INOR 795.** Antifungal and anti-parasitic transition metal complexes of linked, bridged tetraazamacrocyclic. T.J. Hubin, S.J. Archibald, M. Jacob, B. Tekwani, F. Khan

**INOR 796.** Unsymmetric bis-tetraazamacrocyclic transition metal complexes as CXCR4 antagonists. D.G. Jones, C. Baker, C.D. Garcia, A.N. Walker, D. Schols, P. Symmers, S.J. Archibald, T.J. Hubin

**INOR 797.** Binding events of zinc finger proteins. E. Joung, S. Park, S. Lee

**INOR 798.** Synthesis, characterizations, and DNA-binding and cytotoxicity studies of organorhenium naproxenol complexes. S. Azemati, S. Pramanik, S.K. Mandal, A.J. Winstead

**INOR 799.** Kinetic-mechanistic studies on methemoglobin generation by biologically active thiosemicarbazone iron (III) complexes. M.T. Basha, P.V. Bernhardt

**INOR 800.** Investigation of bimetallic asymmetric ruthenium(II) complexes and their DNA interactions. K. Thomas, M.T. Mongelli

**INOR 801.** Withdrawn.

**INOR 802.** Ruthenium-caged P450 inhibitors for dual antitumor activity. A. Zamora, E. Wachter, D.K. Heidary, C.A. Denning, E.C. Glazer

## Section A

San Diego Convention Center  
Hall D

### Coordination Chemistry: Synthesis & Characterization

S. A. Koch, *Organizer*

**6:00 - 8:00**

**INOR 803.** Synthesis, characterization, and CO-releasing properties of rhodium carbonyl complexes containing terpyridine derivatives ligand. B. Zhu, X. Wei, Q. Zhao, J. Xie

**INOR 804.** Bidirectional non-innocence of formazanate in ruthenium complexes. A. Mandal, G.K. Lahiri

**INOR 805.** Synthesis and characterization of new molybdenum(V) complexes with *N*-salicylidene-2-aminothiophenol. N.V. Kolacia

**INOR 806.** Reaction dynamics of simple polyoxometalate ions in water. M.R. Spriet, E.M. Villa

**INOR 807.** Organometallics complexes with triazene ligands functionalized with hindered imidazoles. J. Camarena, V. Miranda Soto, M.P. Parra Hake, D.B. Grotjahn

**INOR 808.** Mixed-valence triruthenium clusters with hydrophobic ligands. M.J. Glover, D.J. SantaLucia, A.L. Eckermann

**INOR 809.** Four new coordination polymers based on p-Terphenyl-3,3',5,5'-tetracarboxylic acid: Syntheses, structures, and photoluminescent properties. C. Zheng

**INOR 810.** Investigating the robustness of disassembly-reassembly methods for the formation of heterometallic MOFs. A. Marton, S. Baudron, M. Hosseini

**INOR 811.** Organometallic complexes of a new electron-rich diketiminato ligand. M.A. Land, K.E. Ylijoki, K. Robertson, P.T. Lee, D. Vidovic, J.A. Clyburne

**INOR 812.** Isomerism and magnetic characteristics of iron heteroscorpionates. K. Demaree, P. Desrochers

**INOR 813.** Synthesis, structural characterization and luminescent behavior of heteroleptic zinc(II) complexes employing novel asymmetric *N,N*-heterocyclic ligands. H. Schoechert, I.M. Klein, S. Kraft, K.L. Cunningham, J.T. Mague, W.F. Wacholtz

**INOR 814.** Computational modeling and analysis of stable 14 electron hemi-chelated Pd-Cr complexes. D. Anstine, J. Djukic

**INOR 815.** Biologically inspired manganese cluster chemistry. D.J. Jovine, M. Zdilla, S. Vaddypally

**INOR 816.** Investigating the electronic and structural properties of trans Co<sup>III</sup>-cyclam acetylides. S.D. Banziger, T. Ren

**INOR 817.** Synthetic strategy for multi-layered Pd(II) complexes via transannular  $\pi$ - $\pi$  interactions. H. Lee, O. Jung

**INOR 818.** 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

**INOR 819.** Novel ligands for organometallic catalysis. B. Wicker, K.M. Gass, M.T. St. Lawrence, Y. Wang, J.H. Davis, R. Sykora

**INOR 820.** Square-planar and octahedral isomers of a Ni(II) complex with a labile sulfur-centered ligand. T. Chivers, J. Konu, S. Haggman, A. Mansikkamaki, I.S. Morgan, H. Tuononen, R. Thirumoorthi, M. Lahtinen

**INOR 821.** Progress towards the synthesis of ligand-free copper(I) carboxylates. H.M. Kidd, S.L. Sandri, A.T. Royappa

**INOR 822.** Synthesis, structural characterization, and magnetic properties of tetranuclear copper(II) and cobalt(II) complexes of Schiff base ligands. Metal catalyzed formation and stabilization of acetal. S.S. Tandon, S.D. Bunge, L.K. Thompson

**INOR 823.** Synthesis and structural characterization of dinuclear 3d-4f complexes, dinuclear (Eu), tetranuclear (Ni), and hexanuclear (Dy) complexes of a Schiff base ligand. S.D. Bunge, S.S. Tandon, V. Hogan, R.R. Boyle

**INOR 824.** Synthesis of 3-functionalized verdazyls. T. Pan, D.J. Brook, A. Herrera

**INOR 825.** Effect of intermolecular forces and linker on metal organic framework secondary structure. M. Johnson, B.A. Doyle, C. Bauer

**INOR 826.** Coordination chemistry of sulfur and selenium oxidized derivatives of tris(2-pyridyl)phosphine with Co(II), Ni(II), Cu(II), Zn(II), and Cd(II) nitrates. A. Bevan, C. Fairfield, A.K. Frampton, D. Pericic, N.A. Piro, W.S. Kassel

**INOR 827.** Solventless and solvent-mediated synthesis and optoelectronic properties of brightly luminescent Ag(I) and Cu(I) azolate/quinoxaline complexes. A.R. Hinkle, K. Reyes, K. Maxwell, S. Hutcheson, M. Wilk, V. Nesterov, M. Omary

**INOR 828.** Synthesis and characterization of Cu(I) and Ag(I) tetrazolate complexes toward active or passive components of electronic devices. R.M. Almotawa, A. Cimino, V. Nesterov, M. Omary, M.A. Omary

**INOR 829.** Synthesis, characterization, and reactivity of small, solvent supported molybdenum clusters. S.C. Haefner

**INOR 830.** Synthesis, single crystal X-ray crystallography and computational studies of Co(II) complex of trimethoprim, [Co(TMP)<sub>2</sub>S<sub>2</sub>]. P.A. Aijbade

**INOR 831.** Synthesis, characterization, and coordination chemistry of poly(2-pyridyl-phosphines) bridged by various linkers. C. Fairfield, N.A. Piro, W.S. Kassel



INOR **832**. Mid-to-late first-row transition-metal complexes of tris(2-pyridyl) phosphine (PPy<sub>3</sub>) and its oxide. **A. Spitzer**, C. Fairfield, A.K. Frampton, N.A. Piro, W.S. Kassel

INOR **833**. Synthesis towards symmetric substituted verdazyl 2 x 2 grid complexes. **B. Ploof**, D.J. Brook, C. Fleming, E. Johnson

INOR **834**. Synthesis of new imine-containing ligand scaffolds for metalloenzyme mimics. **T.M. Dunn**, J.A. Dopke, R.J. Staples

INOR **835**. Bulk synthesis of TCNQ radical anion salts with chemical vapor deposition studying their crystal structure for applications in memory devices. **G.N. Gonzalez**

INOR **836**. Withdrawn.

INOR **837**. Structural studies of manganese carbonyl complexes derived from an anthracene scaffold appended with pyridine, aryl-thioether and aryl-thiolate donors. **T.A. Manes**, M.J. Rose

INOR **838**. Synthesis and electronic description of tetra- and pentametallic, mixed-metal, mixed-valent manganese-cobalt oxido clusters. **A. Nguyen**, D. Suess, L.E. Darago, D.S. Levine, T. Tilley

## Section A

San Diego Convention Center  
Hall D

### Electrochemistry

B. L. Lucht, *Organizer*

6:00 - 8:00

INOR **839**. Consequences of reduction of (T(p-X)PP)Ru(NO)Cl (X= H, Cl, Me, OMe). **J. Zink**, M.J. Shaw, G.B. Richter-Addo

INOR **840**. Analysis of a four H-bond array using cyclic voltammetry: Introducing a new redox center to strengthen dimerization. **B. Tamashiro**, G. Darzi, D.K. Smith

INOR **841**. Proton-coupled electron transfer in an electroactive three hydrogen bond DDA array capable of binding an AAD guest. **R. He**, D.K. Smith

INOR **842**. Novel approaches to the chemical application of electrochemical materials for conducting materials. **E.J. Parish**, M. Hsiao, H. Honda, T. Wei

INOR **843**. Design of a microfluidic electrochemical DNA/RNA hybridization sensor. **J.M. Philippe**, M.C. Buzzeo

INOR **844**. Fluorinated porphyrin as a metal-free electrocatalyst for hydrogen generation. **Y. Wu**, D. Villagran

INOR **845**. Functionalization of Si(111) with sterically spaced molecular wires intercalated within ALD-deposited metal oxides for electron transfer applications. **F. Konopka**, M.J. Rose

## Section A

San Diego Convention Center  
Hall D

### Environmental & Energy-Related Inorganic Chemistry

S. A. Koch, *Organizer*

6:00 - 8:00

INOR **846**. Kinetics of the electrochemical reduction of CO<sub>2</sub> by Re(I) bipyridine complexes: Role of solvents and electrolytes. **J. Nganga**

INOR **847**. Probing structures, spin states, redox properties, and thermodynamics of Co-OEC analogs using broken-symmetry density functional theory. **S. Niu**, E.N. Brothers, M.B. Hall

INOR **848**. Withdrawn.

INOR **849**. Synthesis and study of the photo-physic, excited-state properties, and photolabilization pathways of cyclometalated Ir(III)-Pt(II) and Ir(III)-Ir(III) bimetallic complexes bridged by dipyriddyipyrazine (dpp). **Y. Cho**, S. Kim, D. Cho, H. Son, S.O. Kang

INOR **850**. Oxygen reduction reaction electrocatalysts based on LaFe<sub>2</sub>CO<sub>1-x</sub>O<sub>3</sub> thin films prepared by spray-pyrolysis. **D. Dervishogullari**, L.R. Sharpe

INOR **851**. Ionic conductivities of silyl and carbonate blend electrolytes. **L.J. Lyons**, I. Dixon-Anderson, T. Robinson

INOR **852**. Ni-based electrochemical catalysis for water splitting. **Y. Wang**, G. Wang, Y. Huang, X. Duan

INOR **853**. Essential cation-π interaction in a psychrophilic electron transfer protein. **N. Dalchand**, K.S. Montero, G.J. Salerno, M.C. Buzzeo, J.S. Magyar

INOR **854**. Improved electrical energy storage using nanofiller modified fly-wheels. **T.J. Boyle**, T.N. Lambert, N.S. Bell, W.K. Miller

INOR **855**. Withdrawn.

INOR **856**. Measuring siliceous zeolites for Xe/Kr separations. **A. Sharma**, L. Nemeth, K.V. Lawler, P. Forster

INOR **857**. Development of a photochemical and electrochemical detector of thiocyanate in marine environments. **A.R. McCabe**, C.A. Sweet, C.R. Rockwell, B.S. Sheetz, C. Murphy

INOR **858**. Ecotoxicity study during DEET degradation by ozone. **L. Li**, J. Lee, K. Yeung

INOR **859**. Molecular orbital engineering of a panchromatic cyclometalated Ru<sup>II</sup> dye for p-type dye sensitized solar cells. **M. He**, Z. Ji, Z. Huang, Y. Wu

INOR **860**. Methionine ligand substitution processes provide dynamic stabilization of a psychrophilic metalloprotein. **N.K. Asous**, S.J. Barth, S.K. Lone, K.S. Montero, M.C. Buzzeo, J.S. Magyar

INOR **861**. Metal uptake and regulation in a methanogenic archaeon from the tar pits at Rancho La Brea, Los Angeles. **J. Lee**, P.M. Magyar, J.S. Magyar

INOR **862**. Overexpression, purification, and characterization of a cytochrome P450-type alkane monooxygenase from a psychrophilic marine bacterium. **G.J. Salerno**, J.S. Magyar

INOR **863**. Overexpression and purification of a putative iron uptake protein from the marine diatom *Phaeodactylum tricornutum*. **J. Chou**, K. Farrell, E.M. Shoenfelt, B.C. Bostick, J.S. Magyar

INOR **864**. Protein delivery of a Ni catalyst to photosystem I for light-driven hydrogen production. **S.C. Silver**, J. Niklas, O. Poluektov, P. Du, D.M. Tiede, L.M. Utschig-Johnson

INOR **865**. Water splitting through metal oxide photocatalysts: Effect of shape anisotropy, nature of co-catalysts, and surface properties. **K. Latimer**, D. Daniels, K. Senevirathne

INOR **866**. Organosilyl electrolyte conductivities, lithium transference numbers, and solvation shells via PFG-STE NMR diffusion experiments and their application in lithium-ion batteries. **C. Mulligan**, L.J. Lyons

INOR **867**. Optimization and characterization of high-performance CuFeMgW oxide based semiconductors for solar photocatalysis. **C.A. Sharpe**, L.R. Sharpe

INOR **868**. 3-D Interconnected mesoporous tantalum nitride as a novel water splitting photocatalyst. **H. Kang**, S.H. Tolbert

INOR **869**. Bioaccumulation of selenium in the model bryophyte *Physcomitrella patens*. **J. Carsella**, D.C. Crans, S.J. Bonetti, D. Lehmpuhl

INOR **870**. Post-synthetic alkylamine modification on metal-organic frameworks with isostructures for CO<sub>2</sub> capture. **H. Li**, H. Zhou

## Section A

San Diego Convention Center  
Hall D

### Inorganic Catalysts

S. A. Koch, *Organizer*

6:00 - 8:00

INOR **871**. Chlorite dismutation to chlorine dioxide by an [Fe<sup>III</sup>-TAML] complex. **M. Ramachandra**, J. Park, S.D. Hicks, W. Nam, M.M. Abu-Omar

INOR **872**. Increasing ligand denticity: A strategy for a better water oxidation catalyst (WOC). **F. Saeedifard**, J.M. Kamdar, D.C. Mareluis, D.B. Grotjahn

INOR **873**. Improving the efficiency nickel-bisphosphine hydrogen gas production catalysts by lowering overpotential. **A.P. Cardenas**, E.S. Wiedner, M. Helm, A.M. Appel, M.J. O'Hagan

INOR **874**. Synthesis and reactivity of a secondary phosphine ligand with Ni(0) and Ni(II). **N.J. Downes**, T.W. Chapp

INOR **875**. Withdrawn.

INOR **876**. New metals (V, Pd, Ru) and new amide pendant-arms for cross-bridged tetraazamacrocyclic oxidation catalysts. **M. Gorbet**, G. Yin, T.J. Hubin

INOR **877**. Photocatalytic metal-organic frameworks for the aerobic oxidation of arylboronic acids. **X. Yu**, S. Cohen

INOR **878**. Efficient nickel-catalyzed transfer hydrogenation of ketones using ethanol as solvent and hydrogen donor. **N. Castellanos**

INOR **879**. Light-driven dual metal catalysis. **M. Gelwicks**

INOR **880**. Electrocatalytic materials composed of Earth-abundant elements for the hydrogen and oxygen evolution reactions. **J. Mondschein**, J.F. Callejas, C.F. Holder, J.M. McEaney, R.E. Schaak

INOR **881**. Unusual <sup>13</sup>C NMR shift in "tilted" n-heterocyclic carbene complexes explained. **L. Falivene**, L. Cavallo

INOR **882**. Understanding the distinctive electronic structure of Re and Ru tris(thiolate) complexes and its role in chemistry. **H. Tang**, M.B. Hall

INOR **883**. Design and investigations of peptidic platforms on the electrocatalytic reduction of carbon dioxide by a rhenium bipyridine-based complex. **S.A. Chabolla**, C.W. Machan, S. Sahu, E. Dellamaria, J. Yin, M.K. Gilson, F.A. Tezcan, C.P. Kubiak

INOR **884**. Observation and reactivity studies of an unusual RhI intermediate in H<sub>2</sub> evolution catalysis. **L. Aguirre Quintana**, H.B. Gray, J.R. Winkler, J.D. Blakemore

INOR **885**. Aqueous stability and catalytic HER activity of [(DHMP)<sub>2</sub>Ni][BF<sub>4</sub>]<sub>2</sub> under various pH conditions. **S. Ruelas**, C. Tsay, J. Yang

INOR **886**. Hydrodesulfurization of dibenzothiophene using bimetallic and trimetallic: Cobalt, nickel, tungsten sulfide. **D.F. Gonzalez**, J.S. Sollner, J. Parsons

INOR **887**. Aqueous solution palladium catalyzed Suzuki cross coupling reactions: The effect of base and base concentrations. **T. Olson**, J. Parsons

INOR **888**. Metal organic frameworks as catalysts for organic photoredox transformations. **M.W. Logan**, Y. Lau, Y. Zheng, M. Hettinger, R. Marks, M. Hosler, Y. Yuan, F. Uribe-Romo

INOR **889**. Mechanistic investigation of proton reduction by cobaloximes: Insight from H<sub>2</sub> oxidation kinetics. **S.A. Del Ciello**, J.R. Winkler, J.C. Peters, H.B. Gray

INOR **890**. Withdrawn.

INOR **891**. Molecular catalyst incorporation in conductive coordination polymer scaffolds for heterogeneous electrocatalytic carbon dioxide reduction. **G. Merlen**, M.L. Clark, S.A. Chabolla, C.P. Kubiak

## Section A

San Diego Convention Center  
Hall D

### Inorganic Spectroscopy

V. C. Popescu, *Organizer*

6:00 - 8:00

INOR **892**. Mössbauer spectroscopy and electronic structure of bimetallic iron-nitrosyl complexes. **V.C. Popescu**, M. Cohara, P. Ghosh, M.Y. Darenbourg

INOR **893**. Spectroscopic studies of five-coordinate cobalt (II) model complexes: Fluorine substituted hydroxamic acids. **C.D. James**, T. Kuehn, C.N. Worley, D.L. Tierney

INOR **894**. Large and affected by charge: Synthesis and analysis of binaphthoquinone and dibenzoxanthene compounds. **T. Haden**, S.M. Kruse, W. Cross Lopez, J. Herring, S.K. Hurst

INOR **895**. Group 5 (VB) metals speciation in fused chlorides: A spectroelectrochemical study. **I.B. Polovov**, V.A. Volkovich, B.D. Vasin, T.R. Griffiths

INOR **896**. Molybdenum(IV) and tungsten(IV) species in fused chlorides: A spectroscopy study. **V.A. Volkovich**, A.B. Ivanov, B.D. Vasin, I.B. Polovov, T.R. Griffiths

INOR **897**. Measurement of electron delocalization energy in hydrogen-bonded mixed valent Ru<sub>2</sub>O acetate clusters. **T.M. Porter**, G. Canzi, J. Goeltz, C.P. Kubiak

INOR **898**. Excited-state electron transfer from CdSe quantum dots to TiO<sub>2</sub>: Influence of the properties of molecular linkers on electron transfer within mesoporous films. **M.J. Awad**, K.R. Liwosz, D. Watson

INOR **899**. Fiber optic reflectance spectroscopy and multispectral imaging used to assess cadmium sulfide degradation in cadmium yellow paint in paintings by Louise Herreshoff. **M. Stephenson**, B. Becker, E. Timas, **E.S. Uffelman**, P. Hobbs, J. Mass, J. Delaney, K.A. Dooley

INOR **900**. ESR of the heavy-fermion YbRh<sub>2</sub>Si<sub>2</sub>. **C.C. Beedle**, R.D. McDonald, Z. Fisk, N. Harrison, J. Singleton

INOR **901**. Toward ratiometric metal ion sensors based upon thermoresponsive polymers: Polymer collapse and aggregation detected by fluorescence and light scattering. **L. Fulton**, L. Nyranshuti, W. Seitz, R.P. Planalp

INOR **902**. Measurement of NMR relaxation rates in a series of cobalt (II) β-diketonates. **R.R. Baum**, D.L. Tierney

INOR **903**. Stabilization of a combined phenolphthalin/ Cu(II)/EDTA reagent used for the spectrophotometric determination of aqueous cyanide. **S.J. Chalk**, N. Gutierrez

## Section A

San Diego Convention Center  
Hall D

## Interplay of Structure &amp; Transport Properties in Materials for Energy

K. Kovnir, B. C. Melot, *Organizers*

6:00 - 8:00

INOR **904.** Correlating exciton transport with structural properties in lead sulfide (PbS) nanocrystal films. M.C. Weidman, W.A. Tisdale

INOR **905.** Inkjet printing of water-processible polyaniline films for clean energy applications. Y. Hu, M.E. Hagerman

INOR **906.** Effect of polyhedral rotational distortion on the electrochemical properties of polyanionic intercalation electrode materials. S. Zhou, B.C. Melot, R.L. Brutchey, G. Barim

INOR **907.** Synthesis and characterization of boron phosphide. K. Woo, K. Kovnir

## Section A

San Diego Convention Center  
Hall D

## Lanthanide &amp; Actinide Chemistry

A. De Bettencourt Dias, *Organizer*

6:00 - 8:00

INOR **908.** Determination of magnetic anisotropy and ligands effect in  $D_{4h}$  molecules with slow magnetic relaxation. D. Paez

INOR **909.** Separation of 4f- and 5f-elements in a "fused salt - liquid metal" system. V.A. Volkovich, D.S. Maltsev, S.Y. Melchakov, L.F. Yamshchikov, I.B. Polovov

INOR **910.** Hydrothermal synthesis of lanthanide sulfites and sulfates. J.T. Dvogan, E.M. Villa

INOR **911.** Aluminum-gadolinium master-alloy for aerospace application: Synthesis and properties. I.B. Polovov, A.V. Krylosov, K.V. Maksimtsev, S.V. Belikov, V.A. Volkovich

INOR **912.** Synthesis of a library of divalent europium cryptates. L.E. Hopper, M.J. Allen

INOR **913.** Synthesis of heterometallic rare earth metal precursors to single-molecule magnets with molybdenum and tungsten tetrasulfide bridges. M.D. Boshart, J.W. Ziller, W.J. Evans

INOR **914.** Computational study of divalent transuranic actinides. G. Chen, F.U. Furche

INOR **915.** Withdrawn.

INOR **916.** Organic ligands for actinide extraction in alkaline conditions. E.V. Govor, E. Vasileiadou, S. Kandel, R.G. Raptis, K. Kavallieratos

INOR **917.** Gemini surfactant-based Ln(III) complexes for bioprobe applications. M. Cendejas, A. McAdams, L. Elmendorf, P.S. Barber

## Section A

San Diego Convention Center  
Hall D

## Metal-Oxygen Oxidants in Synthesis &amp; Biology: Beyond Metal- Oxo Species

T. A. Jackson, M. T. Kieber-Emmons, *Organizers*

6:00 - 8:00

INOR **918.** X-ray absorption spectroscopic characterization of the diferric peroxo intermediate of human deoxyhypusine hydroxylase in the presence of its protein substrate. A. Jasniewski, L. Engstrom, V. Vu, L. Que

INOR **919.** Is ferryl a side-product or an intermediate in catalysis of L-tryptophan dioxygenation by human indoleamine 2,3-dioxygenase (hIDO1)? I.M. Chrisman, L.S. Dameron, V.V. Smirnov

INOR **920.** Modulating dioxygen activation of manganese corrolazines. H.M. Neu, D.P. Goldberg

INOR **921.** Characterization and reactivity of a Mn(III)-alkylperoxo species supported by an amide-containing ligand. J. Parham, G. Wijeratne, T.A. Jackson

INOR **922.** Characterization and oxygen reactivity of a flavonoid-bound manganese complex supported by a scorpionate ligand. M. Denler, T.A. Jackson

INOR **923.** Electrochemical investigations of peroxomanganese(III) complexes. A.A. Massie, E. Anxolabehere, T.A. Jackson

INOR **924.** Formation, characterization, and O-O bond activation of a peroxomanganese(III) complex supported by a cross-clamped cyclam ligand. H.E. Colmer, T.A. Jackson

INOR **925.** Lignin: Utilizing stable metal-oxyl complexes to initiate radical depolymerization. T. Carroll, G. Menard

INOR **926.** Insights into Mn(III)-OH reactivity: Experimental and theoretical investigations into the role of electronic structure on hydrogen atom abstraction. D. Rice, A. Burr, G. Wijeratne, T.A. Jackson

INOR **927.** Redox-active ligand mediated oxyl-type O-atom transfer from an exceptionally high valent oxorhenium complex. J.A. Hill, J.D. Soper

## Section A

San Diego Convention Center  
Hall D

## Nanoscience

R. M. Richards, *Organizer*

6:00 - 8:00

INOR **928.** Colloidal synthesis and transformation of ZnO nanoparticles. J.L. Fenton, J.M. Hodges, R.E. Schaak

INOR **929.** Cation exchange in quantum dots: Lessons from the Zn/Pb system. W.R. Tilluck, S. Benjamin, C. Mings, A.L. Morris, P.G. Van Patten

INOR **930.** Controlling the surface modification of magnetic iron oxide nanoparticles: Understanding the binding of benzoic acid and catechol-derived ligands. K.V. Korpany, D. Majewski, C.T. Chiu, S.N. Cross, A.S. Blum

INOR **931.** One-step ligand exchange for the synthesis of superparamagnetic aqueous-stable iron oxide nanoparticles by mechanochemical milling. K.V. Korpany, C. Mottillo, J. Bachelder, P. Dong, S. Trudel, T. Friscic, A.S. Blum

INOR **932.** Periodic arrays of gold ellipse dimer nanoantennae with 10-nm gaps as highly active and tunable SERS substrates. A.M. Jubb, Y. Jiao, G. Eres, S. Retterer, B. Gu

INOR **933.** Influence of ZnO particle size and morphology on photocatalytic degradation of malachite green. J.D. Harris, C.C. Pena, S.C. Bryant, A.J. Christy, A.E. Harris, J.E. Cowen, J.J. Pak

INOR **934.** Studies towards the formation of novel gold copper alloyed anti-neoplastic agents. B.M. Benin, M. Goomann, S. Huang

INOR **935.** Dendrimer modified silica nanoparticles as fluorescent chemosensors for the detection of copper and cyanide. A. Luhrs, K. Lyashkevych, C. Feider, L.D. Margerum

INOR **936.** Multi-step cation exchange of PbS quantum dots. A. Morris, W. Tiluck, S. Benjamin, C. Mings, P. Patten

INOR **937.** Aqueous phase synthesis of metal nanoparticles and hybrid nanocomposites with controlled geometries. A. Penn, T. Abeywickrama, H.P. Rathnayake

INOR **938.** Catalytic activity of ultrasmall copper nanoparticles synthesized with a plant-based reducing agent. S.K. St Angelo, G.A. Ferko

INOR **939.** Controlling the exciton dissociation rates in semiconductor nanocrystal films. N.N. Kholmicheva, M. Zamkov

INOR **940.** Lowering the valence band of  $Cu_2ZnSnS_4$  through anion substitution: Can it be done? M. Thompson, J. Vela-Becerra

INOR **941.** Gas-phase synthesis of clusterfullerenes. P.W. Dunk, A.G. Marshall, H.W. Kroto

INOR **942.** Surface doping of colloidal nanocrystal quantum dots with transition metal complexes. H. Crotty, J. Vela-Becerra

INOR **943.** Target-specific mesoporous silica nanoparticles for combination therapy of cisplatin and gemcitabine to treat cancer. E.D. Fink, S. Yang, M.P. Alvarez-Berrios, J.L. Vivero

INOR **944.** Ground state properties and non-adiabatic dynamical studies of  $Pb_{1-x}X_x/Cd_{32}Y_{32}$  ( $X, Y = S, Se, Te$ ) core/shell quantum dots. P.K. Tamukong

INOR **945.** Withdrawn.

## Section A

San Diego Convention Center  
Hall D

## Organometallic Chemistry: Applications to Materials &amp; Polymer Science

N. S. Radu, *Organizer*

6:00 - 8:00

INOR **946.** polyMOFs: Exploring polymer structure effects on metal-organic frameworks. S. Ayala, Z. Zhang, H. Nguyen, S.A. Miller, S. Cohen

INOR **947.** Preparation of metal thiolate complexes for controlled synthesis of nanomaterials. S. Pickle, A.W. Holland

## Section A

San Diego Convention Center  
Hall D

## Organometallic Chemistry: Applications to Organic Transformations

N. S. Radu, *Organizer*

6:00 - 8:00

INOR **948.** C-CN cleavage using palladium supported by a dippe ligand. L. Munjanja, C. Torres-Lopez, W.D. Jones

INOR **949.** Understanding copper-catalyzed oxidative decarboxylative coupling reactions through the reactivity of copper benzoate and copper aryl complexes. K. Bustin, E. Aguilera, C. Burlas, J.M. Hoover

INOR **950.** Synthesis and reactivity of aminovinyl carbene complexes. R.M. Padilla, A. Feliciano, J. Tamariz, F. Delgado

INOR **951.** Sterically-controlled C-H borylation of aryl phosphines. E.E. Albitz, N. Huynh, T.B. Clark

INOR **952.** Synthesis of alkene-appended dodecaborates. D.T. Buening, J.A. Dopke, R.J. Staples, K.N. Westdorf, A.J. Ramirez

INOR **953.** Studies toward the mechanism of amine-directed, iridium-catalyzed C-H borylation of *N,N*-dimethylbenzylamines. C.M. Oliver, K.A. McGarry, T.B. Clark

## Section A

San Diego Convention Center  
Hall D

## Organometallic Chemistry: Synthesis &amp; Characterization-Late Transition Metals

N. S. Radu, *Organizer*

6:00 - 8:00

INOR **954.** Mono- and binuclear Au(I)-complexes of 1,2,3-triazolylidenes: Synthesis, characterization, and trends in catalysis and properties. L. Hettmanczyk, M. van der Meer, S. Hohloch, B. Sarkar

INOR **955.** Development of new phosphorescent platinum complexes emitting in the deep red to near infrared region. R. Mroz, T. Power, S. Huo

INOR **956.** C-H and C-P activation by a redox non-innocent ligand supported iron dinitrogen complex. C. Ghosh, T.L. Groy, A.C. Bowman, R.J. Trovitch

INOR **957.** Perfluoro-olefin, carbene, and carbene complexes of (PNP)Rh. C.J. Pell, Y. Zhu, R. Huacuja, O. Ozerov

INOR **958.** Tris(3,5-dimethylpyrazol-1-yl)methane and 1,1,1-tris-(3,5-dimethylpyrazol-1-yl)-2-(trimethylsilyloxy)ethane platinum compounds: Synthesis, reactivity and structure. B.P. Quillian, T.B. Gunnoe, A. Lorbecki

INOR **959.** Reactivity of bi(pyrazol-1-yl)acetic acid ligands with diiodo( $\eta^6$ -*p*-cymene) ruthenium(II). B.P. Quillian, A.E. Fields

INOR **960.** Synthetic heterocycles and their applications in energy and advanced electronics. N.C. Tice, C. Snyder, D.L. Smith

INOR **961.** Photophysical properties of platinum group compounds bearing modified pyridine ligands. S.N. Natoli, L.M. Hight, D.R. McMillin

INOR **962.** Facile aerobic alkylation of rhodium porphyrins with alkyl halides. W. Yang, H. Zuo, Y.W. Lai, S. Feng, S.Y. Pang, E.K. Hung, Y.C. Yu, F.Y. Lau, Y.H. Tsoi, K.S. Chan

INOR **963.** Synthesis, characterization and reactivity of late transition metal complexes stabilized by bi- and tridentate ligands. S.H. Schreiner, J. Seo

INOR **964.** Small molecule activation with transition metal-silylene complexes. A.M. Bartrom, W. Harman

INOR **965.** Synthesis and structural determination of mono- and dinuclear late transition metal ferrocenyl complexes. S.H. Schreiner, P. Koirala

Technical program information known at press time.

The official technical program for the 251st ACS National Meeting is available at: [www.acs.org/sandiego2016](http://www.acs.org/sandiego2016)

**INOR 966.** Low-valent 3d metals in weak ligand fields for bio-inspired small molecule activation. **P. Pairs, W. Harman**

**INOR 967.** Synthesis and reactivity of high-valent organometallic nickel complexes bearing trifluoromethyl ligands. **J.R. Bour, N. Camasso, M.S. Sanford**

**INOR 968.** Reactivity of bis-protic *N*-heterocyclic carbene (bis-PNHC) complexes of iridium(III). **J.L. Gomez Lopez, V. Miranda Soto, M.P. Parra Hake, D.B. Grotjahn, A.L. Rheingold**

**INOR 969.** Activation of small molecules using transition metal silylene and germylene complexes. **M. Barrientos, W. Harman**

**INOR 970.** Co(CNA<sup>AlMe2</sup>)<sub>2</sub>, an isolobal analogue of Co(CO)<sub>4</sub>, and its reactivity. **C. Chan, J.S. Figueroa**

## Section A

San Diego Convention Center  
Hall D

### Solid-State Inorganic Chemistry

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

#### 6:00 - 8:00

**INOR 971.** Investigation of vanadium-based bronze materials for the detection of peroxide based explosives. **A.A. Allothman, N.F. Materer, Z. Allothman, A.W. Ablett**

**INOR 972.** Geometrical and functional properties of organic ligands on gas sorption properties of metal-organic framework materials. **T.X. Trieu, X. Zhao, X. Bu**

**INOR 973.** Solid state synthesis of copper iron selenostannates. **S.A. Donnelly, B.J. Bellott**

**INOR 974.** Synthesis and characterization of CO<sub>2</sub> chemisorption sites in TMOS/CH<sub>3</sub>OH/H<sub>2</sub>O xerogels. **R. Neuweiler, E.G. Look, H.D. Gafney**

**INOR 975.** Tacticity control of organic polymers inside MOFs via [2+2] photo-polymerization reactions. **I. Park, R. Medishetty, A. Chanthapally, H. Lee, C. Mulljanto, Z. Zhang, H. Quah, S. Lee, M.J. Zaworotko, J.J. Vittal**

**INOR 976.** Comparison of the negative thermal expansion and behavior on compression for CaZrF<sub>6</sub>, CaNbF<sub>6</sub> and MgZrF<sub>6</sub>. **B. Hester**

**INOR 977.** Competing broken inversion symmetry and oxygen octahedral sliding phenomena in *n*=1 Ruddlesden popper derivative HRTIO<sub>4</sub> (R=Nd, Sm, Eu, Gd, and Dy) family. **F. Brown, A. Sen Gupta, H. Akamatsu, M. An Nguyen, T. Mallouk, V. Gopalan**

**INOR 978.** Development of an aqueous synthesis for zinc oxide nanoparticles with biologically benign capping agents. **J. Zinna, M.C. Gelabert**

**INOR 979.** Hydrothermal synthesis of metal homo- and heteropolychalcogenide compounds. **E.G. Yerdon, C.C. Raymond**

**INOR 980.** Synthesis and single crystal structure of (OC)<sub>2</sub>W(Ph<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>PPh<sub>2</sub>)<sub>2</sub>W(CO)<sub>6</sub>. **H. Drake, K.A. Wheeler, B.J. Bellott**

## Section A

San Diego Convention Center  
Hall D

### Supramolecular Chemistry: A Crown & Anchor Approach

A. E. Gorden, *Organizer*

#### 6:00 - 8:00

**INOR 981.** Molecular recognition of uranyl using salen ligand chemosensors. **M. Eddy, E.E. Hardy, A.E. Gorden**

**INOR 982.** Combination of texaphyrin and platinum(IV) prodrugs as a potential new anticancer therapy. **G. Thiabaud, Z.H. Siddik, J.L. Sessler**

**INOR 983.** Dynamic synthesis of diazaborole based oligomers and macrocycles. **S. Lokugama, C. Manankandayalage, D.E. Gross**

**INOR 984.** Allosteric regulation in supramolecular capsules, cages, and polyhedra. **A. d'Aquino, C.A. Mirkin**

**INOR 985.** Design foldamers from fragments: Chloride encapsulation and switchable double helices. **Y. Liu, A. Sengupta, K. Raghavachari, A.H. Flood**

**INOR 986.** Investigation of CB[7] binding effects on organic chromophores. **C.H. Battle, G.H. Aryal, T.A. Grusenmeyer, J. Jayawickramarajah**

**INOR 987.** Evolving small library of nipecotate and isonipecotate cored derivatives for acetylcholine esterase inhibition. **N. Beltrami, D. Calderon, L.P. Dennis, S. Hickmann, E.F. Walsh, H. William, M. Torok, D. Sikazwe, J.M. Davis**

**INOR 988.** Studies of deep-cavity cavitands. **J.H. Jordan, B.C. Gibb**

**INOR 989.** Synthesis and characterization of dipyrinones as supramolecular building blocks. **Z. Nichols, M.T. Huggins, A. Schrock, K. Barnes, T. Jarvis, A. Fisch**

**INOR 990.** Synthesis and characterization of novel fluorescent boron containing molecule. **N.S. Jackson, A.R. Schroeder, S.E. Harrell, M.T. Huggins, A. Schrock, P.P. Vaughan, K. Molek**

**INOR 991.** Exploitation of new five-coordinate vanadyl complexes for comparative uranyl studies and application to metal sequestration. **J. Niklas, A.E. Gorden**

**INOR 992.** Targeting the terminus in peptide recognition by synthetic receptors. **A.R. Urbach**

**INOR 993.** Oxazolidinone-based small molecule libraries for the selective recognition of therapeutically relevant RNA. **B. Morgan, R.N. Culver, B. Blachut, A.E. Hargrove**

**INOR 994.** Expanded porphyrin cyclo[1]furan[1]pyridine[4]pyrrole: A hybrid macrocycle displaying aromatic character upon cation complexation. **J.T. Brewster, I. Ho, Z. Zhan, J.L. Sessler**

**INOR 995.** Molecular recognition of uranyl using a resin supported salen 2-quinoxalino ligand. **C.D. Tutson, A.E. Gorden**

**INOR 996.** Uranyl extractions using a solid supported quinoxalino based salen ligand. **M. West, A.E. Gorden**

**INOR 997.** Analysis of π-π stacking and higher order dimensional crystal packing in recently characterized salphenazine complexes. **E.E. Hardy, A.E. Gorden**

**INOR 998.** Self-assembled pyridine-dipyrrolate cages. **H. Zhang, V. Lynch, J. Lee, E.V. Anslyn, J.L. Sessler**

**INOR 999.** Calix[4]pyrrole-based metal-organic frameworks (MOFs). **J. Lee, V. Lynch, N. Waggoner, S.K. Kim, S.M. Humphrey, J.L. Sessler**

**INOR 1000.** Energetic components of aryl CH•••X<sup>-</sup> hydrogen bonds: Field and resonance effects. **B.W. Tresca, R.J. Hansen, M.M. Haley, D.W. Johnson**

**INOR 1001.** Application of 'Texas-sized' molecular box in molecular device. **Y. Yang, H. Gong**

**INOR 1002.** Redox chemistry of pyrrole-based ligands in transition metal complexes. **K. Lincoln, R. Gautam, E. Tomat**

**INOR 1003.** In-vitro and intracellular metal chelation properties of sirtuin inhibitor sirtinol. **R. Gautam, E. Akam, E. Tomat**

**INOR 1004.** Towards selective ion-pair sensing based on anion and cation complexation and co-extraction: Dual-host combinations of fluorescent sensors for ammonium and nitrate. **T.M. Jonah, C.L. Cortes, R.A. Currie, K. Kavallieratos**

**INOR 1005.** Molecular cluster metalloligand for the synthesis of dual cluster metal-organic frameworks. **C. Bejger, J. Yu, D.W. Paley, M.L. Steigerwald, C.P. Nuckolls**

## Section A

San Diego Convention Center  
Hall D

### Transition Metal Chemistry in DNA & RNA Regulation

P. Chen, S. L. Michel, *Organizers*

#### 6:00 - 8:00

**INOR 1006.** Bioanalytical approaches to measure iron speciation in plasma of patients treated with iron-nanoparticle drug products. **H.M. Neu, A.D. Smith, A. Wilks, J.E. Polli, M.A. Kane, T.Y. Ting, S.L. Michel**

**INOR 1007.** In-cell fluorescence imaging of platinum anticancer compounds detected using click chemistry. **A.D. Moghaddam, J.D. White, M.M. Haley, V. DeRose**

**INOR 1008.** CPSF30, an RNA binding 'zinc-finger' protein with a 2Fe-2S cluster. **G.D. Shimberg, J. Michalek, A. Rodrigues, B.E. Zucconi, S. Ghosh, K. Sureshchandra, G.M. Wilson, T.L. Stemmler, S.L. Michel**

### Industrial Research at the Interface of Inorganic Chemistry & Polymer Science

*Sponsored by POLY, Cosponsored by BMGT and INOR†*

## WEDNESDAY MORNING

### Section A

San Diego Convention Center  
Room 30B

### Interplay of Structure & Transport Properties in Materials for Energy

B. C. Melot, *Organizer*

K. Kovnir, *Organizer, Presiding*

**8:30 INOR 1009.** Influence of lattice flexibility on ionic diffusion in materials for energy storage. **B.C. Melot**

**9:00 INOR 1010.** Electron transport in Ga<sub>2</sub>In<sub>6</sub>Sn<sub>2</sub>O<sub>16</sub>: The role of the 7-coordinate site. **K. Rickert**

**9:20 INOR 1011.** Exploring new electrode materials for Li-ion batteries: Structure and electrochemistry. **G. Rousse**

**9:50 Intermission.**

**10:10 INOR 1012.** Thermochemical synthesis of earth-abundant phosphorus-rich metal phosphides and metal thiophosphates for catalytic water splitting applications. **E.G. Gillan**

**10:30 INOR 1013.** Probing function and failure in energy materials with hard X-ray tools. **K.W. Chapman**

**11:00 INOR 1014.** First-principles modeling of Li diffusion in V<sub>2</sub>O<sub>5</sub> as cathode material of Li ion batteries. **S. Suthirakun, A. Genest, N. Roesch**

**11:20 INOR 1015.** Structure-function relationships in electrolytes for reversible magnesium batteries. **B.M. Bartlett, A.J. Crowe**

## Section B

San Diego Convention Center  
Room 30C

### Transition Metal Chemistry in DNA & RNA Regulation

P. Chen, *Organizer*

S. L. Michel, *Organizer, Presiding*

V. DeRose, *Presiding*

**8:30 INOR 1016.** *In vitro* selection and characterization of metal-specific DNAAzymes and their applications in imaging metal ions in living cells. **Y. Lu, K. Hwang, P. Wu, C.E. McGhee, S. Torabi**

**9:00 INOR 1017.** Modulation of DNA/RNA-protein interactions with substitution-inert platinum-metal compounds. **N. Farrell**

**9:30 INOR 1018.** RNA and DNA targets of platinum anticancer compounds detected using click chemistry. **A.D. Moghaddam, K. Plakos, R.M. Cunningham, J.D. White, M.M. Haley, V. DeRose**

**10:00 INOR 1019.** Luminescent zinc fingers: From zinc sensors to sequence-specific RNA sensors. **O. Seneque, L. Raibaut, M. Isaac, C. Cepeda, S.L. Michel, S. Eliseeva, S. Petoud**

**10:30 Intermission.**

**10:50 INOR 1020.** *In vivo* inhibition of zinc finger transcription factors by cobalt(III) Schiff base complexes. **T.J. Meade**

**11:20 INOR 1021.** Fe-S cluster biosynthesis provides cofactors to activate proteins that drive gene regulation. **T.L. Stemmler**

**11:50 INOR 1022.** DNA-mediated signaling. **J.K. Barton**

## Section C

San Diego Convention Center  
Room 30D

### Metal-Oxygen Oxidants in Synthesis & Biology: Beyond Metal- Oxo Species

T. A. Jackson, *Organizer*

M. T. Kieber-Emmons, *Organizer, Presiding*

**8:00 INOR 1023.** Role of carboxylic acids in iron-mediated peroxide activation: are peroxycarboxylates involved? **E. Rybak-Akimova, M.C. Piquette, S.G. McKenzie, G. Yang, O. Makhlynets, T. Palluccio**

**8:25 INOR 1024.** Mechanisms and purview of C-H-bond activation by mid-valent metal superoxide complexes. **J.M. Bollinger, C. Krebs**

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**8:50 INOR 1025.** Thermodynamics and mechanistic insights into C-H bond activation by the Cu(III)-OH core. **W.B. Tolman**

**9:15 INOR 1026.** Steric and electronic control of proton-coupled electron-transfer reactions of mononuclear hydroxomanganese(III) complexes. **T.A. Jackson, D.B. Rice, A. Burr, A.W. Howcroft**

**9:40 INOR 1027.** Iron porphyrin electrocatalysts for oxygen reduction. **J.M. Mayer, M. Pegis, B.A. McKeown, S. Raugel, N. Kumar**  
**10:05 Intermission.**

**10:15 INOR 1028.** Bio-inspired metal-oxido and metal-hydroxido species. **A. Borovik**

**10:40 INOR 1029.** Dioxxygen activation by a tricopper-dinitrogen complex. **G. Di Francesco, L.J. Murray**

**11:05 INOR 1030.** Superoxo and peroxo intermediates in oxygenase reactions. **J.D. Lipscomb, B. Rivard, M.S. Rogers, C.J. Knoot, E.G. Kovaleva**

**11:30 INOR 1031.** High valent mononuclear iron-oxo species in catalytic O-O cleaving and forming reactions. **M. Costas, O. Cusso, A. Company, Z. Codola, J. Serrano, J. Lloret-Fillol, X. Ribas**

**11:55 INOR 1032.** Mononuclear metal-O<sub>2</sub>(H) adducts in oxidative nucleophilic and electrophilic reactions. **J. Cho**

## Section D

San Diego Convention Center  
Room 30E

### Memorial Symposium Honoring Karen J. Brewer

*Cosponsored by HIST†  
Financially supported by  
Washington State University*

**M. T. Mongelli, S. C. Rasmussen, Organizers**  
**J. White, Presiding**

**8:30 INOR 1033.** Excited states of transition metal complexes: Optimizing reactions for solar energy conversion and photochemistry. **C. Turro, K.R. Dunbar**

**9:00 INOR 1034.** Design, synthesis, spectroscopic, electrochemical, and biological studies of strained ruthenium(II) and ruthenium(II)-platinum(II) complexes. **A. Jain, K. Wyland, E. Hoffman, D. Davis, C. Brecht**

**9:30 INOR 1035.** New mechanisms in dye-sensitized solar cells: Catalyzing two-electron-transfer halide redox chemistry at sensitized TiO<sub>2</sub>. **H. Chen, J.M. Cardon, J. Angsono, J. Glancy-Logan, S. Ardo**

**9:50 INOR 1036.** Radically new compounds to combat methicillin resistant *Staph. aureus* (MRSA): Metal complexes as antimicrobials. **J.S. Merola, G. Karpin, D.M. Morris, C.M. DuChane, J.O. Falkingham, M.F. Ehrich**

**10:20 Intermission.**

**10:35 INOR 1037.** Stability of Ru(II), Ru(II),Pt(II) and Ru(II),Rh(II),Ru(II) supramolecular complexes containing enantiomerically pure light absorbing subunits. **A. Wagner, K.S. Brewer**

**11:05 INOR 1038.** Light-activatable Ru-based anticancer complexes in a new light. **S.L. Hopkins, B. Siewert, S.H. Askes, L.N. Lameijer, P. Veldhuizen, R. Zwier, S. Bonnet**

**11:35 INOR 1039.** Redox-active intercalating ligands (RAIL) against cancer: A new approach to using ruthenium polypyridyl complexes as potential anti-cancer drugs. **F.M. MacDonnell, N. Alatrash, C. Griffith, A. Dayoub**

**12:05 INOR 1040.** Supramolecular poly-metallic architectures in the treatment of malignant glioma. **J.A. Rodriguez Corrales, J. Zhu, A. Dominijanni, J.L. Robertson, K.S. Brewer**

## Section E

San Diego Convention Center  
Room 31A

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

**S. A. Koch, Organizer**

**P. C. Glazer, Presiding**

**8:30 INOR 1041.** Iron(II) complex as pH-responsive paraCEST MRI contrast agent: Towards imaging of acidosis conditions. **P.B. Tsitovich, J.R. Morrow**

**8:50 INOR 1042.** Ruthenium and platinum antitumor complexes and their activation with 980-nm light. **E. Ruggiero, L. Salassa**

**9:10 INOR 1043.** Targeting specific nucleic acid structures and proteins with ruthenium complexes. **P.C. Glazer**

**9:30 INOR 1044.** Bifunctional compounds as novel theranostic agents for Alzheimer's disease. **L.M. Mirica**

**9:50 Intermission.**

**10:00 INOR 1045.** Role of hydrogen bonding,  $\pi$ - $\pi$  stacking interactions, twist-angle, and solvation on B-DNA. **J. Poater**

**10:20 INOR 1046.** Withdrawn.

**10:40 INOR 1047.** Moving light-based cancer therapy from concept to reality with metaldrug photosensitizers. **S.A. McFarland, H. Yin, S. Monro, T. Sainuddin, M. Pinto, M. Hetu**

**11:00 INOR 1048.** Insights into the biological activities of clavaniins, potent antimicrobial peptides from tunicate hemocytes. **A.M. Angeles Boza, S. Juliano**

## Section F

San Diego Convention Center  
Room 31B

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

**C. G. Lugmair, Organizer**

**J. E. Cloud, V. Doan-Nguyen, Presiding**

**8:30 INOR 1049.** Reducing the large volume change in alloy anodes through porous nanoscale architecture. **T.C. Lin, J.B. Cook, J.N. Weker, E. Detsi, S.H. Tolbert**

**8:50 INOR 1050.** Porous solid electrolytes for advanced lithium ion batteries. **J.E. Cloud, S. Biswas, S.L. Suib**

**9:10 INOR 1051.** Effect of rotational polyhedra distortions on guest ion intercalation in anti-NASICON Fe<sub>3</sub>(MoO<sub>4</sub>)<sub>3</sub>. **G. Barim, S. Zhou, B.C. Melot, R.L. Brutchey**

**9:30 INOR 1052.** Unraveling the mechanism of transition metal sulfide conversion electrodes with local structure methods. **V. Doan-Nguyen, M.M. Butala, M. Lumley, R. Seshadri**

**9:50 Intermission.**

**10:05 INOR 1053.** Graphite-conjugated catalysis. **S. Chu, T. Fukushima, M. Jackson, S. Oh, M. O'Reilly, Y. Surendranath**

**10:25 INOR 1054.** Electro-catalytic oxidation of glycerol on free-standing monolithic nanoporous silver. **Y. Liang, E. Detsi, S.H. Tolbert**

**10:45 INOR 1055.** Modular method for non-covalent attachment of homogeneous electrocatalysts to electrode surfaces. **B.R. Lydon, A. Germann, J. Yang**

**11:05 INOR 1056.** Single and multi-doped transition metal (Mn, Fe, Ni and Co) ZnO and its electrocatalytic activities for oxygen reduction reaction. **M.R. Shakil, A. El-Sawy, H. Tassim, S.L. Suib**

## Section G

San Diego Convention Center  
Room 31C

### Chemistry of Materials: Metal Organic Frameworks

**C. G. Lugmair, Organizer**

**S. H. Pang, C. T. Saouma, Presiding**

**8:30 INOR 1057.** Flexible Ti- and Zr-MOFs based on 1,4-*trans*-cyclohexanedicarboxylate linkers. **B. Bueken, F. Vermoortele, H. Reinsch, M. Cliffe, M. Wharmby, C. Tsou, D.E. Vanpoucke, R. Ameloot, V. Van Speybroeck, A. Goodwin, F. Taulelle, J.M. Mayer, D. De Vos**

**8:50 INOR 1058.** Protein-based metal-organic frameworks. **J. Bailey, F.A. Tezcan**

**9:10 INOR 1059.** Computational study of the dehydration process of the NU-1000 MOF. **A. Mavrandonakis, A.E. Platero Prats, L.C. Gallington, Y. Liu, J.T. Hupp, O.K. Farha, K.W. Chapman, C.J. Cramer**

**9:30 INOR 1060.** Withdrawn.

**9:50 Intermission.**

**10:05 INOR 1061.** Rendering water unstable Cu<sub>2</sub>(NH<sub>2</sub>btc)<sub>2</sub> moisture-resistant via post synthetic modification. **H. Rubin, M.M. Reynolds**

**10:25 INOR 1062.** Thermodynamic considerations for CO<sub>2</sub> reduction at Zr-based MOFs. **C.T. Saouma, T. Elkin, M. Bhattacharya**

**10:45 INOR 1063.** Understanding the formation of defects on metal-functionalized metal-organic frameworks. **G. González Miera, A.E. Platero Prats, P.J. Chupas, K.W. Chapman, B. Martin-Matute**

**11:05 INOR 1064.** Effect of acid gas exposure on the external surfaces of ZIF-8. **S.H. Pang, C.W. Jones, R.P. Lively**

## Section H

San Diego Convention Center  
Room 32A

### Inorganic Catalysts

**S. A. Koch, Organizer**

**R. N. Austin, Presiding**

**8:00 INOR 1065.** O-O bond formation in woc by iridium complexes. **A. Poater, L. Cavallo**

**8:20 INOR 1066.** Cobalt complexes supported by a ferrocene-based ligand as redox switches for hydroelectrochemical reactions. **S. Shepard, P. Diaconescu**

**8:40 INOR 1067.** Mechanistic studies of oxygen atom transfer in [ONO]Re complexes. **J.M. Hoffman, S.N. Brown**

**9:00 INOR 1068.** Cobalt cubane water oxidation catalysts: On the way to photosystem II. **F. Evangelisti, R. More, F. Hodel, S. Luber, G.R. Patzke**

**9:20 INOR 1069.** New ideas for hydrogen-efficient direct deoxygenation catalysts. **R.N. Austin, L. Grabow, B. Frederick, R. Nelson, B. Baek, P. Ruiz, M. Wheeler**

**9:40 INOR 1070.** Water oxidation pathways using a cobalt oxide dimer catalyst. **P. Petrovic, S. Zoric, E. Brothers, P.T. Anastas**

**10:00 INOR 1071.** Withdrawn.

**10:20 Intermission.**

**10:30 INOR 1072.** Electrocatalytic H<sub>2</sub> production is favored over formate production by including a proton shuttle on [Fe<sub>3</sub>N(CO)<sub>12</sub>]. **N.D. Loewen, E.J. Thompson, M. Kagan, C. Bañales, T.W. Myers, J. Fettinger, L.A. Berben**

**10:50 INOR 1073.** Mechanistic details and thermodynamic insights for electrocatalytic reduction of CO<sub>2</sub> or H<sup>+</sup> by metal carbonyl clusters. **A. Taheri, L.A. Berben**

**11:10 INOR 1074.** Modification of electrode surfaces with Ni(II) cyclam, CO<sub>2</sub> reduction catalyst. **A. Zhanaidarova**

**11:30 INOR 1075.** Covalent attachment of molecular electrocatalysts to high surface area carbon materials. **B. Johnson, Z.R. Jones, S.L. Scott, L.A. Berben**

**11:50 INOR 1076.** Overlooked reaction involving a catalyst, [Co(dmgBF<sub>2</sub>)(OH<sub>2</sub>)<sub>2</sub>], and a sacrificial electron donor, triethylamine during the production of hydrogen in acidified acetonitrile: A mechanistic study that must not be ignored! **M.J. Celestine, M.A. Lawrence, J. Combs, C.E. Galbraith, L.S. Joseph, A. Holder**

## Section I

San Diego Convention Center  
Room 32B

### Lanthanide & Actinide Chemistry

**A. De Bettencourt Dias, Organizer**

**S. T. Liddle, D. A. Penchoff, Presiding**

**8:30 INOR 1077.** Uranyl hybrid materials: Synthesis and characterization. **M. Payne**

**8:50 INOR 1078.** Phosphorus-stabilized rare earth(III) and (IV) methanediides: Structure, bonding, and magnetism. **S.T. Liddle, M. Gregson, E. Lu, F. Tuna, E. McInnes, W. Lewis, A. Blake**

**9:10 INOR 1079.** Synthesis and characterization of thorium-chalcogen multiple bonds. **D.E. Smiles, G. Wu, T.W. Hayton**

**9:30 Intermission.**

**9:40 INOR 1080.** Supramolecular assembly of actinide bearing hybrid materials: structural systematics and properties. **R. Surbella, K.L. Pellegrini, B. McNamara, D.E. Meier, J. Schwantes, C.L. Cahill**

**10:00 INOR 1081.** Organometallic actinide complexes with nitrogen-rich ligands. **K.A. Maerzke, K. Browne, P. Yang, N. Henson, J.L. Kiplinger, J.M. Veauthier**

**10:20 INOR 1082.** Towards low limit SERS detection of uranyl ions with tailor made bifunctional ligands. **J.F. DeJesus, M.J. Trujillo, D.A. Penchoff, J.A. Bradshaw, J.P. Camden, D.M. Jenkins**

**10:40 Intermission.**

**10:50 INOR 1083.** Investigation of organo-actinide metal complexes with soft-donor ligands through reactivity studies. **A. Behrle, J.R. Walsensky**

Technical program information  
known at press time.

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**11:10 INOR 1084.** Nitrogen-rich, organometallic complexes of thorium and uranium with 5-methyl-1H-tetrazole. **K. Browne**, K.A. Maerzke, N.E. Travia, N. Henson, D.E. Morris, B. Scott, P. Yang, J.L. Kiplinger, J.M. Veauthier

**11:30 INOR 1085.** Synthesis of  $(C_2H_5SiMe_3)_4U$  reveals that a  $(C_2H_5SiMe_3)_3UCI/(C_2H_5SiMe_3)_3UMe$  mixture is more crystalline than the pure compounds. **C.J. Windorff**, M.R. MacDonald, J.W. Ziller, W.J. Evans

## Section J

San Diego Convention Center  
Room 33A

### Main Group Chemistry

T. W. Hudnall, *Organizer*

S. Aldridge, *Presiding*

**8:30 INOR 1086.** Oxidation of carbene-stabilized main group diatomic molecules. **Y. Wang**, P. Wei, G.H. Robinson

**8:50 INOR 1087.** Bottleable (amino)(carboxy) radicals derived from cyclic (alkyl)(amino) carbenes. **J. Mahoney**, D. Martin, C.E. Moore, A.L. Rheingold, G. Bertrand

**9:10 INOR 1088.** Application of a donor-acceptor strategy to generate molecular main group element precursors to nanodimensional materials. **A.K. Swarnakar**, T.K. Purkait, J.G. Veinot, E. Rivard

**9:30 INOR 1089.** Molecular precursor to phosphathyne: Synthesis, characterization, and further reactivity. **W.J. Transue**, A. Velian, M. Nava, C. Womack, J. Jiang, G. Hou, X. Wang, R. Field, C.C. Cummins

**9:50 INOR 1090.** Encapsulated peroxide dianion in solution and the solid state: Fundamental properties and reactivity with CO and CO<sub>2</sub>. **M. Nava**, S. Zhang, N. Lopez, C.C. Cummins

**10:10** Intermission.

**10:20 INOR 1091.** Metal-free dehydrogenation of amine-boranes by tunable *N*-heterocyclic iminoboranes. **M. Lui**, N. Paisley, R. McDonald, M. Ferguson, E. Rivard

**10:40 INOR 1092.** Bond activation by highly reactive low valent germanium complexes. **S. Aldridge**, A. Rit

**11:00 INOR 1093.** Development of frustrated Lewis pairs featuring antimony(V) acids. **D. Tofan**, F.P. Gabbaï

**11:20 INOR 1094.** Boron, silicon, and phosphorus catalysts for the reduction of CO<sub>2</sub>. **T. Cantat**, N. von Wolff, E. Blondiaux, G. Lefevre, J. Berthet, P. Thuery

**11:40 INOR 1095.** Synthesis and properties of bidentate Lewis acids with large binding pockets. **C. Chen**, F.P. Gabbaï

**12:00 INOR 1096.** Distiboranes based on *ortho*-phenylene backbones: Synthesis and anion binding. **D. You**, M. Hirai, F.P. Gabbaï

## Section K

San Diego Convention Center  
Room 33B

### Organometallic Chemistry: Catalysis

N. S. Radu, *Organizer*

J. Okuda, O. Serrano, *Presiding*

**8:30 INOR 1097.** Carbon dioxide hydrogenation by late transition metal phosphine and *N*-heterocyclic carbene complexes. **M. Reineke**, A. Lilio, C.P. Kubiak

**8:50 INOR 1098.** Lewis acid enhancement in catalytic CO<sub>2</sub> reduction at low cost metals. **Y. Zhang**, **W.H. Bernskoetter**, N. Hazari

**9:10 INOR 1099.** Hydrosilylation of carbon dioxide catalyzed by triphenylborane. **J. Okuda**

**9:30 INOR 1100.** Carbon dioxide reduction to formate by a multi-functional, redox-active borane. **J. Taylor**

**9:50 INOR 1101.** Cascade conversion of carbon dioxide to methanol: New catalytic, kinetic, and mechanistic insights. **D.C. Samblanet**, M.S. Sanford

**10:10** Intermission.

**10:20 INOR 1102.** Photochemical reduction of carbon dioxide using a CN-modified *fac*-Mn(bpy)(CO)<sub>3</sub> catalyst. **P. Cheung**, C.W. Machari, A. Malkhasian, J. Agarwal, C.P. Kubiak

**10:40 INOR 1103.** Small molecule activation by mid-valent group 6 metal complexes supported by a sterically-reduced monocyclopentadienyl, amidinate ligand environment. **L.M. Duman**, L.R. Sita

**11:00 INOR 1104.** Synthesis of stereoregular and cyclic poly(lactic acid) using an iron-based catalyst. **J.A. Byers**, A. Kaur, C.M. Manna, L. Yablon, B. Li, F. Haefner

**11:20 INOR 1105.** Fully aliphatic aziridination employing a macrocyclic *N*-heterocyclic tetracarbenes iron(II) catalyst. **P.P. Chandrachud**, H.M. Bass, D.M. Jenkins

**11:40 INOR 1106.** Ester hydrogenation by an octahedral iron-amino hydride catalyst: DFT comparisons of bifunctional and ion-pair slippage mechanisms. **F. Hasanayn**, A. Abotaka

**12:00 INOR 1107.** Substitution of labile solvent ligands of an iron(II) NHC complex by isocyanides. **A. Lindhorst**, S. Haslinger, J. Kueck, M. Cokoja, A. Pothig, F.E. Kuehn

### Computational Materials & Nanoscience: Theory Meets Experiment

#### Forum: Materials Genome & Materials Informatics

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#### Heavy Element Inorganic Chemistry: A Tribute to Al Sattelberger

*Sponsored by NUCL, Cosponsored by INOR‡*

#### Supramolecular Chemistry

*Sponsored by ORGN, Cosponsored by INOR*

## WEDNESDAY AFTERNOON

### Section A

San Diego Convention Center  
Room 30B

#### Interplay of Structure & Transport Properties in Materials for Energy

K. Kovnir, *Organizer*

B. C. Melot, *Organizer, Presiding*

**1:30 INOR 1108.** Crystal chemistry and transport properties of novel layered Li pnictides. **K. Lee**, **K. Kovnir**

**2:00 INOR 1109.** Silicon clathrates for electrochemical energy storage applications. **C.K. Chan**

**2:20 INOR 1110.** Characterization of multi-valent electrochemical reactions in spinel oxide hosts. **J. Cabana**

**2:50 INOR 1111.** Rational design of heterometallic molecular precursors for the synthesis of energy-related materials. **E. Dikarev**, Z. Wei, H. Han, C.M. Lieberman

**3:20** Intermission.

**3:40 INOR 1112.** Structure and transport of lithium ions in lithium garnet oxides as solid electrolytes for lithium-ion batteries. **W. Lai**

**4:10 INOR 1113.** Germanium nanoparticle synthesis involving other group IV elements. **K.A. Newton**, A.L. Holmes, W. Blacklock, S. Kauzlarich

**4:30 INOR 1114.** Rational nanostructure design for high performance Mg rechargeable batteries. **Y. Yao**

### Section B

San Diego Convention Center  
Room 30C

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

S. A. Koch, *Organizer*

V. V. Smirnov, *Presiding*

**1:30 INOR 1115.** Examining outer-sphere effects on coordination chemistry using disulfide bond networks in engineered metalloprotein scaffolds. **L. Churchfield**, F.A. Tezcan

**1:50 INOR 1116.** Aryl-amine oxygenation mechanism for a diiron enzyme involved in antibiotic biosynthesis. **A. Komor**, B. Rivard, L. Que, J.D. Lipscomb

**2:10 INOR 1117.** Effect of Lewis acids on transition metal complexes. **M. Swart**, M. Gruden, K. Ray, F. Meyer

**2:30 INOR 1118.** Binding of a potent pyridine inhibitor in an iron-sulfur enzyme IspH and NO in the non-heme center of a biosynthetic nitric oxide reductase model. **Y. Zhang**

**2:50 INOR 1119.** Design of protein-based hybrid catalysts for renewable fuel production. **D. Sommer**, A. Roy, M. Vaughn, G. Ghirlanda

**3:10 INOR 1120.** Nitrosyl hydride (nitroxyl) complexes of iron porphyrins. **E.G. Abucayon**, R.L. Khade, Y. Zhang, G.B. Richter-Addo

**3:30** Intermission.

**3:40 INOR 1121.** Synthesis and reductive coupling reactivity of tripodal iron isocyanide complexes. **J.M. Hoover**, A. Gowda, J.L. Petersen

**4:00 INOR 1122.** Effects of ionic liquids on stability, structure, and reactivity on biological macromolecules. **H.U. Valle**, T.A. Rogers, T. Al-Mohanna, J.P. Emerson

**4:20 INOR 1123.** Optimizing immobilization of ferrocene peptide bioconjugates for biosensor development. **M. Goulet**

**4:40 INOR 1124.** Electrochemical characterization of isolated nitrogenase cofactors. **J. Yang**, B.R. Lydon, N. Sickerman, C. Lee, Y. Hu, M. Ribbe

**5:00 INOR 1125.** Tryptophan radical in azurin: Effects of deuteration and metal substitution on quantum yields of fluorescence and radical formation. **J. Liang**, J. Rivera, J.E. Kim

**5:20 INOR 1126.** Why heme enzymes that decyclize free tryptophan react as dioxygenases: Mechanistic study on O<sub>2</sub> activation and timing of the O-O bond cleavage in indoleamine 2,3-dioxygenase (hIDO1). **I.M. Chrisman**, L.S. Dameron, **V.V. Smirnov**

### Section C

San Diego Convention Center  
Room 30D

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

C. G. Lugmair, *Organizer*

B. M. Leonard, S. Marinescu, *Presiding*

**1:30 INOR 1127.** Imobilized one dimensional cobalt dithiolene metal organic surface (MOS) for efficient electrochemical and photoelectrochemical H<sub>2</sub> evolution from water. **C.A. Downes**, S.C. Marinescu

**1:50 INOR 1128.** Two-dimensional cobalt dithiolene metal-organic surfaces (MOS) as immobilized catalysts for the conversion of acidic water to H<sub>2</sub>. **A.J. Clough**, J.W. Yoo, M.H. Mecklenburg, S. Marinescu

**2:10 INOR 1129.** Ligand removal from CdS quantum dots for enhanced photocatalytic H<sub>2</sub> generation in pH neutral water. **C. Chang**, K.L. Orchard, B.C. Martindale, E. Reiser

**2:30 INOR 1130.** Synthesis and water splitting electrocatalysis of metal carbide compounds. **B.M. Leonard**

**2:50** Intermission.

**3:05 INOR 1131.** One- and two-dimensional cobalt dithiolene metal-organic surfaces (MOS) for efficient electrochemical and photoelectrochemical H<sub>2</sub> evolution from water. **S. Marinescu**, A.J. Clough, C.A. Downes, J.W. Yoo

**3:25 INOR 1132.** Effect of interlayer anions on [NiFe]-LDH nanosheet water oxidation activity. **B.M. Hunter**, J.R. Winkler, H.B. Gray, **A.M. Mueller**

**3:45 INOR 1133.** Nanoparticulate RuO<sub>2</sub> deposited on practical electrode substrates: Efficient water oxidation from vanishingly small loadings of an expensive platinum-group metal. **C.N. Chervin**, P. DeSario, E. Nelson, M.B. Sassin, J. Long, D.R. Rolison

**4:05 INOR 1134.** In situ spectroscopies of mixed-metal nanosheet water oxidation catalysts made by pulsed laser ablation in liquids. **B.M. Hunter**, J.R. Winkler, H.B. Gray, A.M. Mueller

**4:25 INOR 1135.** Designing nickel based ceramics as catalysts for the hydrogen evolution reaction combining theoretical and experimental observations. **M. Ledendecker**, H. Schlott, B. Meyer, M. Antonietti, M. Shalom

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## Section D

San Diego Convention Center  
Room 30E

### Memorial Symposium Honoring Karen J. Brewer

*Cosponsored by HIST†  
Financially supported by  
Washington State University*

M. T. Mongelli, S. C. Rasmussen, *Organizers*  
M. Richter, *Presiding*

**1:30 INOR 1136.** Catalytic water oxidation: From Ru(II) to Fe(III). L. Wickramasinghe, L. Tong, R. Zong, R. Zhou, R.P. Thummel

**2:00 INOR 1137.** Ru(II)-anthraquinone complexes: redox and spectroscopic properties and light-activated interactions with DNA. J.K. White, T.A. White, C. Turro

**2:30 INOR 1138.** Tyrosine-histidine mimic with stepwise oxidation and concerted reduction by proton coupled electron transfer. G. Manbeck, E. Fujita, J.J. Concepcion

**3:00 INOR 1139.** What I learned from Karen Brewer about teaching undergraduates. P.A. Deck

**3:30** Intermission.

**3:45 INOR 1140.**  $\pi$ -Extended metal thiophenedithiolenes: Synthetic approaches to tuning electronic and optical properties. K. Konkol, E. Uzelac, C.M. Amb, S.C. Rasmussen

**4:15 INOR 1141.** Light that pleases the world in science: The Karen Brewer's effect on my academic career. A. Holder

**4:45 INOR 1142.** New hydrophilic supramolecular complex for the photocatalytic production of hydrogen from aqueous solutions. T. Canterbury, S.M. Arachchige, R.B. Moore

**5:15 INOR 1143.** Photoredox reactions of Pt(II)  $\sigma$ -metalated bis-pyridylbenzene complexes: Photoreduction and H<sub>2</sub> generation in chromophore-sacrificial donor systems. A.D. Kulkarni, A.C. Neuberger, R.H. Schmehl

## Section E

San Diego Convention Center  
Room 31A

### Chemistry of Materials: Nanomaterials

C. G. Lugmair, *Organizer*  
R. Beaulac, M. W. Lee, *Presiding*

**1:30 INOR 1144.** Formation and interlayer decoupling of colloidal MoSe<sub>2</sub> nano-flowers. D. Sun, S. Feng, M. Terrones, R.E. Schaak

**1:50 INOR 1145.** Multiscale simulations of formation and dissolution of nanomaterials in liquid cells. S. Sen, P. Kral

**2:10 INOR 1146.** Facile synthetic approach to MoS<sub>2</sub> monolayer-PbSe QDs hetero-structures. Q. Ding, S. Jin

**2:30 INOR 1147.** Solution-liquid-solid (SLS) approach to colloidal nitride semiconductor nanomaterials. R. Beaulac, N. Karan, Y. Chen, Z. Liu

**2:50 INOR 1148.** Cubic Sn<sub>3</sub>Ge<sub>1-x</sub> nanoalloys: Beyond bulk composition limit. K. Ramasamy, J.M. Pietryga, S. Ivanov

**3:10** Intermission.

**3:25 INOR 1149.** Amine-copper (II) formates for the generation high conductivity copper films at low temperatures: Towards printing copper on PET. C. Paquet, T. Lacelle, B. Deore, A. Kell, I. Korobkov, S. Lafreniere, P.R. Malenfant

**3:45 INOR 1150.** Radical functionalization of boron nitride nanotubes. T. Sainsbury

**4:05 INOR 1151.** Polyarylboranes: A new and diverse class of small, metal-free quantum dots exhibiting high fluorescence quantum yields. M.W. Lee

**4:25 INOR 1152.** Fabrication of aluminum nanoparticles in constricted environments. C.O. Nyapete, P.A. Jelliss, S.W. Buckner

**4:45 INOR 1153.** Oxide-free functionalized silicon nanowires for versatile applications. J. Veerbeek, J. Huskens

## Section F

San Diego Convention Center  
Room 31B

### Chemistry of Materials: Synthesis & Properties

C. G. Lugmair, *Organizer*  
M. P. Campos, B. Fokwa, *Presiding*

**1:30 INOR 1154.** Experimental and theoretical studies of the hard borides A<sub>3</sub>MB<sub>2</sub> (A = Nb, Ta; M = Fe, Ru, Os). R. Touzani, M. Mbariki, B. Fokwa

**1:50 INOR 1155.** Nanostructuring of superhard materials. M. Yeung, G. Akopov, R. Mohammadi, R.B. Kaner

**2:10 INOR 1156.** Characterization and surface organization of ligand substituted Mn<sub>2</sub> single molecule magnets. N.M. Khatiri, M. Pablico-Lansigan, K.D. Pires, S.E. Lofland, J.A. Borchers, P. Butler, M. Pileni, K. Plass, D. Keavney, S.L. Stoll

**2:30 INOR 1157.** Lanthanides-TTF complexes displaying single molecule magnet behaviour and luminescence. L. Ouahab, F. Pointillart

**2:50 INOR 1158.** New mixed-valence Mn<sub>3</sub> and Mn<sub>2</sub> clusters: Single-molecule magnetism and base-catalyzed transformation of alcohol into hemiacetals. O.A. Adebayo, K.A. Abboud, G. Christou

**3:10** Intermission.

**3:25 INOR 1159.** Tunable library of substituted thiourea and selenourea precursors to metal chalcogenide nanocrystals. M.P. Campos, J.S. Owen, M.P. Hendricks, I. Jen-La Plante, G.T. Cleveland, R.A. Swain, A.W. Graham

**3:45 INOR 1160.** One-step synthesis of core/shell nanocrystals with a graded interface. L. Hamachi, I. Jen-La Plante, J.S. Owen

**4:05 INOR 1161.** Solution-phase conversion of bulk oxides to metal chalcogenides. C. McCarthy, R.L. Brutchey

**4:25 INOR 1162.** Magneto-optical properties of europium sulfide-europium selenide solid solutions in the bulk and nanoscale. N. Rosa, H.A. Dalafa, A. Kawashima, S. Omagari, T. Nakanishi, Y. Hasegawa, S.L. Stoll

**4:45 INOR 1163.** Alkylation of CdSe nanocrystals with organometallic reagents. P. Chen, N.C. Anderson, Z. Norman, J.S. Owen

## Section G

San Diego Convention Center  
Room 31C

### Electrochemistry

B. L. Lucht, *Organizer*  
M. J. Rose, *Presiding*

**1:30 INOR 1164.** Chemically and electrochemically triggered assembly of viologen radicals: From the control of the  $\pi$ -dimerization to molecular switches. A. Milet, E. Saint-Aman, C. Kahlfuss, G. Bucher

**1:50 INOR 1165.** Bonding and function of nickel-phosphine H<sub>2</sub> catalysts to silicon(111) photoelectrodes: C-C covalent attachment and metal-oxide-phosphonate adsorption. M.J. Rose, J. Seo, H. Kim

**2:10 INOR 1166.** Composite  $n$ -Si(111) | R | metal-oxide photoelectrodes: Effect of interfacial organic linkers on charge transfer and ALD-based growth of TiO<sub>2</sub> ultra-thin films. R. Pekarek, M.J. Rose

**2:30 INOR 1167.** Investigating the mechanism of O<sub>2</sub> reduction with iron porphyrin electrocatalysts in the context of structure: Activity relationships. M. Pegis, N. Kumar, F.S. Menges, S. Raugel, M.A. Johnson, J.M. Mayer

**2:50 INOR 1168.** Dynamics of deposition, stripping, and passivation for Mg batteries. D.J. Wetzel, A.A. Gewirth, R.G. Nuzzo

**3:10 INOR 1169.** Fully-integrated wearable sensor array for multiplexed perspiration analysis. W. Gao, S. Emaminejad, H. Nyein, S. Challa, R.W. Davis, A. Javey

## Section H

San Diego Convention Center  
Room 32A

### Organometallic Chemistry: New Ligand Platforms

N. S. Radu, *Organizer*  
S. K. Hurst, *Presiding*

**1:30 INOR 1170.** Towards the stabilization of late transition oxo and imido complexes by cyclic (alkyl)(amino)carbenes (CAACs). D. Munz, J. Chu, M. Melaimi, R. Jazzar, G. Bertrand

**1:50 INOR 1171.** Oxidation chemistry facilitated by cryptand encapsulated M-O-M complexes. J. Stauber, E.D. Bloch, K.D. Vogiatzis, L. Gagliardi, D.G. Nocera, C.C. Cummins

**2:10 INOR 1172.** Selective two-electron reduction of carbon monoxide mediated by molybdenum complexes supported on an asymmetric phenol phosphine ligand. S. Riduan, J.A. Buss, T. Agapie

**2:30 INOR 1173.** Heterolytic activation of C-H bonds via bifunctional transition metal platforms. E.B. Hulley, W. Christman, T. Morrow

**2:50 INOR 1174.** Curved carbon-rich polyaromatic ligands: Convex and concave binding of multiple metal ions. S.N. Spisak, Z. Zhou, N.J. O'Neil, Z. Wei, M.A. Petrukhina

**3:10 INOR 1175.** Withdrawn.

**3:30 INOR 1176.** Photophysically innocent boron cluster ligand scaffolds for organic light emitting diode materials. K. Kirlikovali, J.C. Axtell, A. Gonzalez, A.C. Phung, S. Khan, A.M. Spokoyniy

**3:50 INOR 1177.** Activation of a gold catalyst by oxidation of a redox-noninnocent chlorostibine Z-ligand. H. Yang, F.P. Gabbaï

**4:10 INOR 1178.** Exploring the promises of open cage fullerene coordination. A. Aghabali, M.M. Olmstead, A.L. Balch

**4:30 INOR 1179.** Synthesis of a series of aryl-14H-dibenzo[a,j]xanthene derivatives. S.K. Hurst

## Section I

San Diego Convention Center  
Room 32B

### Inorganic Spectroscopy

S. A. Koch, *Organizer*  
V. C. Popescu, *Organizer, Presiding*

**1:30** Introductory Remarks.

**1:35 INOR 1180.** Computational prediction on nuclear resonance vibrational anisotropy applied to Iron porphyrates. Q. Peng, R.W. Scheidt

**1:55 INOR 1181.** Probing valence orbitals using Co K $\beta$  X-ray emission. F. Li, E. Farquhar

**2:15 INOR 1182.** Homogenous approaches to solar hydrogen production from water. K. El Roz, R.S. Khnazyer, F.N. Castellano

**2:35 INOR 1183.** Cobalt and zinc complexes of hexamine cage ligands with multiple conformations in solution. L. Alcock, G. Cavigliasso, R. Stranger, A. Willis, J. Hook, D. Lawes, S. Ralph

**2:55 INOR 1184.** Withdrawn.

**3:15** Intermission.

**3:25 INOR 1185.** Unexpected photoluminescence enhancement from cyclometalated Ir(III) complexes in water. M. McGorty, R.S. Khnazyer, A. Singh, Y.G. Yingling, F.N. Castellano

**3:45 INOR 1186.** Effect of transition metal ions on the thermal transition of poly-N-isopropylacrylamide. L. Fulton, W. Seitz, R.P. Planalp

**4:05 INOR 1187.** Photo-induced electron and energy transfer in Heisenberg spin-coupled donor-acceptor complexes. D.M. Arias-Rotondo, J.K. McCusker

**4:25 INOR 1188.** Instrumentation for cyclotron resonance and electron spin resonance in high fields/frequencies. C.C. Beedle, R.D. McDonald, N. Harrison, J. Singleton

**4:45 INOR 1189.** Access to a second-order excited-state quenching mechanism. W.B. Swords, G.J. Meyer

**5:05 INOR 1190.** Tracking the excited state equilibrium in an Ir(III) bichromophore system: A combined time resolved spectroscopy and computational study. J. Yarnell, F.N. Castellano

## Section J

San Diego Convention Center  
Room 33A

### Organometallic Chemistry: Applications to Organic Transformations

N. S. Radu, *Organizer*  
K. Szabo, *Presiding*

**1:30 INOR 1191.** Probing early transition metals with macrocyclic tetracarbene ligands for catalytic aziridination. L.C. Keller, G.R. Elpittia, P.P. Chandrachud, D.M. Jenkins

**1:50 INOR 1192.** Ring expansion reactions of the anti-aromatic borole to prepare conjugated heterocycles. C. Martin

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**2:10 INOR 1193.** Rhodium catalyzed C-H activation and hydroamination in a highly selective redox [4+2] imine/alkyne annulation. **R.S. Manan, P. Zhao**

**2:30 INOR 1194.** Application of rhodium-bis(diazaphospholane) catalyzed asymmetric hydroformylation in the enantioselective synthesis of quaternary aldehydes and sequence specific oligoesters. **F. Foarta, C.R. Landis**

**2:50 INOR 1195.** Asymmetric transformations using 1,1-disubstituted olefins as challenging substrates. **O. Pamies, M. Dieguez**

**3:10 INOR 1196.** Organometallic chemistry of adamantane: Toward novel functionalization of diamondoid hydrocarbons. **D. Armstrong, F. Taullaj, U.W. Fekl**

**3:30 INOR 1197.** General and green protocol for the allylation of tautomeric amidic nucleophilic centers through palladium catalysis. **S. Vemula, D. Kumar, G.R. Cook**

**3:50 INOR 1198.** Withdrawn.

**4:10 INOR 1199.** Alkyl carbon-nitrogen bond formation from Ir<sup>III</sup>. **T.E. Stevens, T.R. Cundari, K.I. Goldberg**

**4:30 INOR 1200.** Catalysis at metal-metal bonds. **C. Uyeda, T. Steiman, S. Pal, Y. Zhou**

**4:50 INOR 1201.** Metal mediated fluorination with fluoro-benziodoxole reagents. **K. Szabo**

## Section K

San Diego Convention Center  
Room 33B

### Organometallic Chemistry: Catalysis

N. S. Radu, *Organizer*

J. S. Figueroa, *Presiding*

**1:30 INOR 1202.** Effect of ligand exchange processes in asymmetric catalysis and redox chemistry of rare earth alkali metal BINOLate heterobimetallic complexes. **J.R. Robinson, J. Gu, P.J. Carroll, P.J. Walsh, E.J. Scheller**

**1:50 INOR 1203.** Mesoionic carbenes in copper(I) catalyzed reactions. **S. Hohloch, L. Suntrup, F. Duecker, B. Sarkar**

**2:10 INOR 1204.** Pd-Cy\*Phine catalyzed copper-free sonogashira cross-coupling: Mechanism and insights from electronic structure calculations. **A.M. Mak, Y. Lim, H. Jong, E.G. Robins, C. Johannes, M.B. Sullivan**

**2:30 INOR 1205.** Ligand-free copper catalyzed hydrazination of terminal alkynes. **J. Peltier, R. Jazzar, M. Melaimi, G. Bertrand**

**2:50** Intermission.

**3:00 INOR 1206.** Theoretically-guided optimization of new ligand libraries for asymmetric reduction and C-C bond coupling reactions. **M. Diéguez, O. Pamies**

**3:20 INOR 1207.** Well-defined molybdenum isocyanide catalysts for regioselective hydrostannation. **K. Mandla, J.S. Figueroa**

**3:40 INOR 1208.** Withdrawn.

**4:00 INOR 1209.** Development of a rhodium(I) catalyst for single-step styrene production. **B.A. Vaughan, M. Webster-Gardiner, S. Karbalaeei Khani, T.R. Cundari, T.B. Gunnoe**

**4:20 INOR 1210.** New developments in the catalytic dehydrogenative borylation of terminal alkynes and the applications of alkynylboronates. **C.J. Pell, C. Lee, O. Zherov**

**4:40 INOR 1211.** Analysis on olefin hydrosilylation catalyzed by a cationic nickel allyl complex. **Y. Choe, J. Mathew, Y. Nakajima, S. Shimada, k. sato**

**5:00 INOR 1212.** Influence of Lewis acids on organometallic species. **J. Becica, D. Chen, L.V. Dinh, G. Dobreiner**

## Computational Materials & Nanoscience: Theory Meets Experiment

### Forum: Powering the Future: Novel Materials for Solar Cell Technologies

*Sponsored by MPPG, Cosponsored by COMP, ENFL, INOR, ORGN and POLY*

### Heavy Element Inorganic Chemistry: A Tribute to Al Sattelberger

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### Supramolecular Chemistry

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## THURSDAY MORNING

### Section A

San Diego Convention Center  
Room 30B

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

S. A. Koch, *Organizer*

K. N. Green, C. T. Saouma, *Presiding*

**8:30 INOR 1213.** Cobalt (III) complexes as pro drugs for cancer therapy. **C. Zhang, M. Sutherland, L. Chiang, R. Clarke, J. Thompson, C. Walsby, T.J. Storr**

**8:50 INOR 1214.** Pyridol derived N-heterocyclic amines and applications in catalysis and medicine. **K.N. Green, S.M. Brewer, H.M. Johnston, M. Burnett**

**9:10 INOR 1215.** Titanium(IV) serum transferrin structure: New insight into the use of chemical transferrin mimetics for Ti(IV) anticancer drug development. **A.D. Tinoco, S.A. Loza-Rosas, A.M. Vázquez, K.I. Rivero, L.M. Negrón, M. Saxena, S. Sharma, N. Zambrana, T.B. Parks**

**9:30 INOR 1216.** Evaluating the potential of deferasirox, a commercial chemical transferrin mimetic, in Ti(IV) anticancer drug design. **S.A. Loza-Rosas, A.M. Vázquez, K.I. Rivero, L.M. Negrón, T.B. Parks, A.D. Tinoco**

**9:50** Intermission.

**10:00 INOR 1217.** Structural features that influence photochemical reactivity and phototherapeutic activity of Ru(II) polypyridyl complexes. **E. Wachter, A. Zamora, Y. Sun, D.K. Heidary, E.C. Glazer**

**10:20 INOR 1218.** Redox-activated MRI contrast agents to detect oxidative stress. **C.T. Saouma, C. Mathis**

**10:40 INOR 1219.** Disulfide-masked thiosemicarbazone prochelators targeting the iron metabolism of cancer. **E. Akam, E. Tomat**

### Section B

San Diego Convention Center  
Room 30C

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

C. G. Lugmair, *Organizer*

S. Gage, R. Sardar, *Presiding*

**8:30 INOR 1220.** Improving the efficiency and stability of photochemical CO<sub>2</sub> reduction mediated by dye-sensitized ternary system (dye/TiO<sub>2</sub>/Re(I)). **H. Son, C. Pac, S.O. Kang, W. Dong-II, J. Lee**

**8:50 INOR 1221.** Withdrawn.

**9:10 INOR 1222.** Synthesis and photocatalytic properties of ternary metal halide nanocrystals. **B. Yin, B. Sadtler**

**9:30 INOR 1223.** Spectroscopic investigations of surface-immobilized molecular photocatalysts for CO<sub>2</sub> reduction. **M.E. Louis, T. Fenton, G. Li**

**9:50 INOR 1224.** Anisotropically shaped perovskite nanostructures synthesis and photovoltaic applications. **R. Sardar, M. Teunis**

**10:10** Intermission.

**10:25 INOR 1226.** Perovskite mysteries revealed: Amorphous and dopant phases studied by annealing, <sup>207</sup>Pb ssNMR, and XRD. **B. Rosales, L. Men, S. Cady, J. Vela-Becerra**

**10:45 INOR 1227.** Tiny TiN: Solution ammolysis reactions towards nanoparticulate titanium nitride and titanium-niobium nitride alloys. **J. Brancho, B.M. Bartlett**

**11:05 INOR 1228.** Size-controlled synthesis of later transition metal nitrides by templating using mesoporous silica. **S. Gage, M.R. Davidson, C.A. Cadigan, S. Pylypenko, B.G. Trewyn, R.M. Richards**

**11:25 INOR 1229.** Bendable zeolite membranes for pervaporation separation. **B. Wang, P. Dutta**

### Section C

San Diego Convention Center  
Room 30D

### Chemistry of Materials: Metal Organic Frameworks

C. G. Lugmair, *Organizer*

M. E. Anderson, O. Miljanic, *Presiding*

**8:30 INOR 1230.** Metal-organic frameworks as scaffolds for probing HSAB properties. **T.A. Makal**

**8:50 INOR 1231.** 2D metal-organic frameworks as supramolecular building blocks for constructing ordered arrays of aromatic panels. **L.M. Lifshits, M. Zeller, J.K. Klosterman**

**9:10 INOR 1232.** Developing design rules for MOF thin film integration. **M.E. Anderson**

**9:30 INOR 1233.** Chemical vapour deposition of zeolitic imidazolate framework thin films. **I. Stassen, M. Styles, G. Greci, H. Van Gorp, W. Vanderlinden, S. De Feyter, P. Falcaro, D. De Vos, P. Vereecken, R. Ameloot**

**9:50 INOR 1234.** Synthesis and property of porous coordination polymer nano/micro-materials. **W. Sun**

**10:10** Intermission.

**10:25 INOR 1235.** Investigation of the surface properties and potential application areas of novel copper based metal organic framework synthesized by solvothermal and microwave assisted method with different heating and drying temperatures and durations, washing and filtration procedure. **A. Yurdusen, Y. Yurum**

**10:45 INOR 1236.** Withdrawn.

**11:05 INOR 1237.** Structure transitions of the Zr<sub>6</sub>(O)<sub>4</sub> clusters in NU-1000 and related MOFs. **A.E. Platero Prats, L.C. Gallington, A. Mavrandonakis, Y. Liu, J.T. Hupp, O.K. Farha, C.J. Cramer, K.W. Chapman**

**11:25 INOR 1238.** Nitrogen-rich porphyrinic metal-organic frameworks synthesized by postsynthetic metathesis method: From inert material to active catalyst. **X. Wang, H. Zhou**

**11:45 INOR 1239.** Withdrawn.

### Section D

San Diego Convention Center  
Room 30E

### Chemistry of Materials: Nanomaterials

C. G. Lugmair, *Organizer*

C. W. Li, J. D. Rinehart, *Presiding*

**8:30 INOR 1240.** Solution-processed semiconductor materials for electronic and thermoelectric devices. **Z. Lin, A. Yin, Y. Huang, X. Duan**

**8:50 INOR 1241.** Multidimensional functional graphene materials and their applications. **T. Fan, S. Tong, S. Mo, Y. Yu, Y. Liu, Y. Min**

**9:10 INOR 1242.** Optimizing permanent magnetic materials through post-synthetic modification on the single-domain level. **J.D. Rinehart, P. Adelman**

**9:30 INOR 1243.** End-bonded contacts for carbon nanotube transistors with low, size-independent resistance. **Q. Cao**

**9:50 INOR 1244.** Optical characterization of oxides and selenites of bismuth doped with Li<sup>+</sup>, Eu<sup>3+</sup> and Mn<sup>4+</sup>. **J. Ortiz Q, I. Zumeta Lubé, D. Diaz**

**10:10** Intermission.

**10:25 INOR 1245.** Surface reactivity of lead sulfide nanocrystals. **I. Rreza, J.S. Owen**

**10:45 INOR 1246.** Band-edge potentials of colloidal semiconductor nanocrystals. **C. Brozek, G.M. Carroll, D.R. Gamelin**

**11:05 INOR 1247.** Intercolloidal charge transfer between ZnO nanocrystals and amorphous TiO<sub>2</sub> nanoparticles. **J. Lora, R. Mitsuhashi, J.M. Mayer**

**11:25 INOR 1248.** Distinctive, selective ligand binding sites on CdS nanocrystals affecting energy and charge transfer. **X. Li, L. Slyker, V. Nichols, G. Pau, C.J. Bardeen, M. Tang**

**11:45 INOR 1249.** Tailoring the surface of colloidal ZnO quantum dots for efficient photocatalytic charge transfer. **C.W. Li, P. Alivisatos**

**12:05 INOR 1250.** Proton coupled electron transfer at nanocrystals: Effects of protons on ZnO redox chemistry. **C. Valdez, J.M. Mayer**

### Section E

San Diego Convention Center  
Room 31A

### Coordination Chemistry: Characterization & Applications

S. A. Koch, *Organizer*

D. J. Brook, *Presiding*

**8:00 INOR 1251.** Using a Ru(II) building block and a rapid screening approach to identify nucleic acid selective "light switch" compounds. **E. Wachter, D. Moyá, E.C. Glazer**

**8:20 INOR 1252.** Rhodamine based turn-on fluorescent sensor for the detection of chromium ions. **R. Madawala, E. Sinn**

**8:40 INOR 1253.** New class of heterobimetallics with potential for CO<sub>2</sub> activation. **A.M. Lunsford, K. Goldstein, M. Cohan, M.Y. Darensbourg**

**9:00 INOR 1254.** Effect of redox-inactive metals toward reactivity of biomimetic Fe complexes. **T. Chantarojsiri, J. Yang**

**9:20 INOR 1255.** Four-electron reductive coupling of carbon monoxide: Evidence for dicarbyne and terminal carbide reaction intermediates. **J.A. Buss, T. Agapie**

**9:40 INOR 1256.** Metal-assisted (Zn, Au) thiolate-disulfide exchange: Explorations of the mechanism using 2D NMR. **G.S. Garusinghe, A.E. Bruce, M.R. Bruce**

10:00 Intermission.

10:10 **INOR 1257.** Evidence for valence tautomerism in the iron and cobalt complexes of verdazyls. **D.J. Brook, C. Fleming, B. Ploof**

10:30 **INOR 1258.** Synthesis and characterization of novel gold (III) thiolate complexes. **M. Johnson**

10:50 **INOR 1259.** Synthesis, characterization, crystallography, and antimicrobial activity of novel gold(II) complexes with phosphine ligands (L<sub>2</sub>) tris(4-methoxy-3,5-dimethylphenyl)phosphine and (L<sub>2</sub>) Bis(2-methoxyphenyl) chlorophosphine. **K.J. Brown**

11:10 **INOR 1260.** Why MLCT excited-states make poor photoacids, and how to overcome it. **C.P. Ramirez, S. Ardo**

11:30 **INOR 1261.** Chemical and spectroscopic characterization of a monomeric Ni(II)-OH complex derived from water. **N. Lau, A. Borovik**

11:50 **INOR 1262.** Dinitrogen activation by a zerovalent cobalt complex: Exploiting its reducing power. **I. Reim, B.J. Cook, M. Pink, S. Bidwell, R.L. Lord, K.G. Caulton**

12:10 **INOR 1263.** Generation of coordinatively unsaturated, Lewis acidic manganese(I) complexes via controlled *cis*-labilization of CO. **D.W. Agnew, J.S. Figueroa**

## Section F

San Diego Convention Center  
Room 31B

### Coordination Chemistry: Synthesis & Characterization

S. A. Koch, *Organizer*

Z. Assefa, P. Desrochers, *Presiding*

8:00 **INOR 1264.** Withdrawn.

8:20 **INOR 1265.** Ruthenium polypyridyl complexes with antimony-substituted cyclometalating ligands. **A.M. Christianson, F.P. Gabbaï**

8:40 **INOR 1266.** Effects of the  $\mu_4$ -bridging atom in a tetranuclear iron cluster on the activation of nitric oxide. **C. Reed, T. Agapie**

9:00 **INOR 1267.** Thermally mediated decoherence in high-spin, nuclear spin-free transition metal complexes. **J. Zadrozny, D.E. Freedman**

9:20 **INOR 1268.** Investigating computational, structural, physicochemical and biological properties of a family of pyridoxine-lanthanide metal complexes. **A. Saha, C.E. Stouder, K. Warren, C.W. Padgett, A.L. Stewart, K.S. Aiken, S.M. Landge, A. Amonette**

9:40 **INOR 1269.** Structure and photoluminescent properties of dinuclear and tetranuclear Au(I) and Ag(I)-complexes with 1-methylbenzimidazole diphenylphosphine (MBDP) ligand. **Z. Assefa, D.E. Jenkins**

10:00 **INOR 1270.** Iron and cobalt chemistry of ferrocenyl substituted hydrotris(pyrazolyl)borate ligands. **D.C. Cummins, K.H. Theopold, G.P. Yap**

10:20 Intermission.

10:30 **INOR 1271.** Synthesis of a masked terminal nickel(II) sulfide via reductive deprotection. **N.J. Hartmann, G. Wu, T.W. Hayton**

10:50 **INOR 1272.** Curious stability of binuclear alkyl hydrides of chromium and their reaction with hydrocarbons. **Y. Hung, K.H. Theopold, G.P. Yap**

11:10 **INOR 1273.** Highly-reduced complexes of platinum and palladium supported by *m*-terphenyl isocyanides. **B.R. Barnett, J.S. Figueroa**

11:30 **INOR 1274.** Bimetallic indium complexes for the polymerization of cyclic esters. **P. Kelley, P. Mehrhodavandi**

11:50 **INOR 1275.** Chromium complexes of the redox-active [ONO] ligand and oxygen-atom transfer reactivity. **A. Hollas, A.F. Heyduk**

12:10 **INOR 1276.** Rapid synthesis of a functional resin-supported scorpionate and its copper(I, II), rhodium(I), and chromium(III) complexes. **P. Desrochers, A. Pearce, T.R. Rogers**

## Section G

San Diego Convention Center  
Room 31C

### Environmental & Energy-Related Inorganic Chemistry

S. A. Koch, *Organizer*

J. D. Blakemore, J. Yang, *Presiding*

8:00 **INOR 1277.** Withdrawn.

8:20 **INOR 1278.** Development of bis(arylimino)acenaphthene (BIAN) copper complexes as visible light harvesters for photovoltaic and artificial photosynthetic applications. **J. Kee, Y. Lu, R. Ganguly, H. Soo**

8:40 **INOR 1279.** Solvation effects on transition metal hydricity and electrocatalytic aqueous hydrogen production. **J. Yang, C. Tsay, B. Livesay, S. Ruelas**

9:00 **INOR 1280.** Proton-hydride tautomerism in hydrogen evolution catalysis. **J.D. Blakemore, L.M. Aguirre Quintana, S.I. Johnson, J.R. Winkler, H.B. Gray**

9:20 **INOR 1281.** Reusable materials in chemical sensing utilizing supramolecular  $pK_a$  shifts. **N. Saleh**

9:40 **INOR 1282.** Manifold of excited states and density of acceptors: Disentangling excited state electron injection into nanoporous titania. **D.F. Ziegler, Z.A. Morseth, L. Wang, D.L. Ashford, M.K. Brennaman, E. Grumstrup, E.C. Brigham, M.K. Gish, R. Dillon, L. Alibabaei, G.J. Meyer, T.J. Meyer, J.M. Papanikolas**

10:00 **INOR 1283.** Cation-dependent charge recombination to solution phase electron acceptors in dye-sensitized solar cells. **B.N. DiMarco, R.M. O'Donnell, G.J. Meyer**

10:20 Intermission.

10:30 **INOR 1284.** Nanoporous black silicon as a platform for photoelectrochemical hydrogen production: Exciting catalysts and nailing down the flatband potential. **N.C. Anderson, N.R. Neale**

10:50 **INOR 1285.** Hydrogenation of CO<sub>2</sub> and dehydrogenation of formic acid using Cp\*Ir complexes with imidazoline ligands. **Y. Himeida, N. Onishi, M.Z. Ertem, A. Tsuruzaki, Y. Manaka, J.T. Muckerman, E. Fujita**

11:10 **INOR 1286.** Hybrid molecule-nanocrystal photon upconversion across the visible and near-infrared. **Z. Huang, X. Li, M. Mahboub, B. Yip, J. Rubalcava, K.M. Hanson, V. Nichols, H. Le, C.J. Bardeen, M.L. Tang**

11:30 **INOR 1287.** Ternary Zn/Al/Ir layered hydroxide as efficient water oxidation catalyst. **L. Fagiolarì, A. Scafuri, F. Costantino, R. Vivani, A. Macchioni**

11:50 **INOR 1288.** Synthesis and surface chemistry of cadmium carboxylate passivated CdTe nanocrystals from cadmium bis(phenyltelluroate). **M.P. Campos, J.S. Owen**

12:10 **INOR 1289.** Distance-dependent energy transfer pathway between CdSe nanoparticles and anthracene during hybrid inorganic-organic upconversion. **X. Li, R. Zavala, M. Tang**

## Section H

San Diego Convention Center  
Room 32A

### Lanthanide & Actinide Chemistry

A. De Bettencourt Dias, *Organizer*

E. Borbas, J. Monteiro, *Presiding*

8:30 **INOR 1290.** Structural trends and solution behavior of actinide and lanthanide thiocyanate complexes. **R. Wilson, T.J. Carter, S. Skanthakumar, L. Soderholm**

8:50 **INOR 1291.** Chemical and electrochemical approaches to recycling rare-earth metals. **J.A. Vigil, L.J. Small, T.N. Lambert, R.F. Hess, T.J. Boyle, M. Kelly**

9:10 **INOR 1292.** Integrated toolkit of synchrotron X-ray and atomistic simulations for rare earth element refinery. **B. Qiao, G. Ferru, M. Olvera De La Cruz, R.J. Ellis**

9:30 Intermission.

9:40 **INOR 1293.** Reactivity of [K(18-crown-6)]([C<sub>5</sub>H<sub>9</sub>(SiMe<sub>3</sub>)<sub>2</sub>]<sub>2</sub>Th), the first complex containing thorium in the formal +2 oxidation state. **R. Langeslay, M. Fieser, J.W. Ziller, F.U. Furché, W.J. Evans**

10:00 **INOR 1294.** Sequestering uranium from seawater: Accurate predictions of thermochemistry and structural properties. **D.A. Penchoff, C. Peterson, J.P. Camden, D.M. Jenkins, A.K. Wilson**

10:20 **INOR 1295.** Open frameworks assembling from selected *f*-elements and various di-carboxylic acids. **R.A. Zehnder, M. Zeller**

10:40 Intermission.

10:50 **INOR 1296.** Recycling rare earth elements using ionic liquids: An electrochemical approach. **R.F. Hess, T.J. Boyle, J. Sears, L.J. Small, T.N. Lambert, D.R. Kammiller**

11:10 **INOR 1297.** Biologically (RE)levant metals: Model studies of a new rare-earth dependent methanol dehydrogenase. **W.L. Dornier, P.J. Carroll, E.J. Schelter**

11:30 **INOR 1298.** X-ray absorption spectroscopy of actinium and americium. **M. Ferrier, E.R. Batista, J.M. Berg, E. Birnbaum, J. Cross, J. Engle, K. John, S.A. Kozimor, V. Radchenko, B. Stein**

## Section I

San Diego Convention Center  
Room 32B

### Organometallic Chemistry: Catalysis

N. S. Radu, *Organizer*

D. Ess, *Presiding*

8:30 **INOR 1299.** Computation and experiment reveal unique reactivity and mechanisms of heterobimetallic and homobimetallic catalysts. **D. Ess**

8:50 **INOR 1300.** Ligand substituent effects on enantio- and regioselectivity in carbophilic catalysis with metal-acyclic diaminocarbene complexes. **A. Ruch, X. Zhang, F. Kong, L.M. Slaughter**

9:10 **INOR 1301.** Metal-carbon bond functionalization in the context of methane oxidation. **R.J. Nielsen, M. Cheng, W.A. Goddard**

9:30 **INOR 1302.** Exploiting electrophilic interactions to go beyond traditional pathways in hydrogenations with Wilkinson's catalyst. **J.E. Perea-Buceta, I. Fernández, S. Heikkinen, K. Axenov, A. King, T. Niemi, M. Nieger, M. Leskela, T. Repo**

9:50 **INOR 1303.** On the mechanism of the dual metal catalysis. **A. Poater, S. Vummaleti, L. Falivene**

10:10 **INOR 1304.** Highly enantioselective allylic alkylations in water. **J. Eppinger, D. Sawant**

10:30 **INOR 1305.** Base-free and acceptorless ruthenium-catalyzed dehydrogenative coupling of alcohols to esters. **D. Nguyen, R. Gauvin, G. Raffia, L. Zhang, L.C. Demailly, P. Fongarland, S. Dasset, P. Sebastien, F. Dumeignil**

10:50 Intermission.

11:00 **INOR 1306.** Redox non-innocent ligand supported manganese complexes for solar-fuel generation. **T.K. Mukhopadhyay, T.L. Groy, R.J. Trovitch**

11:20 **INOR 1307.** Transition-metal-catalyzed decarbonylation of biomass-derived carboxylic acids: A DFT study. **M.A. Ortuno, B. Dereli, C.J. Cramer**

11:40 **INOR 1308.** Light activated H<sub>2</sub> release from amine borane by [FeFe]ase mimics. **J. Blank, A. Lunsford, S. Moncho Escriva, S. Haas, M. Sohail, E.N. Brothers, M.Y. Darensbourg, A. Bengali**

## Section J

San Diego Convention Center  
Room 33A

### Organometallic Chemistry: Synthesis & Characterization-Late Transition Metals

N. S. Radu, *Organizer*

J. M. O Connor, *Presiding*

8:30 **INOR 1309.** Reactivity of Cp\*Co(IPr) with E-H Bonds: Experimental and computational studies of oxidative addition to a 16 electron Co(I) fragment. **J. Andjaba, C.A. Bradley**

8:50 **INOR 1310.** Withdrawn.

9:10 **INOR 1311.** Conversions of a metallocyclobutene to conjugated dienes. **P. Qin, B. Cenzano-Fong, K.K. Baldrige, R.L. Holland, J.M. O Connor**

9:30 **INOR 1312.** Structure and reactivity of a Ru(0) N-heterocyclic carbene pincer complex. **A. Sasayama, C.P. Kubiak**

9:50 **INOR 1313.** Reactions of pincer-type Pd<sup>II</sup>-Me complexes with molecular oxygen. **K. Smoll, W. Kaminsky, K.I. Goldberg**

10:10 **INOR 1314.** Withdrawn

10:30 **INOR 1315.** Synthesis and reactivity of (C<sub>2</sub>F<sub>5</sub>-PONOP) pincer complexes of iridium. **P. Miller, J. Addams, T. Parson, D.M. Roddick**

10:50 **INOR 1316.** DFT Calculations of spectra and binding mechanisms of bimetallic complexes. **A.L. Cooksy, H. Amouri**

11:10 **INOR 1317.** Stimuli induced, "on-off" ligation in a simple [Cu<sub>2</sub>(dppm)<sub>2</sub>(solvent)<sub>2</sub>]<sup>2+</sup> system. **T.M. Brown, V.J. Catalano**

11:30 **INOR 1318.** New paramagnetic rhodium(II) dimers without Rh-Rh bonds. **D. Zhu, A. Sharma, C. Wiebe, P.H. Budzelaar**

## Section K

San Diego Convention Center  
Room 33B

## Solid-State Inorganic Chemistry

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

J. Chan, *Presiding*

**8:30 INOR 1319.** Piezoelectrics: Putting the "squeeze" on new materials. A. Manjon-Sanz, T. Surta, R. McQuade, M. Dolgos

**8:50 INOR 1320.** Local order parameters: Descriptors for databases, synthesizability, interstitial relaxation, and diffusion paths. N.E. Zimmermann, M. Haranczyk

**9:10 INOR 1321.** Influence of Sn<sup>2+</sup>-substitution on the local structure of the Pb-free ferroelectric perovskites (Sr,Sn)TiO<sub>3</sub> and (Ba,Ca,Sn)TiO<sub>3</sub>. G. Laurita, K. Page, S. Suzuki, R. Seshadri

**9:30 INOR 1322.** Local structure influence on the insulator-metal transition in complex palladium oxides. L. Lamontagne, G. Laurita, M. Knight, H. Yusuf, R. Seshadri

**9:50 INOR 1323.** M&M process for ferrite synthesis. A.W. Apblett, A. Vecoven

**10:10** Intermission.

**10:25 INOR 1324.** Withdrawn.

**10:55 INOR 1325.** Withdrawn.

**11:15 INOR 1326.** Withdrawn.

**11:35 INOR 1327.** Synthesis, crystal growth, structural and magnetic characterization of NH<sub>4</sub>MCl<sub>2</sub>(HCOO), M = (Fe, Co, Ni). J.T. Greenfield, K. Kovnir

**11:55 INOR 1328.** Structural properties of ammonia borane/polymer composites. O. Gunaydin-Sen, R. Gangineni, S. Pati, R. Suwari

## Computational Materials &amp; Nanoscience: Theory Meets Experiment

## Forum: The Future of Spectroscopies: Quantum &amp; Classical Fields; Theoretical Perspectives

Sponsored by MPPG, Cosponsored by COMP, ENFL, INOR, ORGN and POLY

## Heavy Element Inorganic Chemistry: A Tribute to Al Sattelberger

Sponsored by NUCL, Cosponsored by INOR†

## THURSDAY AFTERNOON

## Section A

San Diego Convention Center  
Room 30B

## Chemistry of Materials: Materials for Energy &amp; Catalytic Applications

C. G. Lugmair, *Organizer*

L. A. Fredin, M. Yadav, *Presiding*

**1:30 INOR 1329.** Potential of imogolite nanotubes as (co-)photocatalyst: A linear-scaling density functional theory study. E. Poli, J.D. Elliott, G. Teobaldi

**1:50 INOR 1330.** High energy hot electron generated from Mn-doped quantum dots: A new way to enhance photocatalysis. Y. Dong, J. Choi, H. Jeong, D. Son

**2:10 INOR 1331.** Understanding the photochemistry of earth abundant iron light harvesters for sensitization. L.A. Fredin

**2:30 INOR 1332.** One-pot synthesis of photocatalytically active metal chalcogenide aerogels. D.A. Ramirez, B. Pacheco, L. Luberski, L. Hope-Weeks

**2:50 INOR 1333.** New family of earth-abundant materials for solar energy conversion applications. K. Ramasamy, H. Sims, S. Ivanov, A. Gupta

**3:10** Intermission.

**3:25 INOR 1334.** Withdrawn.

**3:45 INOR 1335.** Organic-inorganic hybrid catalyst for alkane oxidation. M. Yadav, A.J. Karkamkar

**4:05 INOR 1336.** Sol-gel synthesis of composite Cu/ZnO/Y<sub>2</sub>O<sub>3</sub> nanomaterials as potential heterogeneous catalysts. R. Baghi, R.W. Lord, L. Hope-Weeks

**4:25 INOR 1337.** Immobilization of transition metal complexes on composite surfaces: Metal sensing and catalysis. E. Rosenberg, G. Abbott, J. Ross, R. McVay

**4:45 INOR 1338.** Palladium intercalated in the walls of mesoporous silica for robust, high temperature catalytic applications. R.M. Richards, S. Gage, M. Davidson, M. Menart, Y. Ji, J. Leong, S. Pylypenko, B.G. Trewyn, C. Ngo, S. Kodambaka

## Section B

San Diego Convention Center  
Room 30C

## Chemistry of Materials: Metal Organic Frameworks

C. G. Lugmair, *Organizer*

K. V. Lawler, A. Mavrandonakis, *Presiding*

**1:30 INOR 1339.** Light gas separations and storage with MOFs via DFT modeling, synthesis, and pressurized induced structural changes. T.M. Nenoff, D.F. Sava Gallis, M.V. Parkes, J. Greathouse, M. Rodriguez, K. Chapman

**1:50 INOR 1340.** MOF crystal chemistry paving the way to gas storage needs: Aluminum-based soc-MOF for CH<sub>4</sub>, O<sub>2</sub>, and CO<sub>2</sub> storage. D. Alezi, Y. Belmabkhout, M. Suyetin, M. Eddaoudi

**2:10 INOR 1341.** Separation of xylene isomers in the metal-organic frameworks CO<sub>2</sub>(dobdc) and CO<sub>2</sub>(m-dobdc): Adsorption differences and unexpected framework flexibility. M. Kapelewski, E.D. Bloch, M.I. Gonzalez, M.R. Hudson, D. Reed, G. Barin, C.M. Brown, J.R. Long

**2:30 INOR 1342.** polyMOFs as a strategy to obtain water tolerant materials for selective carbon dioxide separations. Z. Zhang, S. Cohen

**2:50 INOR 1343.** Multi-functional rare-earth porphyrinic shp-MOF platform meets the needs for gas storage, catalysis, and electron sensitizer. Z. Chen, K. Adil, Y. Belmabkhout, M. Eddaoudi

**3:10 INOR 1344.** Dramatic tuning on carbon dioxide uptake through pore space partition. X. Zhao, Q. Zhai, X. Bu, P. Feng

**3:30** Intermission.

**3:45 INOR 1345.** Computational investigation of C1-C2 hydrocarbons interacting with the open-metal sites of the MIL-127 framework. A. Mavrandonakis, V. Bernaldes, L. Gagliardi, C.J. Cramer

**4:05 INOR 1346.** Importance of a precise crystal structure for simulating gas adsorption in nanoporous materials. K.V. Lawler, Z. Hulvey, P. Forster

**4:25 INOR 1347.** Reversible, low-concentration carbon monoxide binding in a metal-organic framework utilizing a unique spin state change mechanism. D. Reed, J.R. Long

**4:45 INOR 1348.** Carbon dioxide chemical fixation on metal-organic framework (MOF) platforms. W. Gao, S. Ma

**5:05 INOR 1349.** Evaluating Ni<sub>2</sub>(m-dobdc) and other metal-organic frameworks for high-pressure hydrogen storage. M. Kapelewski, T. Runcevski, H. Jiang, K. Hurst, T. Gennett, S. Fitzgerald, J.R. Long

**5:25 INOR 1350.** Extraordinary versatility of the metal-organic framework UiO-66-NH<sub>2</sub> for toxic chemical removal. G.W. Peterson, J.B. DeCoste

## Section C

San Diego Convention Center  
Room 30D

## Chemistry of Materials: Nanomaterials

C. G. Lugmair, *Organizer*

J. Florek, I. Jen-La Plante, *Presiding*

**1:30 INOR 1351.** Compact voltage sensitive nanocrystals for the imaging of neuron activity. I. Jen-La Plante, L. Hamachi, J.S. Owen

**1:50 INOR 1352.** Mesoporous silica nanoparticles: Selective surface functionalization and particle size control for optimal theranostic performances. M. Bouchoucha, R. C.-Gaudreault, M. Fortin, F. Kleitz

**2:10 INOR 1353.** Exploring disulfide and metal-mediated bonding as design principles for protein self-assembly. R. Subramanian, F.A. Tezcan

**2:30 INOR 1354.** Enzymatically responsive nanoparticle superlattices. S.N. Barnaby, R.V. Thayer, M.B. Ross, K. Brown, G.C. Schatz, C.A. Mirkin

**2:50 INOR 1355.** Synthesis of nanoinks using novel precursors for advanced Direct Write applications. L.J. Treadwell, T.J. Boyle, A. Cook, N.S. Bell

**3:10** Intermission.

**3:25 INOR 1356.** Molecular magnets gone dimensional. S.A. Corrales, T. Jenkins, D. Pistey, N. Mhesri, B. Voss, A.M. Mowson, G. Christou, A. Ozarowski, C. Lampropoulos

**3:45 INOR 1357.** Withdrawn.

**4:05 INOR 1358.** Nanoporous organo-functionalized materials as selective and regenerable sorbents for rare earth extraction. J. Florek, A. Mushtaq, E. Juère, F.G. Fontaine, D. Larivière, F. Kleitz

**4:25 INOR 1359.** Supercapacitors based on CuSbS<sub>2</sub> nanoplates. K. Ramasamy, R. Gupta, H. Sims, S. Ivanov, A. Gupta

**4:45 INOR 1360.** Observing different electronic sites in reduced titanium dioxide nanoparticles. J. Peper, J.M. Mayer

## Section E

San Diego Convention Center  
Room 31A

## Coordination Chemistry: Synthesis &amp; Characterization

S. A. Koch, *Organizer*

P. Chandrasekaran, *Presiding*

**1:30 INOR 1361.** Coordination chemistry of N-heterocyclic thione (NHT) and selone (NHSE) derivatives of caffeine. M. Styrón, D. Rabinovich

**1:50 INOR 1362.** Synthesis and characterization of bimetallic coordination complexes of tris(2-pyridyl)phosphine and its derivatives. A.K. Frampton, C. Fairfield, N.A. Piro, W.S. Kassel

**2:10 INOR 1363.** Magnetism of two-coordinate transition metal complexes. P. Bunting, J.R. Long

**2:30 INOR 1364.** Radical stabilization and ligand-based redox chemistry on oligopyrrolic fragments. R. Gautam, E. Tomat

**2:50 INOR 1365.** Towards terminal high-valent metal-oxo motifs on multimetallic scaffolds. G. de Ruiter, N.B. Thompson, T. Agapie

**3:10 INOR 1366.** Effects of methyl viologen on aminoethylglycine-functionalized [Ru(bpy)<sub>3</sub>]<sup>2+</sup> with pendant phenothiazines. B. Biber, M. Williams

**3:30 INOR 1367.** Structural properties of silver(I) and mercury(II) coordination polymers based on benzene-1,2,4,5-tetrathioether. P. Chandrasekaran, S. Kakumanu, T. Selby-Karani

**3:50** Intermission.

**4:00 INOR 1368.** Tetranuclear complexes as precursors for the rational design of pentanuclear oxido clusters reminiscent of the oxygen evolving complex in photosystem II. H. Lee, E. Tsui, T. Agapie

**4:20 INOR 1369.** Extremes of π-backdonation: The isolation of a m-terphenyl isocyanide stabilized Co-carbyne. C.C. Mokhtarzadeh, J.S. Figueroa

**4:40 INOR 1370.** Withdrawn.

**5:00 INOR 1371.** Modular approach to tuning the equatorial ligand field strength around a series of Co<sup>II</sup>-OH complexes with hydrogen bonding cavities in trigonal symmetry. J. Jones, A. Borovik

**5:20 INOR 1372.** Withdrawn.

**5:40 INOR 1373.** Intramolecular arene C-H and C-F activation by multimetallic tetramanganese clusters relevant to the oxygen-evolving complex of photosystem II. K.M. Carsch, G. de Ruiter, T. Agapie

## Section F

San Diego Convention Center  
Room 31B

## Nanoscience

R. M. Richards, *Organizer, Presiding*

**1:30 INOR 1374.** Photoinduced electron donor/acceptor processes between colloidal CdSe quantum dots and nitroxide free radicals. P. Dutta, R. Beaulac

**1:50 INOR 1375.** Hydrothermal synthesis of substitutionally-doped transition metal ions in SrTiO<sub>3-δ</sub> colloidal nanocrystals. W. Harrigan, S.E. Michaud, K.A. Lehuta, K.R. Kittilstved

**2:10 INOR 1376.** Electronic transport in self-assembled gold nanoparticle-molecular networks. P. Zhang, C. Papadopoulos

**2:30 INOR 1377.** Plasmonic metallurgy enabled by DNA. M.B. Ross, J.C. Ku, B. Lee, C.A. Mirkin, G.C. Schatz

**2:50 INOR 1378.** N-heterocyclic carbene precursors for Ag, Ag<sub>2</sub>S and Ag<sub>2</sub>Se nanocrystals syntheses. H. Lu, R.L. Brutchey

**3:10** Intermission.

**3:30 INOR 1379.** Tuning the magic size of atomically precise gold nanoclusters via isomeric methylbenzenethiols: Small change makes big difference. Y. Chen, R. Jin

**3:50 INOR 1380.** Computationally guided synthetic approaches to nanoscale metal carbide/nitride materials. S. Gage, C.A. Cadigan, C. Ciobanu, S. Pylypenko, B.G. Trewyn, R.M. Richards

**4:10 INOR 1381.** Mixed halide organolead perovskites: Dimensionality control and role of excess precursor on photoluminescence stability. L. Men, D. Freppon, U. Bhattacharjee, F. Zhu, B. Rosales, J.W. Petrich, E.A. Smith, J. Vela-Becerra

**4:30 INOR 1382.** Exploring the surface chemistry of semiconductor nanocrystals: From CdS to CsPbI<sub>3</sub>. H. Andaraarachchi, J. Vela-Becerra



## Section G

San Diego Convention Center  
Room 31C

## Organometallic Chemistry: Catalysis

N. S. Radu, *Organizer*

S. N. Brown, M. Findlater, *Presiding*

**1:30 INOR 1383.** Transition metal oxos as frustrated Lewis pairs. E.A. Ison, N.S. Lambic

**1:50 INOR 1384.** Ligand-centered dehydrogenation reactions of metal bis- and tris-iminoxolones. S.N. Brown

**2:10 INOR 1385.** Pt(II) complexes supported on mesoporous silica nanoparticles: New catalyst for olefin hydroarylation. T.S. Gray, P. Kunal, M.M. Otting, N. Hirscher, J.R. Andreatta, L.G. Habgood, B.G. Trewyn, T.B. Gunnoe

**2:30 INOR 1386.** Withdrawn.

**2:50 INOR 1387.**  $sp^2$  C-H activation and C-C coupling catalyzed by Cu(I) complex with the ambiphilic ligand 8-quinolylidimesitylborane. S.R. Tamang, J.D. Hoefelmeyer

**3:10** Intermission.

**3:20 INOR 1388.** C-H activation by a titanium neopentylidene complex. D. Ninkovic, E. Brothers, S. Zaric, M.B. Hall

**3:40 INOR 1389.** Ir(III)-arene complexes as active catalysts for the oxidation of  $sp^3$  C-H bonds. S. Hohloch, S. Kaisers, F. Duecker, A. Bolje, R. Maity, J. Kosmirj, B. Sarkar

**4:00 INOR 1390.** Alkane dehydrogenation co-catalyzed by an iridium(III) complex and Lewis acids. Catalyst design and mechanistic study. Y. Gao, C. Guan, Z. Syed, T.J. Emge, A.S. Goldman

**4:20 INOR 1391.** Palladium complexes with electron-poor biscarbenes. P. Piernaria

## Section H

San Diego Convention Center  
Room 32A

## Organometallic Chemistry: Synthesis &amp; Characterization-Late Transition Metals

N. S. Radu, *Organizer*

D. B. Grotjahn, *Presiding*

**1:30 INOR 1392.** Ligands possessing C- and N-donors for ruthenium catalyzed water oxidation: Synthesis, characterization, and electrochemistry. A.G. Nash, D.B. Grotjahn

**1:50 INOR 1393.** High-valent Pd and Ni complexes supported by 1,4,7-trimethyl-1,4,7-triazacyclononane. M. Watson, L.M. Mirica

**2:10 INOR 1394.** Synthesis, characterization, and reactivity of mononuclear palladium complexes bearing nitrogen and carbon-donor ligands. N. Ruhs, N.P. Rath, L.M. Mirica

**2:30 INOR 1395.** Late transition metal complexes of protic bifunctional ligands: Activation of molecular oxygen. W.D. Bailey, R.A. Kemp, K.J. Goldberg

**2:50 INOR 1396.** First late transition metal cyclopentadienyl chelate complexes with silylphosphane or secondary phosphane tethers. I. Werner, S. Heinisch, H. Butenschon

**3:10 INOR 1397.** Withdrawn.

**3:30 INOR 1398.** Synthesis and reactivity of copper hydride nanoclusters. T.D. Nguyen, G. Wu, T.W. Hayton

**3:50 INOR 1399.** Development and investigations into a bispyrazolyl mono-triazolyl heteroscorpionate platinum system. K. Lavoie, B. Frauhiger, P. White, J.L. Templeton

**4:10 INOR 1400.** Synthesis and characterization of  $(\text{N}4)\text{M}(\text{COD})$  ( $\text{R} = \text{Me}$  or  $\text{tBu}$ ,  $\text{M} = \text{Rh}$  or  $\text{Ir}$ ) complexes. K. Fuchigami, L.M. Mirica

**4:30 INOR 1401.** Incorporating a proaza-phosphatrane donor into a tripodal ligand. Z. Thammavongsy, I. Kha, J. Yang

**4:50 INOR 1402.** Towards transition metal complexes having 1,3-benzoxaphosphole ligands. A. Grimm, J. Protasiewicz

## Section I

San Diego Convention Center  
Room 32B

## Main Group Chemistry

T. W. Hudnall, *Organizer*

A. M. Spokoiny, *Presiding*

**1:30 INOR 1403.** Tin catalyzed hydrophosphination of secondary phosphines. J.P. Stelmach, R. Waterman

**1:50 INOR 1404.** Cationic gallium and indium complexes as Lewis acids for molecular catalysis: Structure-stability-activity relationships. V. Gandon

**2:10 INOR 1405.** Computational evidence for bond activation by main-group metals. D. Ess

**2:30 INOR 1406.** Mechanistic insight into ligand-based proton transfer reactions with a molecular aluminum complex. T. Sherbow, L.A. Berben

**2:50 INOR 1407.** Synthesis and characterization of low-valent aluminum clusters. L. Stevens, Y. Peng, D. Mayo, S.M. DeCarlo, P. Zavalij, K.H. Bowen, B.W. Eichhorn

**3:10** Intermission.

**3:20 INOR 1408.** Selective vertex cross-coupling of bromo-carboranes using electron-rich phosphine ligands. R.M. dziedzic, L.M. Saleh, S.L. Stevens, A.M. Spokoiny

**3:40 INOR 1409.** Hydrogen peroxide and dihydroperoxy alkane adducts of phosphine oxides as solid, stoichiometric, and soluble oxidizing agents. S. Ahn, J. Bluemel

**4:00 INOR 1410.** S-block grind: Mechanochemical synthesis of bulky allyl complexes of the s-block metals. N.R. Rightmire, T.P. Hanusa

**4:20 INOR 1411.** Lewis acidic properties of tryarylstibines. M. Yang, F.P. Gabbai

**4:40 INOR 1412.**  $\text{B}(\text{C}_6\text{F}_5)_3$  - A unique  $\pi$ -Lewis acid: Rearrangement and carboboration reactions. M.M. Hansmann

**5:00 INOR 1413.** Forming new bonds: Ditopic organoboranes in reduction reactions. T. Kaese, M. Wagner

## Computational Materials &amp; Nanoscience: Theory Meets Experiment

## Forum: Exciting Aspects of Excitation Dynamics &amp; Dissociation at the Nanoscale

Sponsored by MPPG, Cosponsored by COMF, ENFL, INOR, ORGN and POLY

## MEDI

## Division of Medicinal Chemistry

W. Young, *Program Chair*

## BUSINESS MEETINGS:

**MEDI Executive Committee Business Meeting,** 8:30 AM: Sun

**MEDI Division Business Meeting,** 4:30 PM: Sun

**Long Range Planning Committee,** 6:00 PM: Mon

## SUNDAY MORNING

## Section A

San Diego Convention Center  
Room 6F

## Bromodomain Inhibition: BETs &amp; Beyond

A. S. Duerfeldt, W. D. Schmitz, *Organizers, Presiding*

**9:00** Introductory Remarks.

**9:05 MEDI 1.** Bromodomain inhibitors: from chemical probe to clinic candidate. J. Qi

**9:35 MEDI 2.** New benzazepine and pyridopyrazinone BET-inhibitors for cancer treatment. N. Schmees

**10:05 MEDI 3.** BET proteins: Biology beyond cancer. G.V. Denis, J.T. Deeney, A.C. Belkina, O.O. Shirihai, B.E. Corkey

**10:35 MEDI 4.** From epigenetic mechanism to targeted therapy. M. Zhou

**11:05 MEDI 5.** Discovery and development of a potent dual TRIM24/BRPF1 bromodomain inhibitor, IACS-9571, using structure-based drug design. W.S. Palmer, G. Poncet-Montagne, G. Liu, A. Petrocchi, N. Reyna, G. Subramanian, J. Theroff, M. Kost-Alimova, J. Bardenhagen, E. Leo, H. Sheppard, T. Tieu, S. Xi, Y. Zhan, S. Zhao, M. Barton, G. Draetta, C. Toniatti, P. Jones, M. Geck Do, J. Andersen

**11:35 MEDI 6.** Hijacking ubiquitin E3 ligases using PROTAC technology to effectively degrade BRD4 and achieve anti-tumor efficacy. Y. Qian, J. Lu, K. Raina, M. Altieri, D. Gordon, A. Rossi, J. Wang, H. Dong, X. Chen, K. Siu, J. Winkler, C.M. Crews, K. Coleman, A. Crew

## Section B

San Diego Convention Center  
Room 6E

## General Orals

W. B. Young, *Organizer*

J. B. Schwarz, *Presiding*

**8:30 MEDI 7.** Scaffold hopping and optimization of maleimide based porcupine inhibitors. A. Poulsen, S.Y. Ho, W. Wang, J. Alam, A.J. Duraiswamy, G.R. Lin, S.H. Ang, E.S. Tan, M.A. Lee, Z. Ke, B. Madan, D. Virshup, L. Ding, V. Manoharan, C.Y. Shan, L.C. Bing, V. Pendharkar, K. Sangthongpitag, T.H. Keller

**8:50 MEDI 8.** Solubility sorted: Solid form disruption to improve solubility. C. Groom, E. Davis, J. Cole

**9:10 MEDI 9.** Targeting the transcriptional activation of human oncogenes with small molecules. D. Sun

**9:30 MEDI 10.** Alternative core development around HCV NS5A inhibitor MK-8742 scaffold. L. Tong, J.A. Kozlowski, W. Yu, C.A. Coburn, P.T. Meinke, A.G. Nair, M.P. Dwyer, O. Selyutin, S.B. Rosenblum, Y. Jiang, R. Liu, E. Asante-Appiah, S. Agrawal, E. Xia, S. Curry, P. Ingravallo

**9:50 MEDI 11.** Identification of a novel series of indole core protein modulators of the hepatitis B virus. S.D. Kuduk, A.M. Lam, C. Esperitu, R. Vogel, K. Klumpp, L. Flores, G.D. Hartman

**10:10 MEDI 12.** Evolution of synthetic cannabinoid designer drugs. S. Banister, M. Longworth, J. Stuart, R. Kevin, M. Glass, R. Gerona, M. Connor, I. McGregor, M. Kassiou

**10:30 MEDI 13.** Development of novel and selective factor IXa inhibitors. T. Zhang

**10:50 MEDI 14.** Selective deubiquitylase inhibitors for cancer immunotherapy. J. Wu, S. Kumar, G. Fegley, F. Wang, M. Kodrasov, S. Agarwal, M. Mattern, J. Weinstock

**11:10 MEDI 15.** Novel indole-2-carboxamides are highly potent against drug-sensitive and drug-resistant strains of *Mycobacterium tuberculosis*. J. Stec, O.K. Onajole, S. Lun, W.R. Bishai, A.P. Kozikowski

**11:30 MEDI 16.** Identification of a potent and selective covalent inhibitor of lysophospholipase-like 1 (LYPLAL1). J. Chen, K. Ahn, D. Anderson, M. Boehm, M.F. Brown, Y. Che, K.F. Fennell, K.F. Geoghegan, A.M. Gilbert, J. Gutierrez, J.J. Calloway, A.S. Kalgutkar, A. Lanba, C. Limberakis, T.V. Magee, I. O'Doherty, R. Oliver, B. Pabst, J. Pandit, K. Parris, R. Patel, J.A. Pfefferkorn, T. Rolph, B.P. Schuff, J. Starr, A. Varghese, N.B. Vera, C. Vernochet, J. Yan

**11:50 MEDI 17.** Discovery of CCT251921: A potent, selective and orally bioavailable small molecule modulator of the mediator complex-associated kinases CDK8 and CDK19. A. Mallinger, K. Schiemann, C. Rink, F. Stieber, M. Calderini, M. Stubbs, O. Poeschke, M. Busch, P. Czodrowski, D. Musil, D. Schwarz, M. Ortiz-Ruiz, R. Schneider, M. Valenti, A. de Haven Brandon, P. Workman, T. Dale, D. Wienneke, P. Clarke, C. Esdar, F. Raynaud, s. Eccles, F. Rohdich, J. Blagg

## From Synthesis to Design: Modeling Tools for Medicinal Chemists

Sponsored by COMF, Cosponsored by CINF and MEDI

## SUNDAY AFTERNOON

## Section A

San Diego Convention Center  
Room 6F

## General Orals

W. B. Young, *Organizer, Presiding*

**1:30 MEDI 18.** Discovery of an iminopyridine derivative, TAK-259, as a novel, selective, and orally active  $\alpha_{1D}$  adrenoceptor antagonist with anti-urinary frequency effects. N. Sakauchi, Y. Kohara, A. Sato, T. Suzuki, Y. Imai, Y. Okabe, S. Imai, R. Saikawa, H. Nagabukuro, H. Kuno, H. Fujita, I. Kamo, M. Yoshida

**1:55 MEDI 19.** Minimizing CYP2C9 inhibition of exposed-pyridine inhibitors of NAMPT (nicotinamide phosphoribosyltransferase). M. Zak, N.J. Skelton, T. O'Brien, B.M. Liederer, D. Sampath, J. Oeh, W. Wang, X. Zheng, Y. Ho, P. Yuen, P.S. Dragovich