

## INOR

### DIVISION OF INORGANIC CHEMISTRY

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

## SUNDAY MORNING

### Section A

Marriott Marquis San Diego  
Marina  
Santa Rosa

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

S. A. Koch, *Organizer*  
M. C. Heffern, S. E. Stieber, *Presiding*

**8:30 1.** Investigating the dependence of proinsulin C-peptide on metal micronutrients. **M.C. Heffern**

**8:50 2.** Oxygen uptake in complexes related to [NiFeS] and [NiFeSe] hydrogenase active sites. **X. Yang**, T. Le, L.C. Elrod, M.Y. Darensbourg, M. Hall

**9:10 3.** Mononuclear Cu-aqua and -hydroxido complexes for multielectron processes. **D.L. Ross**, A. Borovik

**9:30 4.** Metal-binding pharmacophores utilizing bioisosteres as novel scaffolds for metalloenzyme inhibition. **B. Dick**, S. Cohen

**9:50 5.** Quantifying nickel nitrosyl coordination modes with X-ray emission spectroscopy and computations. **S.E. Stieber**

**10:10** Intermission.

**10:30 6.** Harnessing P450 biocatalysis with Ru(II)-polypyridyl complexes. **L.E. Cheruzel**

**10:50 7.** Stable end-on ( $\eta^1$ ) superoxocopper(II) complexes that display appreciable substrate reactivity. **J. England**

**11:10 8.** Oxygen intermediates before and after ferryl-oxos in mononuclear nonheme iron enzymes. **S. Iyer**, K. Tidemand, S. Goudarzi, H. Christensen, G. Peters, E.I. Solomon

**11:30 9.** Dioxygen activation by manganese thiolate complexes with tunable ligands. **C. Poon**, M.A. Dedushko, X. Sun, G. Yang, S.A. Toledo, E. Hayes, A. Johansen, J. Rees, S. Stoll, E.V. Rybak-Akimova, J. Kovacs

**11:50 10.** Non-heme iron and 2-oxoglutarate-dependent histone demethylases: Understanding reaction mechanisms, ligand binding and dynamics using QM/MM and MD methods. **C. Christov**, R. Rajeev, S.S. Chaturvedi, T. Karabencheva-Christova

**12:10 11.** Understanding the mechanism of hydrogen peroxide induced carbon monoxide release from a manganese carbonyl. **J. Barrett**, P.C. Ford

### Section B

Marriott Marquis San Diego  
Marina  
Marriott Grand Ballroom Section 9  
**Environmental & Energy-Related Inorganic Chemistry**

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

**8:30 12.** Ultrathin MOF nanosheet based composite membranes for carbon capture. **M. Liu**, Q. Fu, P. Webley, G. Qiao

**8:50 13.** Metal oxide electronic structure determines the direction of electron transfer at dye-sensitized interfaces. **R.E. Bangle**, G.J. Meyer

**9:10 14.** Coordination environment of a polymer-encapsulated cobalt complex for selective electrochemical CO<sub>2</sub> reduction. **Y. Liu**, C.C. McCrory

**9:30 15.** 150MPa of high-pressure H<sub>2</sub>/CO<sub>2</sub> production by formic acid dehydrogenation and continuous separation. **H. Kawanami**, Y. Himeda, M. Iguchi

**9:50 16.** Electrocatalytic H<sub>2</sub> evolution in water by co-mimochrome VI\*a, a synthetic mini-protein. **J. Le**, V. Firpo, V. Pavone, A. Lombardi, K. Bren

**10:10 17.** Functional mapping reveals mechanistic clusters for OER catalysis across (Cu-Mn-Ta-Co-Sn-Fe)O<sub>x</sub> composition and pH space. **J. Haber**, H.S. Stein, D. Guevarra, A. Shinde, R.J. Jones, J.M. Gregoire

**10:30 18.** Open-shell Mo(V) nitrides, phosphides, and carbides: Does radical character dictate coupling chemistry?. **G.A. Bailey**, J.A. Buss, T. Agapie  
**10:50** Intermission.

**11:00 19.** High performance PDMS pervaporation membranes for recovery of *n*-butanol. **J. Lee**, D. Kim, S. Shin, J. Lee

**11:20 20.** Electrochemical total oxidation of multi-carbon substrates by an oxidic cobalt catalyst. **T. Keane**, C. Brodsky, D.G. Nocera

**11:40 21.** Electrocatalytic water oxidation using (bpy)<sub>2</sub>Co-based precursors. **R.L. Holland**, H.M. Tubbs, B.A. McKeown, R.J. Nielsen, W.A. Goddard, T.B. Gunnoe

**12:00 22.** Thermodynamic strategies of hydride tuning for CO<sub>2</sub> reduction. **A.L. Ostericher**, C.P. Kubiak

**12:20 23.** Determining the site of protonation and the hydricity of active-site model complexes of the tungsten- and molybdenum-containing formate dehydrogenases. **T. Kerr**, J.Y. Yang

### Section C

Marriott Marquis San Diego  
Marina  
Marina Ballroom Salon F  
**Chemistry of Materials: Materials for Energy & Catalytic Applications**

C. G. Lugmair, *Organizer*  
D. Primm, Y. N. Regmi, *Presiding*

**8:30 24.** Oxide nanoparticles coated with corrosion resistant metals as anode catalyst layer fillers in proton exchange membrane electrolyzers. **Y.N. Regmi**, E. Tzanetopoulos, N. Danilovic

**8:50 25.** Introducing nanocrystalline CeO<sub>2</sub> and Au-CeO<sub>2</sub> in electrocatalytic HER, OER and electro-oxidation of methanol. **K. Deori**

**9:10 26.** Improving and understanding the hydrogen evolving activity of a cobalt dithiolene metal-organic framework. **K. Chen**, E. Schneider, C. Downes, J. Goodpaster, S.C. Marinescu

**9:30 27.** Synthesis of PtNi tetrahedrons with exceptional activity for hydrogen evolution reaction. **C. Wan**, X. Duan

**9:50 28.** Stabilization of reactive Co<sub>4</sub>O<sub>4</sub> cubane oxygen-evolution catalysts within porous frameworks. **K.M. Van Allsburg**, A.I. Nguyen, M.W. Terban, M. Bajdich, J. Oktawiec, J. Amtawong, M.S. Ziegler, J.P. Dombrowski, K.V. Lakshmi, W.

Drisdell, J. Yano, S.J. Billinge, T. Tilley

**10:10** Intermission.

**10:25 29.** Design of single-site transition metal catalysts for electrochemical oxidation of methane to methanol. **D. Primm**, J. Fornaciari, A.Z. Weber, A.T. Bell

**10:45 30.** Electrocatalytic small molecule transformations using multilayer films of discrete molecular catalysts. **J. Kallick**

**11:05 31.** Understanding structural features for rapid transport in lithium-ion batteries with niobium oxides. **M. Preefer**, R. Seshadri

**11:25 32.** *Operando* X-ray diffraction gives insight into the origin of pseudocapacitance in nano-MoO<sub>2</sub> electrodes. **D. Robertson**, Y. Yao, M. Chin, T.C. Lin, S.H. Tolbert

**11:45 33.** Superhydrophilic and superaerophobic metal-organic frameworks for electrocatalytic oxygen evolution. **F. Xie**, J. Ye, M. Eddaoudi, Z. Tang, Y. Han

### Section E

Marriott Marquis San Diego  
Marina  
Marriott Grand Ballroom Section 8  
**Emerging Research in Molecular Synthesis**

A. C. Brewer, J. M. Hoover, V. A. Schmidt, J. Y. Yang, *Organizers*  
E. B. Hulley, J. Yang, *Presiding*

**8:30 34.** Metal carbonyl clusters as catalysts for fast H<sub>2</sub> evolution. **L.A. Berben**

**9:00 35.** To tether or not to tether: Frustration of electrophilic transition metal systems. **E.B. Hulley**, W. Christman, L. Pap, T. Morrow, N. Arulsamy

**9:30 36.** Developing molecular electrocatalysts and scalable systems for renewable fuels. A. Nichols, S. Hooe, C. Jiang, L. Lieske, **C.W. Machan**

**10:00** Intermission.

**10:15 37.** Storing electrons and protons on redox-active ligands. **A.F. Heyduk**, B.J. Charette

**10:45 38.** Chemical and electrochemical studies of half-sandwich rhodium complexes supported by hybrid [P,N] ligands. **J.D. Blakemore**, J. Hopkins, D. Lionetti, V. Day

### Section F

Marriott Marquis San Diego  
Marina  
Solana  
**Main Group Chemistry**

T. Hudnall, *Organizer*  
M. J. Rose, *Presiding*

**8:30 39.** Readily available primary aminoboranes as powerful reagents for aldimine synthesis. **G.P. Junior**, E.A. Romero, X. Chen, R. Jazzar, G. Bertrand

**8:50 40.** Dispiro-4-bromobenzylaminophosphazenes: Synthesis reactions, spectroscopic and chromatographic properties, crystal structures, biological, and cytotoxic activities. **N. Guven Kuzey**, M. Özgür, N. Asmafiliz, L. Acik, B. Aydin, T. Hokelek, M. Turk, A. Cerci

**9:10 41.** New ligand protonation series of aluminum(III) complexes. **N.A. Phan**, L.A. Berben

**9:30 42.** Life without solvent: Mechanochemical synthesis of bulky main-group allyl species. **R.F. Koby**, T.P. Hanusa

**9:50 43.** Formation of well-defined strong acid sites on oxides. **D. Culver**, W. Huynh, M.P. Conley  
**10:10** Intermission.

**10:20 44.** Photocatalytic reactivity of tellurorhodamine chromophore derivatives towards aerobic oxidation of organic substrates. **I. Rettig**, T. McCormick, J. Van, J. Brauer, L. Lutkus, J. Lohman

**10:40 45.** Adventures in antimony-3d metal chemistry (Mn to Cu): NIR emission, metal deposition, and spin-orbit coupling. **M.J. Rose**, L. Taylor

Section G

Marriott Marquis San Diego  
Marina  
Point Loma

**Organometallic Chemistry: Catalysis - Early Transition Metals**

N. S. Radu, *Organizer*  
A. D. Sadow, *Presiding*

**8:30 46.** Zirconium complexes supported by a ferrocene-based ligand as redox switches for hydroamination reactions. **Y. Shen**, P. Diaconescu

**8:50 47.** Kinetics And mechanism of catalytic aluminol Of 1-alkynes by rare-earth aluminates. **U. Kanbur**, **A.D. Sadow**

**9:10 48.** Niobium-catalyzed ether deoxyhalogenation with silicon halides. **B.F. Parker**, H. Tsurugi, J. Arnold, K. Mashima

**9:30 49.** Substrate determined mechanism of deoxydehydration of polyols by a Mo(VI) catalyst. **S.M. Kilyanek**, R. Tran, K.A. DeNike

**9:50 50.** Synthesis, structure, and reactivity of bulky isocyanides supported unsaturated chromium dianion species. **S. Wang**, J.S. Figueroa

**10:10 51.** Synthesis and reactivity of group 4 complexes supported by redox noninnocent anthracene-bisphenoxide ligands. **M. Bruening**, C. Low, T. Agapie

**10:30 52.** Homoleptic lanthanide alkyl compounds in homogeneous and interfacial hydroboration catalysis. **A.D. Sadow**

**10:50 53.** Ligand substituent effects on the rate of hydrocarbon C-H activation at bent-sandwich tantalum(V) trihydride complexes. **S. Rehbein**

Section H

Marriott Marquis San Diego  
Marina  
Cardiff

**Organometallic Chemistry: New Ligand Platforms**

N. S. Radu, *Organizer*  
T. S. Haddad, D. R. Manke, *Presiding*

**8:30 54.** Cooperative hydrogenolysis in late transition metal-aluminum heterobimetallic complexes. **R.M. Charles**, T.W. Yokley, N.J. Deyonker, T.P. Brewster

**8:50 55.** Synthesizing new "Pacman" ligands for renewable energy applications. **P.E. Sues**, C.A. Ackley, E.M. Archer, N.P. Marshall

**9:10 56.** Synthesis and characterization of 1,1'-dicarbodiimidoferocones and their group IV 1,1'-bisguanidinateferrocene complexes. **O. Esarte Palomero**, R.A. Jones

**9:30 57.** Electropolymerization of new N-heterocyclic carbene (NHC) complexes of Pd, Pt, Rh and Ir featuring a terthiophene backbone. **W. Wang**, R.A. Jones

**9:50 58.** Siloxide podand ligands as a scaffold for molybdenum catalyzed alkyne metathesis: Role of ligand flexibility and Mo-O-Si bond angle on catalytic activity.

**R.R. Thompson**, P. Du, R. Kumar, S. Lee

**10:10 59.** Synthesis, characterization, and reactivity of iridium-aluminum and rhodium-aluminum heterobimetallic complexes. **T. Brewster**, Z. Li, R.M. Charles, T.W. Yokley, S.L. Tran, N.D. Schley, N.J. Deyonker

**10:30 60.** Ligand design for permanent catalytic deactivation. **T.S. Haddad**, A. Romich, J.A. Boatz, R. Blanski, K.B. Ghiassi

**10:50 61.** What difference does an extra CH<sub>2</sub> make? Oxidation chemistry of 16- and 18-atom ringed tetra-NHC iron complexes. J. DeJesus, M. Anneser, X. Powers, S.B. Isbill, K. Blatchford, S. Roy, **D.M. Jenkins**

**11:10 62.** Diferrocenylmercury-bridged diphosphines: Flexible ambiphilic ligands with a unique stereochemical environment. A. Tagne Kuate, R. Lalancette, **F. Jaekle**

**11:30 63.** Design and synthesis of a new hybrid N<sub>2</sub>P<sub>2</sub> tetradentate ligand and its metal complexes. **E.E. Marlier**, S.A. Brunclik, M.H. Nevins, A. Reuter, C.M. Seong

**11:50 64.** Studies on phosphine ligands containing protic imidazolyl groups for the activation of O-H bonds. **B.E. Silva**, A. Sarbajna, A. Sharma, R.N. Nair, Y. Gong, J. Golen, A.L. Rheingold, D. Grotjahn

**12:10 65.** New tren ligands and the reactivity of their metal complexes. **D.R. Manke**

**12:30 66.** Sterically hindered  $\beta$ -diketones: Synthesis and applications in catalysis. **A.S. Crossman**, M.P. Marshak

<section>

**Future Insights into Syngas Conversion Catalysis: Symposium in honor of Burtron H. Davis**

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<section>

**Advances in Catalysis with Ceria & Other Reducible Oxides Model Ceria Catalyst**

Sponsored by CATL, Cosponsored by ENFL, ENVR, INOR and PHYS

**SUNDAY AFTERNOON**

Section A

Marriott Marquis San Diego  
Marina  
Santa Rosa

**Inorganic Young Investigator Awards**

A. De Bettencourt Dias, *Organizer*,  
*Presiding*

**1:30** Introductory Remarks.

**1:35 67.** Rediscovering the crystal chemistry of higher borides. **G. Akopov**

**2:00 68.** Design and synthesis of heterostructured nanoparticle libraries through sequential cation exchange pathways. **J.L. Fenton**, B.C. Steimle, R.E. Schaak

**2:25 69.** Fundamental lessons in carbon fixation chemistry: Molybdenum-mediated reduction of C<sub>1</sub> oxygenates. **J.A. Buss**, T. Agapie

**2:50 70.** Metal-organic framework functionalization: Toward uniform and tunable heterogeneous catalysts. **P. Ji**, W. Lin  
**3:15** Intermission.

**3:25 71.** Comprehensive nanoscale evaluation of layered materials by X-ray microscopy. **L.R. De Jesus**, S. Banerjee, T.E. Mallouk

**3:50 72.** Following the catalyst wherever she goes: Forays into the fundamental behavior of active, on-cycle intermediates in Ru-catalyzed olefin metathesis. **G.A. Bailey**, D. Fogg

**4:15 73.** Accessing rare metal-ligand multiple bonds of early transition metals: Nucleophilic, electrophilic, and radical reactivity. **L. Grant**, D.J. Mindiola, B. Pinter

**4:40 74.** Understanding and redesigning metallic lithium for next-generation batteries. **Y. Liu**, D. Lin, Y. Lin, G. Chen, A. Pei, Y. Li, Y. Cui

Section B

Marriott Marquis San Diego  
Marina  
Marriott Grand Ballroom Section 9  
**Undergraduate Research at the Frontiers of Inorganic Chemistry**

C. Nataro, N. S. Williams, *Organizers*, *Presiding*

**1:30** Introductory Remarks.

**1:35 75.** Toward the synthesis of unprecedented transition-metal nitride molecules. K.D. Herring, G.X. Monasterio, N. Yamamoto, S.C. Addy, A.R. Sumner, A.M.

Dew, M.P. Nguyen, R.J. Wilson, **L.G. Beauvais**, M. Bennett

**1:55 76.** Cooperative reactivity of a redox-active ditopic diazaborole. **N. Kennedy**, C. Cuthbertson, N. Torquato, D.N. Blauch, M.R. Anstey

**2:15 77.** Syntheses, characterization, and reactivity of cobalt(II) SNS pincer complexes. **J.R. Miecznikowski**, M. Lynn, J. Jasinski, E. Reinheimer, B.Q. Mercado

**2:35 78.** Evaluation of air-free glassware using the ketyl test. **L. Carlson**, E.D. Douma, P.T. Truong, M.A. Bowring

**2:55** Intermission.

**3:10 79.** Ambiphilic phosphine boronates by C(sp<sup>2</sup>)-H and C(sp<sup>3</sup>)-H borylation of a diverse class of tertiary phosphines. **K.C. Morris**, S.E. Wright, H. Eichelberger, S. Richardson-Solorzano, T.B. Clark

**3:30 80.** Synthesis of a phenoxazine-based ligand for redox flow battery electrolytes. **C. Hernandez**, D. Thole, D.N. Blauch, M.R. Anstey

**3:50 81.** Water and alkyl Grignards mix for an effective cobalt-catalyzed Kumada coupling of N-aryl chlorides. **M.C. Perry**

**4:10 82.** Translating lessons learned in the platinum group to base metal complexes featuring sterically-demanding amine bis(phenolate) ligands. **B. Wile**

**4:30** Concluding Remarks.

#### Section C

Marriott Marquis San Diego Marina  
Marina Ballroom Salon F

#### Organometallics Distinguished Author Symposium

P. J. Chirik, *Organizer, Presiding*

**1:30** Introductory Remarks.

**1:35 83.** Functionalizing strong C-H bonds with nonheme Fe<sup>V</sup>=O oxidants, seen and unseen. **L. Que**

**2:10 84.** Efficient CO<sub>2</sub> reduction by bioinspired cobalt aminopyridine complexes. **S.C. Marinescu**

**2:45** Intermission.

**3:00 85.** Logical ligand design of iron-based complexes used as catalysts for Suzuki-Miyaura cross-coupling reactions. **J.A. Byers**, M.P. Crockett, A.S. Wong

**3:35 86.** Metal-metal cooperativity in small molecule activations at

bimetallic reaction centers. **T. Tilley**

#### Section D

Marriott Marquis San Diego Marina  
Rancho Santa Fe 2

#### Chemistry of Materials: Nanomaterials

C. G. Lugmair, *Organizer*  
D. Fairen-Jimenez, *Z. Lin, Presiding*

**1:30 87.** Design of highly porous metal-organic frameworks for drug and gene delivery. C. Orellana, S. Haddad, M. Teplensky, **D. Fairen-Jimenez**

**1:50 88.** Syntheses of phase pure ternary layered chalcogenides of Mo and W. **M.M. Li**, S. Ivanov

**2:10 89.** Solution-processable van der Waals thin film electronics. **Z. Lin**

**2:30 90.** Graphene oxide aerogels as electrically-heatable, 3D frameworks for inorganic adsorbent nanoparticles. **D. Xia**, R. Menzel

**2:50 91.** Examining the effect of nanoscale architecture on the thermal conductivity of mesoporous silica thin films. **S. King**, Y. Yan, M. Li, T. Galy, J.S. Kang, M. Marszewski, Y. Li, L. Pilon, Y. Hu, S.H. Tolbert

**3:10** Intermission.

**3:25 92.** Gold nanobipyramids for noninvasive photothermal killing of bacteria. **C. Yang**, T. Kuo

**3:45 93.** Fluorescent surfactant for real-time visualization and dynamics studies of boron nitride nanomaterials. **A. Smith McWilliams**, Z. Tang, S. Ergülen, C.A. de los Reyes, M. Pasquali, A.A. Marti

**4:05 94.** Improving FePt/FePd nanoparticle synthesis for easier processing of magnetic properties. **J.A. Kurish**, S.H. Tolbert

**4:25 95.** Sharp transition from metallic to non-metallic state in gold nanoclusters with atomically tailored optical properties. **T. Higaki**, M. Zhou, R. Jin

#### Section E

Marriott Marquis San Diego Marina  
Marriott Grand Ballroom Section 8

#### Emerging Research in Molecular Synthesis

A. C. Brewer, J. M. Hoover, V. A. Schmidt, J. Y. Yang, *Organizers*

D. C. Lacy, K. J. Stowers, *Presiding*

**1:30 96.** Enabling base-metal catalysis through metalloligand design. **C.C. Lu**, M. Vollmer, B. Ramirez

**2:00 97.** Catalysis at metal-metal bonds. **C. Uyeda**

**2:30 98.** Copper-carbon interfaces: Highly active catalysts from inorganic-organic hybrid materials. **K.J. Stowers**, C. Nguyen-Sorenson, A.J. Matzger

**3:00** Intermission.

**3:15 99.** Design principles in synthetic non-heme (di)oxygenases. **D.C. Lacy**

**3:45 100.** Copper complexes bearing redox active ligands with tunable H-bonding interactions: Synthesis, structure, and reactivity. **I. Garcia-Bosch**

#### Section F

Marriott Marquis San Diego Marina  
Solana

#### Coordination Chemistry: Characterization & Applications

A. Larsen, *Organizer*  
M. I. Gonzalez, G. Mezei, *Presiding*

**1:30 101.** Tertiary phosphines and bisphosphines appended on N-heterocyclic moieties: Transition metal chemistry and catalytic studies. **M.S. Balakrishna**

**1:50 102.** Nitrogen-rich metal coordination complexes for new applications in explosive initiation. **J.M. Veauthier**

**2:10 103.** Synthesis, characterization, equilibrium, and antibacterial studies of Co(II) complex with 4-Hydroxy-N<sup>2</sup>-(3-hydroxy-5-(hydroxy methyl)-2-methylpyridin-4-yl)methylene)benzohydrazide. **V. Chittireddy**

**2:30 104.** Tuning the anion binding selectivity of nanojars by ligand-shell rigidification and controlled acidification. **G. Mezei**

**2:50 105.** Co<sub>2</sub>(pyrazine-2,3-dicarboxylate)<sub>2</sub>(4,4'-bipyridine) 1D porous coordination materials: Enhanced carbon dioxide adsorption at ambient temperature. **S. Urcia-Romero**, R. Arrieta-Perez, A.J. Hernandez

**3:10** Intermission.

**3:15 106.** Zr/Co early-late heterobimetallic (ELHB) complexes: O<sub>2</sub> activation, CO<sub>2</sub> capture, and beyond. **H. Zhang**, C.M. Thomas

**3:35 107.** Taming the chlorine radical: Controlling the reactivity of photogenerated chlorine-atom complexes for selective C-H activation. **M.I. Gonzalez**, D. Gygi, Y. Qin, K. Xia, L. Kramer, D.G. Nocera

**3:55 108.** Modelling surface dinitrogen coordination with a dicobalt macrocycle. **A. Spentzos**, N.C. Tomson

**4:15 109.** Study of the catalytic activity of formamidate bridged Rh<sub>2</sub>(II,II) complexes as a function of the trans effect across the Rh-Rh bond in the axial position. **A. Millet**, C. Turro, K.R. Dunbar

**4:35 110.** Caught in the act: Capturing C-H bond activation with photocrystallography. **D. Gygi**, M. Gonzalez, K. Xia, S. Hwang, D.G. Nocera

#### Section G

Marriott Marquis San Diego Marina  
Point Loma

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

S. A. Koch, *Organizer*  
T. A. Su, *Presiding*

**1:30 111.** Photophysical evaluation of biologically active strained ruthenium(II) polypyridyl complexes. **R.S. Khnayer**

**1:50 112.** Versatile roles of extracellular vesicles in cancer biology: New fluorophores as novel selective nucleic base stains for cellular microvesicles. **K. Wardhani**, A. Levina, G.E. Grau, F. Keene, J. Collins, P.A. Lay

**2:10 113.** Modular ionophore platform for treating copper deficiency in fatty liver disease. **T.A. Su**, C.J. Chang

**2:30 114.** Supramolecular assembly of uridine monophosphate (UMP) and thymidine monophosphate (TMP) with a dinuclear copper(II) receptor. **M. Rhaman**, D.R. Powell, A. Hossain

**2:50 115.** Interaction of DNA with reduced graphene oxides: Electrochemical oxidation of guanines. **J. Kim**, M. Choi, S. Lee

**3:10** Intermission.  
**3:30 116.** Synthesis and characterization of symmetrical and

unsymmetrical copper(II) bis(terpyridine) complexes: Electrochemical and biological studies. **B. Sengottuvelan**, E. Tamilarasu

**3:50 117.** Dinuclear-ruthenium(II) complexes as binders of human telomeric dimeric G-quadruplexes. **J. Weynand**, **A. Decottignies**, **J. Dejeu**, **E. Defrancq**, **B. Elias**

**4:10 118.** Investigation of rhenium tricarbonyl isonitrile complexes as alternatives to platinum anticancer agents. **A.P. King**, S. Marker, J.J. Wilson

**4:30 119.** Oligo tetrapyrrole complexes as efficient photochemotherapeutic agents with remarkably high phototoxicity indices. A. Potocny, R. Riley, E.S. Day, **J. Rosenthal**

**4:50 120.** Photocytotoxicity of dirhodium (II,II) complexes featuring formamidinate bridging ligands with halogen substitution. **E. Song**, C. Turro, K.R. Dunbar

**5:10 121.** Copper (II) selective chelators attenuate copper-overload induced oxidative stress *in vivo*. **A. Rakshit**, K. Khatua, V. Shanbhag, P. Comba, A. Datta

**5:30 122.** Rhenium isonitrile complexes induce unfolded protein response-mediated apoptosis in cancer cells. **S. Marker**, A.P. King, R. Swanda, J.J. Wilson

Section H

Marriott Marquis San Diego Marina  
Cardiff

### Chemistry of Materials: Metal Organic Frameworks

C. G. Lugmair, *Organizer*

M. L. Aubrey, S. K. Elsaidi, *Presiding*

**1:30 123.** Mixed-metal metal-organic frameworks as multifunctional catalysts. **M. Zaheer**

**1:50 124.** Dual-layer MOF@MOF inorganic membranes with tunable gas transport properties for post-combustion CO<sub>2</sub> separation. **S.K. Elsaidi**, M.H. Mohamed, S. Venna, D. Hopkinson

**2:10 125.** Small and smaller: [Pt<sub>12</sub>]@ZIF-8 releases platinum nanoparticles with exceptional mass activity for oxygen electroreduction. **K. Kratzl**, B. Garlyyev, A. Bandarenka, R. Fischer

**2:30 126.** Highly conductive and stable metal-organic frameworks from sulfur chemistry for electrocatalysis applications. **Z. Xu**

**2:50 127.** Structural flexibility and tunability in heteronuclear actinide-based metal-organic frameworks (MOFs). **O.A. Ejegbavwo**, M.D. Smith, N.B. Shustova

**3:10** Intermission.

**3:25 128.** Harnessing synthetic biology to design novel metal-organic frameworks for photocatalytic oxidation. **J.B. DeCoste**, M.F. Lee, S.J. Garibay, A.M. Ploskonka

**3:45 129.** Sol-gel monolithic metal-organic frameworks with enhanced adsorption properties. T. Tian, B. Connolly, m. Casco, Z. Zeng, J. Tan, J. Silvestre Albero, **D. Fairen-Jimenez**

**4:05 130.** Redox doping and electron hopping in conductive metal-organic frameworks. **M.L. Aubrey**, B. Wiers, S. Andrews, T. Sakurai, S. Reyes-Lillo, S. Hamed, C. Yu, L.E. Darago, J.A. Mason, F. Grandjean, G.J. Long, S. Seki, J. Neaton, P. Yang, J.R. Long, M.I. Gonzalez, K. Pedersen, R. Clerac, J. Oktawiec, M. Kapelewski

**4:25 131.** MOF/polymer interactions in composite materials visualized *in situ* with solid-state NMR. **J. Moreton**, P. Duan, S. Tavares, R. Semino, G. Maurin, S. Cohen, K. Schmidt-Rohr

<section>

### 150 Years of the Periodic Table

Sponsored by HIST, Cosponsored by CINF, INOR<sup>‡</sup> and PRES

<section>

### Future Insights into Syngas Conversion Catalysis:

#### Symposium in honor of Burtron H. Davis

Sponsored by CATL, Cosponsored by ENFL, ENVR, INOR and PHYS

<section>

### Advances in Catalysis with Ceria & Other Reducible Oxides Theory of Ceria Catalysts

Sponsored by CATL, Cosponsored by ENFL, ENVR, INOR and PHYS

### SUNDAY EVENING

Section A

Placeholder

### Learning from Nature: Earth-Abundant Metals for Oxidation Catalysis

S. S. David, T. A. Jackson, A. Mukherjee, *Organizers*

#### 5:30 - 7:30

**132.** Synthetic model for “diamond” core intermediates in nonheme diiron enzymes. **S. Banerjee**, W. Rasheed, L. Que

**133.** Mechanism of olefin *cis*-dihydroxylation catalyzed by a bio-inspired non-heme iron complex. **J. Chae**, S. Xu, L. Que

**134.** Stabilizing reactive nonheme oxoiron(IV) complexes supported by a common pentadentate ligand framework. C. Abelson, W. Rasheed, **L. Que**

**135.** High-valent gold-hydroxo complex capable of O-H and C-H bond oxidation. **M. Lovisari**, A. McDonald

**136.** X-ray absorption spectroscopy for elucidating the structure of high-valent nonheme iron complexes. **P. Crossland**, S. Banerjee, W. Rasheed, L. Que

**137.** Characterization of peroxoiron(III)(TMC) complexes. **W. Ching**, L. Que

**138.** Peeking into how aromatic hydroxylation reactions are performed by synthetic Fe<sup>IV</sup>(O) complexes. **Y. Sheng**, A. Darksharapu, J. Prakash, L. Que

**139.** Probing internal motion of Zn(II) bispicen complexes via NMR relaxometry. **T. Jones**, A. Mukherjee

**140.** To rebound or not in hydrogen atom transfer reactions by synthetic nonheme oxoiron(IV) complexes. **S. Xu**, T. Jo, W. Rasheed, J.E. Klein, L. Que

**141.** Characterization and reactivity of [Fe<sup>IV</sup>O(TPA)(L)] and [Fe<sup>IV</sup>O(TQA)(L)]: Influence of the L ligand. **G.L. Tripodi**, J. Roithová

Section B

Placeholder

### Undergraduate Research at the Frontiers of Inorganic Chemistry

C. Nataro, N. S. Williams, *Organizers*

#### 5:30 - 7:30

**142.** VIPER: Community and content for the inorganic classroom. N.S. Williams, C.

**Nataro**, A.K. Bentley, H.J. Eppley, E.R. Jamieson, S. Lin, A.R. Johnson, J.M. Pratt, J.R. Raker, B.A. Reisner, S.R. Smith, J.L. Stewart, L.A. Watson

**143.** Group 13 complexes of 4,6-dihydroxy-10-phenylphenoxazine. **E. Warner**, C. Hernandez, D. Thole, D.N. Blauch, M.R. Anstey

**144.** Suzuki coupling catalyzed by (8-(dimesitylboryl)quinoline)palladium(0) species: Theoretical analysis. **H.S. Rust**, A.J. Achazi, P. Miro

**145.** Synthesis of nickel nitrosyl complexes with bidentate N-heterocyclic carbene ligands. **Z. Zhang**, S.E. Stieber

**146.** Heteroatom pendant bases for ruthenium catalyzed water oxidation. **B.D. Vincenzini**, A.G. Nash, C.J. Breyer, B.E. Silva, D.B. Grotjahn

**147.** Stability of molecular-electrode conjugates in acids and bases. **S.K. Spence**, L. Hallett, S.M. Kilyanek

**148.** Synthesis and characterization of metal-organic framework hydrogel composites. **S. Klein**, L. Zarzar, Y. Liu

**149.** Unique crystalline composites displaying multiple primary zoning events in the solid state and based upon self-assembled coordination polymers: Summary of results. **S.R. Seidel**, A. Zamurd, S. Cornell, K. Godwin, A. Partelow

**150.** Investigation of strontium doped hydroxyapatite coating methods for iron oxide nanoparticles. **C.E. Chamberlain**, K. Libson, A. Washburn, A.L. Eckermann

**151.** Tuning magnetic coupling in organic radical-bridged lanthanide single molecule magnets. **E. Mu**, C. Gould, J.R. Long

**152.** Optimization of light-driven P450 biocatalysts featuring Ru(II)-polypyridine complexes. **B. Foley**, **M. Nguyen**, M. Kato, L.E. Cheruzel

**153.** Synthesis of a gallium metallocavitand nanoparticle for bacterial inhibition. **B.M. Forry**, W.D. Shafer

Section C

Placeholder

### Electrochemistry

N. S. Radu, *Organizer*

5:30 - 7:30

**154.** Electrochemical behaviors of MnBr(CO)<sub>3</sub>bpyCOOH in aqueous solution. **D. Zheng**, L. Sepunaru, P.C. Ford

**155.** Reversible Na-capacity of magnesium-reduced graphitic carbon nitride. B.D. Fahlman, **A.S. Adeyemi**

**156.** Reversible Li- and Na-capacities of BaTiO<sub>3</sub>/p-Si/g-C<sub>3</sub>N<sub>4</sub> nanocomposites. B.D. Fahlman, **M.L. Anger**

**157.** Proton-coupled electrochemistry of catechol-based redox active deep eutectic solvents. **H. Booth**, J.C. Goeltz

**158.** High concentrations of electroactive TEMPOL in various ionic melts. **J.M. Carter**, J.C. Goeltz

Section D

Placeholder

### Emerging Research in Molecular Synthesis

N. S. Radu, *Organizer*

5:30 - 7:30

**159.** Synthesis of cyclopropanes using nickel-catalyzed cross-electrophile coupling reactions. **A. Castro**, E. Lucas, K.A. Hewitt, E.R. Jarvo

**160.** Measuring the influence of metal ion on hydrogen atom reactivity in a series of group 10 complexes with a proton and redox non-innocent ligand. **B. Charette**, A.F. Heyduk

**161.** Probing promoter effects in E selective alkyne semi-hydrogenation. **S. Desai**, J. Ye, T. Islamoglu, O.K. Farha, D.G. Truhlar, C.C. Lu

**162.** Development of molecular electrocatalyst for CO<sub>2</sub> reduction based on nitrogen-based macrocyclic ligands. **L. Lieske**, C.W. Machan

**163.** Electrocatalytic reduction of dioxygen to hydrogen peroxide by a molecular manganese complex with a bipyridine-containing Schiff base ligand. **S.L. Hooe**, A.L. Rheingold, C.W. Machan, D. Dickie

**164.** Electrocatalytic CO<sub>2</sub> reduction with Fe(III) Schiff base-type complexes containing pendent proton relays. **A. Nichols**, S. Hooe, C.W. Machan

Section E

Placeholder

### Inorganic Catalysts

S. A. Koch, *Organizer*

5:30 - 7:30

**165.** Homogeneous reduction of atmospheric carbon dioxide by a neutral zinc complex. **S. Cronin**, m. mashuta, M.J. Shaw, R. Buchanan, C.A. Grapperhaus

**166.** Product and active site studies of biocatalytic copper-based metal-organic frameworks. **R. Tuttle**, H. Rubin, C. Rithner, R.G. Finke, M.M. Reynolds

**167.** Synthesis of air-stable ruthenium and nickel catalysts. **S. Phuangthong**, J.P. Lanorio

**168.** Modification of inorganic catalysts' ligand frameworks for connection to polymeric structures. **V.C. Tafuri**, D. Navarro, H. Ordon, M.R. Radlauer

**169.** Toward (Z)-alkene isomerization. **E. Delgado**, E.R. Paulson, A.L. Rheingold, D.B. Grotjahn

**170.** Computational study of the pKa of transition metal-methyl C-H bonds. **W.M. Grumbles**, T.R. Cundari

**171.** Niobium-doped TiO<sub>2</sub>: Effect of an interstitial oxygen atom on charge state of niobium. **X. Liu**

**172.** Catalytic properties of lanthanum phosphates. **M. Albqmi**, A.W. Apblett

**173.** Seed-induced synthesis of functional MFI zeolite materials: Method, mechanism, and catalytic property. **H. Zhang**, Z. Ye, Y. Tang

**174.** Alkali metal-doped series of Linde-Type L zeolites via hydrothermal processes. **Y. Koh**, W.D. Shafer

**175.** Transition metal dichalcogenides as heterogeneous catalysts for the hydrogenation of nitroarenes. **A. Darling**, Y. Sun, R.E. Schaak

**176.** Exploring salen ligand type inspired from purple-acid phosphatase towards catalyzing pesticides hydrolysis with zinc complexes. **M.M. Allard**, N.T. Le

**177.** Zr- and Hf-based polyhedral oligomeric silsesquioxanes (POSS) as thermally robust catalysts in the Meerwein-Ponndorf-Verley reduction. **S. Garg**, C. Krempner

**178.** Molecular catalysts for CO<sub>2</sub> reduction to CO. **A. Zhanaidarova**, C.P. Kubiak

**179.** Ferrocene-chelating heteroscorpionate complexes in catalysis. **N. Adhmi**

**180.** Photophysical properties of rhenium(i) diimine dicarbonyl complexes containing phenanthroline and bipyridine ligands. **H. Atallah**, F.N. Castellano, C.M. Taliaferro

**181.** Solid-state NMR and density functional theory approaches for the elucidation of structure for inorganic complexes. **W. Huynh**, D. Culver, M.P. Conley

Section F

Placeholder

### Chemistry of Materials

C. G. Lugmair, *Organizer*

5:30 - 7:30

**182.** Hydrothermal crystal growth and characterization of rare earth rhenium and tungsten oxides. **M.T. Kolambage**, C.D. McMillen, J.W. Kolis

**183.** Generalizable top-down nanostructuring method of bulk oxides: Sequential oxygen-nitrogen exchange reaction. **H. Kim**, J. Bang

**184.** Incorporating excess lithium into LiMn<sub>2</sub>O<sub>4</sub> via thermally induced grain fining: Promoted lithium-ion diffusion in Li-excess LiMn<sub>2</sub>O<sub>4</sub>. **G. Lee**, J. Bang

**185.** Highly conductive and stretchable nanocomposite using Ag-Au core-shell nanowires: Applications in wearable and implantable devices. **S. Han**, T. Hyeon

**186.** Two polymorphs of 4,4',5,5'-tetraamino-3,3'-bi-1,2,4-triazolium dinitroformate and their energetic properties. **Y. Xu**, M. Lu

**187.** Solid-phase detoxification of chemical warfare agents using zirconium-based metal organic frameworks and the moisture effects—analyze via digestion. **H. Wang**, J.J. Mahle, T.M. Tovar, G.W. Peterson, M.G. Hall, J.B. DeCoste, J. Buchanan, C.J. Karwacki

**188.** Synthesis and electrochromic properties of morphology-controlled vanadium dioxide nanoparticles. **D. Roh**

**189.** Single-component frameworks for heterogeneous catalytic

hydrolysis of organophosphates in pure water. **S. Garibay**, O.K. Farha, J.B. DeCoste

**190.** Defect-free MOF-based mixed matrix membranes obtained by corona crosslinking. **Y. Katayama**, K.C. Bentz, S. Cohen

**191.** Heterometallic multinuclear metal-organic frameworks. **O.A. Ejegbavwo**, N.B. Shustova

**192.** Sierpinski molecules, carbon schwarzites and porous materials for catalytic and electronic applications. **Z. Xu**

**193.** Hybrid polymer/inorganic nanoparticle composite nanofibers through cooperative non-covalent interactions. **L. Meng**, Y. Qin

**194.** Charge-separated metal-organic frameworks: Design and application. **S. Thapa**, Y. Qin

**195.** Exploring O<sub>2</sub> adsorption in cobalt triazolate frameworks. **J. Oktawiec**, H.Z. Jiang, J. Vitillo, D. Reed, L.E. Darago, B.A. Trump, V. Bernales, H. Li, K. Colwell, H. Furukawa, C.M. Brown, L. Gagliardi, J.R. Long

**196.** Chemical vapour deposition of zinc oxysulfide for photovoltaics. **M.A. Bhide**, C.J. Carmalt, C.E. Knapp

**197.** Montmorillonite synthesized from natural bentonite. **S. Seo**, J. Kim

**198.** Effect of heavy atom on the photophysics of porphyrin coordination complexes. **A. Aggarwal**, C. Farley, C.M. Drain

**199.** Improving PbS QD SWIR photodetectors using thermal annealing. **J. Jin**, **G. Hwang**

**200.** Development of the facile ITO coating method on flexible substrates using PDMS (polydimethylsiloxane) nanostructures and the spin-coating approaches. **H. Seo**, S. Sul, S. Lee, S. Chae, J. Jung

**201.** Seeded growth of metal nitrides on noble metal nanoparticles to form complex nanoscale heterostructures. **R.W. Lord**, C.F. Holder, J.L. Fenton, R.E. Schaak

**202.** Selective post-synthetic modification of copper sulfide regions in heterostructured nanoparticles. **A.G. Butterfield**, B.C. Steimle, R.E. Schaak

**203.** Synthesis, structures and properties of some recently characterized borates. **D. Neiner**, Y. Sevryugina, D.M. Schubert

**204.** Engineering metastable precursors of two-dimensional MBenes. **L. Alameda**, R.E. Schaak

**205.** Novel electrospun Ti<sub>3</sub>C<sub>2</sub>Tx MXene titania nanocomposites. **S. Debow**, **B.G. DeLacy**, W.R. Creasy, Y. Gogotsi, K. Maleski, D. Kuhn, Z. Zachary

**206.** Nanoballs featuring Lewis acidic and basic sites as efficient bifunctional catalysts for tandem deacetalization-Knoevenagel reaction. **G. Verma**, S. Kumar, Z. Niu, W. Gao, L. Wojtas, S. Ma

**207.** New crystalline porous materials and their gas sorption properties. **X. Bu**, H. Yang, P. Feng

Section G

Placeholder

### Organometallic Chemistry: Catalysis

N. S. Radu, *Organizer*

5:30 - 7:30

**208.** DFT study of double bond cleavage induced by silyl migration in Fe complex. **N. Koga**, A.A. Dahy

**209.** Computational study of methane C-H activation by main group and mixed main group-transition metal complexes. **C. Carter**, **T.R. Cundari**

**210.** Colloidal DMF-protected metal nanoparticles for their use as catalyst in organic transformations. **Y. Obora**

**211.** Indium and yttrium alkoxide catalysts for redox switchable ring opening polymerization. **S. Deng**, P. Diaconescu

**212.** Phosphines on sulfated zirconia: Probes for Brønsted acidity and precursors to catalytically active olefin polymerization sites. **J.E. Rodriguez**, M.P. Conley

**213.** Manganese-catalyzed transfer hydrogenation of nitriles with secondary alcohols as the hydrogen source. **J.A. Garduno**, J.J. Garcia

**214.** Incorporating iridium pincer complexes in polymeric scaffolds for site-isolated catalytic alkane dehydrogenation. **J. Hickey**, T.Z. Myint, M.R. Radlauer

**215.** High efficient pincer oxo-rhenium catalyst for hydrosilylation. **M. Xiong**, M. Abu-Omar

**216.** Bioinspired trimetallic cobalt triphenylenehexathiol complex for

CO<sub>2</sub> reduction reaction. **J. Intrator**, N.M. Orchanian, A.J. Clough, S.C. Marinescu

Section H

Placeholder

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

N. S. Radu, *Organizer*

5:30 - 7:30

**217.** Incorporation of functionalized rhenium(I) bipyridine catalysts into polycarbonates via chain transfer chemistry. **G. Bhat**, T.M. Folsom, A.Z. Rashad, D.J. Darensbourg

**218.** Synthesis and chemical vapour deposition of precursors to zinc oxysulfide. **M.A. Bhide**, C.J. Carmalt, C.E. Knapp

Section I

Placeholder

### Bioinorganic Chemistry

S. A. Koch, *Organizer*

5:30 - 7:30

**219.** Better resolution of hyperfine lines for high-spin cobalt at low frequency, L-band: [Co(D4)(dca)]. **S. Hernández-Anzaldo**, A.K. Girón Moreno, Y. Reyes-Ortega, **W.E. Antholine**

**220.** Interplay of folding, reduction potential, and tryptophan fluorescence in azurin variants. **N.J. McCormick**, A. Cembran, S.M. Berry

**221.** Oxidation of phenols by redox-active copper complexes with tunable hydrogen bonding donor groups. **K. Rajabimoghadam**, I. Garcia-Bosch

**222.** Metal oximate and amidoximate complexes for the catalytic cleavage of carboxylic and phosphate esters. **E. Alpizar-Juárez**, **P. Gomez-Tagle**

**223.** Diastereomeric suite of triscatecholate siderophores: Origin and physiological relevance of Fe(III)-complex chirality. **P. Stow**, Z. Reitz, E. Thomsen, A. Butler

**224.** Reactive intermediates in multicopper oxidase catalysis. **J. Shin**, J.R. Winkler, H.B. Gray

**225.** Combined molecular dynamics and quantum mechanical/molecular mechanical

studies on histone demethylation by KDM4A enzymes. **R. Ramanan**, S.S. Chaturvedi, T. Karabencheva-Christova, C. Christov

**226.** Influence of ligand structure and stereochemistry on the photoreactivity of Fe(III)-siderophore complexes containing  $\beta$ -hydroxyaspartic acid. **C.D. Hardy**, J. Suk, A. Butler

**227.** Computational insights into catalytic mechanism of N $\epsilon$ -methyl lysine demethylation by PHF8. **S.S. Chaturvedi**, R. Ramanan, T. Karabencheva-Christova, C. Christov

**228.** Exploring the mechanism of DNA repair by ALKBH2 enzyme: Multilevel modeling study. **S.O. Waheed**, R. Ramanan, C. Christov, T. Karabencheva-Christova

**229.** Long wavelength light induced CO-release from binuclear rhenium-manganese carbonyl complex. **X. Jiang**, **J. Barrett**, **P.C. Ford**

**230.** Application of graphene quantum dots for NIR light triggered intracellular release of nitric oxide. **C. Guzman**, P. Huang

## MONDAY MORNING

Section A

Marriott Marquis San Diego Marina  
Marina Ballroom Salon F

### ACS Award in Pure Chemistry: Symposium in Honor of Danna Freedman

H. Karunadasa, J. Zadrozny, *Organizers*, *Presiding*

8:30 Introductory Remarks.

8:35 **231.** Platform-based surface ligands for inorganic nanocrystals. **J.A. Mason**, G. Stec, S. Thapa, J. Lee

9:00 **232.** Organic mixed-valency across a five charge states of group 13 complexes. **A. Arnold**, R. Saylor, D. Britt, T. Bass, **L.A. Berben**

9:25 **233.** Chalcogenide based coordination polymers. **J.S. Anderson**, J. Xie, N. Horwitz

9:50 Intermission.  
10:05 **234.** Stibonium cations as Z-type ligands for late transition metals: Impact on catalytic properties. **F.P. Gabbai**

10:30 **235.** Efficient single molecule dirhodium photocatalyst

for H<sub>2</sub> generation using low energy visible to near-IR light. **T.J. Whittemore**, C. Xue, **C. Turro**  
10:55 **236.** Metal semiquinoid magnets: From molecules to materials. **L. Liu**, J. DeGayner, B. Coleman, Y. Wang, A.E. Thorarinsdottir, I. Jeon, **D. Harris**  
11:20 **237.** Nickel-catalyzed coupling promoted by substrate photoexcitation. **J.A. Kalow**  
11:45 Concluding Remarks.

Section B

Marriott Marquis San Diego Marina  
Marriott Grand Ballroom Section 9  
**Learning from Nature: Earth-Abundant Metals for Oxidation Catalysis**

Financially supported by INOR  
S. S. David, A. Mukherjee, *Organizers*  
T. A. Jackson, *Organizer*, *Presiding*

8:30 **238.** Molecular catalysts for water oxidation using first-row transition metals. **G.W. Brudvig**, K.J. Fisher, H.M. Lant, T. Michaelos, L.S. Sharninghausen, R.H. Crabtree

9:00 **239.** *Operando* X-ray spectroscopic studies of heterogeneous water oxidation catalysts. **S. DeBeer**

9:30 **240.** Molecular complexity in inorganic chemistry: Utilizing non-covalent interactions into the molecular designs of metal complexes. **A. Borovik**

10:00 Intermission.

10:10 **241.** Mechanistic and structural analysis of how nonheme-iron enzymes direct different oxidation reactions. **J.M. Bollinger**, A. Boal, C. Krebs, A. Silakov

10:40 **242.** Oxygen intermediates in Cu and Fe zeolites: Correlations to metalloenzymes. **E.I. Solomon**, B.E. Snyder, H.M. Rhoda

11:10 **243.** MUTYH & its metal cofactors: Mitigating menacing mutations and mediating DNA damage responses. **S.S. David**

Section C

Marriott Marquis San Diego Marina  
Solana

### Inorganic Chemistry Lectureship

W. B. Tolman, *Organizer*,

*Presiding*

**8:30** Introductory Remarks.

**8:35 244.** Gold (I) anticancer agents: Building blocks for the synthesis of bimetallic compounds, bioconjugates and nanocarrier payloads. Preclinical studies. **M. Contel**

**9:05 245.** Nanoparticles and polymer-based nanozymes: Harnessing the power of transition metal catalysis for bioorthogonal chemistry. **V.M. Rotello**

**9:35 246.** Iridium luminescent gold nanoparticles in bioimaging and detection. S. King, S. Claire, I. Theofilou, T. Chauhan, R. Bicknell, S. Botchway, P. Murray, **Z. Pikramenou**

**10:05** Intermission.

**10:20 247.** Radiometal-based radiopharmaceuticals for cancer imaging. **J. Lewis**

**10:50 248.** Metallo-supramolecular DNA and RNA recognition combined with nanoscience to achieve bioactivity. **M.J. Hannon**

**11:20 249.** Unveiling the beauty of gold for biomedical applications: From molecular to supramolecular inorganic chemistry. **A. Casini**

**11:50** Concluding Remarks.

Section D

Marriott Marquis San Diego Marina  
Rancho Santa Fe 2

**Inorganic Chemistry for Sustainable Energy & Environment**

L. A. Berben, *Organizer*  
C. P. Kubiak, *Presiding*

**8:30 250.** Fractionation of biomass and upgrading of lignin and cellulose streams. **M.M. Abu-Omar**, J. Truong, R. Nishide, B. Liu, S. Zhao

**9:00 251.** Approaches to the synthesis of weak chemical bonds and application to the synthesis and oxidation of ammonia. **P.J. Chirik**

**9:30 252.** Molecular control of interfacial energy catalysis. M. Jackson, C.J. Kaminsky, S. Oh, M. Pegis, J. Rosenberg, P. Smith, **Y. Surendranath**

**10:00** Intermission.

**10:20 253.** Nitrate-mediated photooxidation of alcohols on CdS nanowires. **B.M. Bartlett**

**10:50 254.** Managing reactivity of hydrides in CO<sub>2</sub> reduction to formate. **L.A. Berben**

**11:20 255.** Carbon dioxide mineralization: Strategy for the provision of building materials, and for carbon management globally. **G.N. Sant**, E. Callagon La Plante, D. Jassby, M. Bauchy, D. Simonetti

Section E

Marriott Marquis San Diego Marina  
Santa Rosa

**Emerging Research in Molecular Synthesis**

A. C. Brewer, J. M. Hoover, V. A. Schmidt, J. Y. Yang, *Organizers*  
M. Dai, C. Roberts, *Presiding*

**8:30 256.** Nickel-catalyzed stereospecific cross-coupling and cross-electrophile coupling reactions. **E.R. Jarvo**

**9:00 257.** Understanding the mechanism of nickel catalyzed cross-coupling and cross-electrophile coupling reactions. **N. Hazari**

**9:30 258.** Using first row transition metals for challenging bond breaking and forming reactions. **C. Roberts**, M.S. Sanford

**10:00** Intermission.

**10:15 259.** Building structural complexity via novel palladium-catalyzed carbonylative reactions. **M. Dai**

**10:45 260.** Novel pyridine-modified 12-membered pyridinophane ligands control iron catalyzed C-C coupling reactivity. **K.N. Green**, M. Mekhail, A. Yepremyan

Section F

Marriott Marquis San Diego Marina  
Marriott Grand Ballroom Section 8  
**Electrochemistry**

N. S. Radu, *Organizer*  
J. C. Goeltz, J. A. Maurer, *Presiding*

**8:30 261.** Unique interfacial thermodynamics of few-layer 2D MoS<sub>2</sub> for (photo)electrochemical catalysis. **M. Carroll**

**8:50 262.** Mechanism of copper dissolution by nitric acid: Unraveling a century of hypotheses. **R. Carlson**, P. Yang, S.M. Clegg, E.R. Batista

**9:10 263.** Core-shell structured zero-valent manganese (ZVM)-sulfur nanohybrid materials for superior performance supercapacitor. K. Jena, **S. Al Hassan**

**9:30 264.** Immobilization of a molecular proton reduction catalyst onto high-surface area silicon photoelectrodes. **C. Hanna**, N.R. Neale, J.Y. Yang

**9:50 265.** Proton-coupled and proton-independent redox active deep eutectic solvents. **J.C. Goeltz**

**10:10 266.** High voltage redox flow batteries: Shattering the kinetic stability window of aqueous electrolyte. **M.P. Marshak**, B.H. Robb, J.M. Farrell

**10:30 267.** *In situ* nanostructuring and stabilization of polycrystalline copper electrodes with organic salt additives promotes CO<sub>2</sub> reduction to ethylene. **A. Thevenon**, A. Rosas-Hernández, J. Peters, T. Agapie

**10:50 268.** Effects of solution pH and film thickness on electrocatalytic CO<sub>2</sub> reduction activity by polymer encapsulated cobalt phthalocyanine. **T. Soucy**, C.C. McCrory

**11:10 269.** Electrodeposition of refractory metals from deep eutectic solvents. **J.A. Maurer**

**11:30 270.** Fine tuning HER and CO<sub>2</sub>RR reaction dynamics via co-substrate addition to Fe tetraphenyl porphyrin. **C.G. Margarit**, C. Costentin, D.G. Nocera

**11:50 271.** Electrochemical and electrocatalytic analysis of Ru(II) complexes with redox-active S<sub>2</sub>N<sub>2</sub> ligands: Applications towards CO<sub>2</sub> reduction. **J.A. Luna**, K.D. Spielvogel, S.M. Loria, F.B. Evans, L.P. Weisburn, G. Durgaprasad, J.M. Keith, M.R. Ringenberg, S.K. Shaw, S.R. Daly

Section G

Marriott Marquis San Diego Marina  
Point Loma

**Organometallic Chemistry: Catalysis - Late Transition Metals**

N. S. Radu, *Organizer*

**8:30 272.** Proton coupled electron transfer by a gold(III)-hydroxide complex. **M. Lovisari**, A. McDonald

**8:50 273.** Nickel-mediated activation of N-H and O-H bonds. **P. Zhao**, S. Acharya, R.S. Manan

**9:10 274.** Nickel-catalyzed cross-electrophile coupling reaction of mesylates for cyclopropane synthesis. **T.A. Thane**, A. Sanford, T. McGinnis, E.R. Jarvo

**9:30 275.** Robust and efficient iridium catalysts having pyridylpyrazole ligands for dehydrogenation of formic acid. **Y. Himeda**, N. Onishi, R. Kanega, E. Fujita

**9:50 276.** New catalytic route to dehydrogenate alkanes by PCP-pincer iridium complexes using proton and electron acceptors. **A. Shada**, A.S. Goldman

**10:10 277.** Alkyne hydroarylations catalyzed by low-valent, co complexes: Mechanism and catalysis. **B.A. Suslick**, T. Tilley

**10:30 278.** Olefin hydroarylation catalyzed by palladium(II) catalysts: Investigation of the reaction selectivity and comparison with Rh catalysts. **X. Jia**, A. Foley, W. Zhu, B.A. Vaughan, B.A. McKeown, T.B. Gunnoe

**10:50 279.** Chemical innovation at heraeus precious metals: Case studies of process and performance improvements from product development. **P.B. Kettler**, R. Walter, P. Walter, M. Gock

**11:10 280.** Observation of a photogenerated nitrenoid intermediates in C-H amination. **D.C. Powers**

**11:30 281.** Environmentally friendly rhodium(I) model catalysts. Z.G. Morerwa, A. Roodt, **G.J. Venter**

Section H

Marriott Marquis San Diego Marina  
Cardiff

**Coordination Chemistry: Synthesis & Characterization**

A. Larsen, *Organizer*  
J. England, K. V. Waynant, *Presiding*

**8:30 282.** Bio-inspired approach to ligand design: Folding single-chain peptoids to chelate a multimetallic cluster. **A.I. Nguyen**, R.K. Spencer, R.N. Zuckermann

**8:50 283.** Structure study of uranyl bisphosphonate-based ligands as potential uranium decorporation agents. **G. Ye**

**9:10 284.** Electron transfer studies of tris(*N*-arylacetamide) metal complexes. **A.F. Cannella**, D.C. Lacy

**9:30 285.** Building a better understanding of binding in redox-active arylazothioformamide ligand systems. **K.V. Waynant**, J. Moberly, M.F. Roll, K.L. Gutman, V. Groner

**9:50 286.** Tetranuclear transition metal clusters with direct metal-metal interactions: Synthesis, electronic structure, and magnetism. **K. Chakarawet**, J. Marbey, S. Hill, J.R. Long

**10:10** Intermission.

**10:15 287.** Carbodicarbene ligand redox noninnocence in highly oxidized first-row transition metal complexes. **J. England**

**10:35 288.** Synthesis and characterization of homobimetallic redox-active macrocycle transition metal complexes with increasing pocket size. **L.M. Thierer**, P. Cui, S. Brooks, Q. Wang, S. Zhang, M. Gau, B. Manor, P. Carroll, N.C. Tomson

**10:55 289.** Tuning properties of coordination cages via ligand functionalization. **G.A. Taggart**

**11:15 290.** Linear cobalt(II) dialkyl complex with a non-Aufbau ground state and very large magnetic anisotropy. **P. Bunting**, M. Atanasov, E. Damgaard-Møller, M. Perfetti, I. Crassee, M. Orlita, J. Overgaard, J. van Slageren, F. Neese, J.R. Long

**11:35 291.** Spectroscopic and photochemical investigations of a thiolate-bridged dinuclear Rh(II,II) complex featuring reversible redox events. **R.P. Coll**, B.S. Dolinar, K.R. Dunbar

<section>

**150 Years of the Periodic Table**  
Sponsored by HIST, Cosponsored by CINF, INOR<sup>2</sup> and PRES

<section>

**Advances in Catalysis with Ceria & Other Reducible Oxides**

**Reactions of Ceria Catalysts**

Sponsored by CATL, Cosponsored by ENFL, ENVR, INOR and PHYS

**MONDAY AFTERNOON**

Section A

Marriott Marquis San Diego Marina  
Marina Ballroom Salon F

**ACS Award in Pure Chemistry: Symposium in Honor of Danna Freedman**

H. Karunadasa, J. Zadrozny, *Organizers, Presiding*

**1:30** Introductory Remarks.

**1:35 292.** Lanthanide-based single-molecule magnets with high blocking temperatures. C. Gould, P. Bunting, A. Vincent, S. Demir, K.R. McClain, L. Darago, K. Chakarawet, M. Gonzalez, K.R. Meihaus, J. Zadrozny, M. Nippe, J.D. Rinehart, S. Teat, B.G. Harvey, W.J. Evans, **J.R. Long**

**2:00 293.** Control of magnetic relaxation via spin bath design. **J. Zadrozny**

**2:25 294.** Halide perovskites under pressure. A. Jaffe, Y. Lin, W. Mao, **H. Karunadasa**

**2:50 295.** Developing a mild and modular route to chemically modified electrodes for photoelectrochemical cells. C. Hanna, **J.Y. Yang**

**3:15** Intermission.

**3:30 296.** Tunable metal oxide materials via assembly of [NaP<sub>3</sub>W<sub>30</sub>O<sub>110</sub>]<sup>14-</sup>. **A.M. Schimpf**

**3:55 297.** Making flexible, transparent electronic devices a reality: Organic polymers, heterojunctions, oxides and beyond. **T.J. Marks**

**4:20 298.** On the selectivity of the reduction of CO<sub>2</sub> on gold electrodes. **D.G. Nocera**

**4:45** Concluding Remarks.

Section B

Marriott Marquis San Diego Marina  
Marriott Grand Ballroom Section 9  
**Learning from Nature: Earth-Abundant Metals for Oxidation Catalysis**

S. S. David, T. A. Jackson, *Organizers*  
A. Mukherjee, *Organizer, Presiding*

**1:30 299.** New insights into oxidation catalysis with copper. **M.T. Kieber-Emmons**, D. Ramirez, P. VanNatta, G. Ali, A. Velarde

**1:55 300.** Geometric and electronic structure contributions to reactivity of Mn–oxygen intermediates. **T.A. Jackson**, J. Parham, M. Denler

**2:20 301.** Copper(I)-dioxygen adduct stabilization and substrate oxidative reactivity. **K.D. Karlin**

**2:50 302.** Reactivity of an alkyl thiolate-ligated Fe<sup>III</sup>-superoxo intermediate derived from dioxygen. **J. Kovacs**, M.N. Blakely, M.A. Dedushko, P. Poon, A. Downing, D. Rogers, P. Gannon

**3:20** Intermission.

**3:30 303.** Going a step beyond nature: Catalyzing aldehyde deformylation with a non-enzymatic metal. **C.R. Goldsmith**, A.C. Saunders

**3:55 304.** Intermediates in aromatic hydroxylation catalyzed by a Rieske monooxygenase. M.S. Rogers, **J.D. Lipscomb**

**4:25 305.** Differentiating between radical rebound hydroxylation versus H-atom transfer with non-heme iron(III)-hydroxo complexes. **A.R. Fout**, M.J. Drummond

**4:50 306.** Site and enantioselective C–H oxidations inspired in nature. M. Milan, M. Scianfanelli, A. Palone, G. Olivo, X. Ribas, M. Bietti, **M. Costas**

**5:20 307.** Cu-promoted hydroxylation of sp<sup>2</sup> and sp<sup>3</sup> C–H bonds: From enzyme modeling to synthetic applications. **I. Garcia-Bosch**

Section C

Marriott Marquis San Diego Marina  
Solana

**Inorganic Nanoscience Award Symposium**

J. Millstone, *Organizer, Presiding*

**1:30 308.** Plasmonic metal oxide nanocrystals. **D.J. Milliron**

**2:15 309.** Details of ligands on nanocrystal surfaces. **C.J. Murphy**

**2:45 310.** Inverse design of interactions for assembly. **T. Truskett**

**3:15 311.** Exploiting interfacial assemblies of nanoparticle surfactants to design reconfigurable materials and devices. **B. Helms**, W. Feng, J. Forth, T.P. Russell

**3:45** Intermission.

**4:00 312.** Prospects and challenges for unity quantum yield nanocrystal lumophores. **P. Alivisatos**

**4:30 313.** Synthesis of multi-component nanocrystals and their application as catalysts to store energy in chemicals. **R. Buonsanti**

**5:00 314.** Dopants and defects in colloidal semiconductor nanocrystals. **D.R. Gamelin**

Section D

Marriott Marquis San Diego Marina  
Rancho Santa Fe 2

**Inorganic Chemistry for Sustainable Energy & Environment**

L. A. Berben, *Organizer, Presiding*

**1:30 315.** Selective reduction of CO<sub>2</sub> to water by molecular catalysts attached to carbon surfaces. **C.P. Kubiak**, A. Zhanaidarova

**2:00 316.** Sustainable and renewable carbon and nitrogen cycles for fuel and crop production. **D.G. Nocera**

**2:30 317.** Advances and research challenges in chemical and materials research for renewable energy conversion, storage, and utilization. **W. Tumas**

**3:00** Intermission.

**3:20 318.** Mechanisms for the activation of supported oxometal complexes for olefin metathesis. **S.L. Scott**, F. Zhang, L. Li, C. Vandervelden, B. Peters

**3:50 319.** Conductive metal-organic frameworks for electrocatalytic H<sub>2</sub> evolution. **S.C. Marinescu**

**4:20 320.** Mechanistic studies of technologically-relevant dye-sensitized and cocatalyst-containing photocatalytic materials. J.M. Cardon, W. Gaieck, K. Tkaczibson, N. Farhang, S. Keene, S. Luo, H. Chen, **S. Ardo**

**4:50 321.** Controlling the electrocatalytic reduction of O<sub>2</sub> to H<sub>2</sub>O/H<sub>2</sub>O<sub>2</sub> using nontraditional porphyrinoid scaffolds. Q. Cai, J. Eddy, T. Qiu, **J. Rosenthal**

Section E

Marriott Marquis San Diego Marina  
Santa Rosa

**Emerging Research in Molecular Synthesis**

A. C. Brewer, V. A. Schmidt, J. Y. Yang, *Organizers*  
J. M. Hoover, *Organizer, Presiding*  
I. Tonks, *Presiding*

**1:30 322.** Cross-electrophile coupling to form Csp<sup>3</sup>-Csp<sup>2</sup>bonds. **D.J. Weix**

**2:00 323.** Cross-coupling with three components and in three dimensions. **K.M. Engle**

**2:30 324.** Unraveling the mechanism of catalytic decarboxylative coupling reactions. **J.M. Hoover**

**3:00** Intermission.

**3:15 325.** Complex molecule synthesis via the enantioselective hydroformylation/hydroacylation/dol sequence. **C.R. Landis**

**3:45 326.** Incorporating aryne chemistry into Ti redox catalytic reactions: Ti-catalyzed synthesis of substituted naphthalenes via *in situ* generated arynes. **I. Tonks, B. Reiner**

**4:15 327.** Identifying catalysts and reactor conditions for tailored polymer rheology. **S.E. Smith, A. Mohan, G. Kiss, J.M. Soulagés**

Section F

Marriott Marquis San Diego Marina  
Marriott Grand Ballroom Section 8  
**Surface Chemistry & Structure in Ligand Protected Nanoparticles**

C. J. Johnson, *Organizer*  
B. Lear, *Organizer, Presiding*

**1:30** Introductory Remarks.

**1:35 328.** Atomically precise gold nanoclusters: Surface structure and implications. **R. Jin**

**2:20 329.** Atomically-precise nanocluster electronic structure and reactivity from atomically-impure syntheses. **C.J. Johnson, A. Cirri, H. Morales, C. Kmiotek**

**2:50** Intermission.

**3:00 330.** Effects of surface structure on the chirality and luminescence of thiolate- and phosphine-stabilized gold nanoclusters. **C.M. Aikens**

**3:45 331.** Chemical control over the electronic structure of discrete gold nanoclusters: Effects of composition, ligand, and solvent environment. **A. Cirri, H. Morales, C. Kmiotek, C.J. Johnson**

**4:15** Intermission.

**4:25 332.** Coherent electronic dynamics in atomically precise nanoclusters. **K.L. Knappenberger**

Section G

Marriott Marquis San Diego Marina  
Point Loma

**Charge & Substrate Transport in 3D Electrocatalytic Materials**

Cosponsored by CATL and ENFL  
A. Hall, C. C. McCrory, *Organizers*  
V. Thoi, *Organizer, Presiding*

**1:30** Introductory Remarks.

**1:35 333.** Designing catalysts for water splitting based on electronic structure considerations. **S. Banerjee**

**2:00 334.** How do interactions between protic cations and polarized bismuth cathodes control the pathway of CO<sub>2</sub> reduction?. **J. Rosenthal**

**2:25 335.** Accessing 3-D in transition-metal phosphide catalysts for water splitting: Challenges and opportunities. **C. Acquah, S. Mutinda, R. Liyanage, D. Li, S.L. Brock**

**2:50 336.** Modulating electrode-electrolyte interfaces for energy conversion reactions. **V. Thoi**

**3:15** Intermission.

**3:30 337.** Water electrolysis on metal oxides for energy conversion: Materials and mechanisms. **P. Strasser**

**3:55 338.** Interfacing metals and compounds for enhancing hydrogen electrochemistry. **Y. Sun**

**4:20 339.** Tailoring the surface of metal nanoparticles for selective electrocatalysis. **C.W. Li**

Section H

Marriott Marquis San Diego Marina  
Cardiff

**Lanthanide & Actinide Chemistry**

A. De Bettencourt Dias, *Organizer*  
K. Carter, D. Mills, *Presiding*

**1:30 340.** Electronic structures of bent, formally two-coordinate lanthanide(III) cations. **H. Nicholas, M. Vonci, C. Goodwin, S. Loo, S. Murphy, D. Cassim, R.E. Wimpenny, E. McInnes, N. Chilton, D. Mills**

**1:50 341.** New insights into solid-phase transformations in the uranyl peroxide system. **T.L. Spano, A. Miskowicz, J.L. Niedziela, M.W. Ambrogio, B.B. Anderson**

**2:10 342.** Uncovering unprecedented uranium species:

From water-stable uranyl(V) to U(IV) POM clusters. **R. Faizova, L. Chatelain, R. Scopelliti, M. Mazzanti**

**2:30 343.** Guest-dependent single-crystal-to-single-crystal phase transitions in a two-dimensional uranyl-based metal-organic framework. **S. Hanna, X. Zhang, K. Otake, R.J. Drout, P. Li, T. Islamoglu, O.K. Farha**

**2:50 344.** Synthesis of an unusual square planar Th(III) complex. **D.N. Huh, J.W. Ziller, W.J. Evans**

**3:10** Intermission.

**3:20 345.** Interactions of unsaturated hydrocarbon ligands with low valent uranium centers. **J.M. Boncella, A.M. Tondreau, B.S. Billow**

**3:40 346.** Tuning reactivity of nitride bridged uranium complexes with amide and siloxide ligands. **C.T. Palumbo, L. Barluzzi, R. Scopelliti, M. Mazzanti**

**4:00 347.** Reactivity of uranyl triperoxide monomers. **A. Arteaga, N. Martin, L.N. Zakharov, M.D. Nyman**

**4:20 348.** Structural chemistry of uranium(IV)-furoate complexes. **N.A. Vanagas, K.E. Knope**

**4:40 349.** Organometallic chemistry of lanthanides: Oxidation states in trompe l'oeil and magnetic sandwiches. **G. Nocton**

**5:00 350.** Condensed and gas phase coordination chemistry of bioinspired chelators with early actinides. **K. Carter, J. Jian, M. Pynch, T. Forbes, W. Dejong, J.K. Gibson, R.J. Abergel**

<section>

**150 Years of the Periodic Table**  
Sponsored by HIST, Cosponsored by CINF, INOR<sup>‡</sup> and PRES

<section>

**Advances in Catalysis with Ceria & Other Reducible Oxides Reactions and Other Metal Oxides**

Sponsored by CATL, Cosponsored by ENFL, ENVR, INOR and PHYS

**MONDAY EVENING**

Section A

Placeholder  
**Sci-Mix**

S. A. Koch, N. S.

Radu, *Organizers*

**8:00 - 10:00**

**134, 138, 139, 141, 143, 145, 146, 147, 150, 152, 154, 155, 157, 158, 159, 162, 163, 164, 165, 169, 170, 183, 184, 187, 190, 191, 193, 199, 201, 204, 206, 212, 213, 214, 220, 222, 223, 224, 225, 227, 228, 229.** See Previous Listings.

**476, 477, 478, 480, 484, 486, 487, 490, 492, 494, 500, 501, 503, 504, 506, 507, 509, 510, 514, 515, 517, 523, 524, 534, 539, 540, 541.** See Subsequent Listings.

**TUESDAY MORNING**

Section A

Marriott Marquis San Diego Marina

Marina Ballroom Salon F

**ACS Award in Pure Chemistry: Symposium in Honor of Danna Freedman**

Cosponsored by PHYS  
H. Karunadasa, J. Zdrozny, *Organizers, Presiding*

**8:30** Introductory Remarks.

**8:35 351.** Applications of coordination chemistry principles to molecular magnetism. **K.R. Dunbar**

**9:00 352.** Giant spins as magnetic nodes and building blocks. **T. Betley**

**9:25 353.** Rationalizing the magnetism of multinuclear single-molecule magnets containing strong single-ion sources of anisotropy through the use of the anisotropic building unit [ErCOT]<sup>+</sup>(COT<sup>2-</sup> = 1,3,5,7-cyclooctatetraenide dianion). **J.D. Rinehart, J. Hilgar, M.G. Bernbeck, A.K. Butts**

**9:50 354.** Quantum magnetism enabled by chemistry: From quantum spin liquids to topological spin waves. **Y. Lee**

**10:15** Intermission.

**10:30 355.** Let's get together! Making bonds between small molecules at multimetallic centers. **L.J. Murray**

**10:55 356.** Quantum sensing using diamond color centers. **H. Park**

**11:20 357.** Award Address (ACS Award in Pure Chemistry sponsored by the Alpha Chi Sigma Fraternity and the Alpha Chi Sigma Educational Foundation): Approaching challenges in physics

with inorganic chemistry. **D.E. Freedman**, M.J. Amdur, K. Collins, S. Coste, M. Fataftah, R.A. Klein, D. Laorenza, T. Pearson, S. Petry, A. Tamerius, C. Yu, A. Altman, L. Sun, J.P. Walsh, J. Zadrozny, M. Graham, S. Clarke

Section B

Marriott Marquis San Diego  
Marina  
Solana

**Chemistry of Materials:  
Nanomaterials**

C. G. Lugmair, *Organizer*  
E. A. Hernandez-Pagan, M. A. Mahmoud, *Presiding*

**8:30 358.** Single-component quasicrystalline nanocrystal superlattices by the flexible polygon tiling rule. **Y. Nagaoka**, O. Chen, H. Zhu

**8:50 359.** Synthesis of ZnS quantum dots: Towards shelling and heterostructures. **E. Bennett**, J.S. Owen

**9:10 360.** Correlated series of Au/Ag nanoclusters revealing the evolutionary patterns of asymmetric Ag doping. **Y. Li**

**9:30 361.** Size-controllable and uniform gold bumpy nanocubes for single-particle-level surface enhanced Raman scattering sensitivity. **Y. Lee**, K. Nam

**9:50 362.** Modulation of tungsten precursor reactivity for control over size and phase of WSe<sub>2</sub> nanocrystals. **J.Q. Geisenhoff**, A.M. Schimpf

**10:10** Intermission.

**10:25 363.** Expanding colloidal hybrid nanoparticles to metal phosphide systems. **E.A. Hernandez-Pagan**, R.E. Schaak

**10:45 364.** Photoreduction of iron oxide nanocrystals. **H. Jung**, B. Zhou, A.M. Schimpf

**11:05 365.** Asymmetric deposition of platinum atoms on gold nanorods induced by a substrate for synthesis of anisotropic bimetallic nanostructures. **M.A. Mahmoud**  
**11:25 366.** Triplet exciton transfer in PbS/CdS core-shell quantum dots with surface-appended chromophores. **C.M. Papa**, S. Garakyaraghi, F.N. Castellano

Section C

Marriott Marquis San Diego  
Marina  
Marina Ballroom Salon D

**Chemistry of Material  
Lectureship & Best Paper Award**

J. M. Buriak, A. De Bettencourt Dias, C. Toro, *Organizers*, *Presiding*

**8:30** Introductory Remarks.

**8:35 367.** Functional properties from molecular dynamics in hybrid perovskite halides. E. Mozur, I.W. Oswald, A. Koegel, A. Maughan, **J.R. Neilson**

**9:10 368.** Competing interactions: Octahedral tilting, organic-inorganic coupling, and charge transport in vacancy-ordered double perovskites. **A. Maughan**, A. Ganose, A.M. Candia, J. Granger, D.O. Scanlon, J.R. Neilson

**9:45 369.** Atomic pair distribution function (PDF) analysis of nanostructured and disordered materials. **S. Billinge**

**10:10** Intermission.

**10:20 370.** Tuning the bandgaps of halide double perovskites. A. Slavney, B. Connor, L. Leppert, J. Neaton, **H. Karunadasa**

**10:45 371.** Defect and carrier transport properties of emerging bismuth based photovoltaics. **A. Ganose**

**11:10 372.** Structural complexities in solids: Understanding functionality through local distortions in perovskite and pyrochlore materials. **G. Laurita**  
**11:35 373.** Key structural and chemical features of defect-tolerant semiconductors. **P. Gorai**

Section D

Marriott Marquis San Diego  
Marina  
Marriott Grand Ballroom Section 9

**Inorganic Chemistry for  
Sustainable Energy &  
Environment**

L. A. Berben, *Organizer*  
S. C. Marinescu, *Presiding*

**8:30 374.** Strategies to enhance electrochemical ammonia production on the surfaces of non-noble metal electrocatalysts. Y. Jang, **K. Choi**

**9:00 375.** CO<sub>2</sub> as a trigger for controlling the properties of surfaces and coatings. **P.G. Jessop**, M.F. Cunningham

**9:30 376.** Developing alternatives to oil as feedstocks for our

chemicals and liquid fuels. **K.I. Goldberg**

**10:00** Intermission.

**10:20 377.** Metal-organic frameworks in light harvesting and energy transfer. **A.J. Morris**, P. Usov, S. Shaikh

**10:50 378.** Renewable methane from green energy and CO<sub>2</sub>: Commercial-scale solution to decarbonize our planet with biological methanation. **M.B. Hein**

Section E

Marriott Marquis San Diego  
Marina  
Santa Rosa

**Emerging Research in Molecular  
Synthesis**

A. C. Brewer, J. M. Hoover, J. Y. Yang, *Organizers*  
V. A. Schmidt, *Organizer*, *Presiding*  
M. Emmert, *Presiding*

**8:30 379.** Beyond static DFT calculations for organometallic reactions in catalysis. **D.H. Ess**

**9:00 380.** Cu-catalyzed MLCT enabled photocycloadditions of non-conjugated pi-systems. **V.A. Schmidt**

**9:30 381.** Development of the copper-catalyzed carboamination reaction. **K.L. Hull**

**10:00** Intermission.

**10:15 382.** Developing data-driven reaction analysis tools for reaction optimization and interrogation. **M.S. Sigman**

**10:45 383.** Mechanistic insights into Fe catalyzed late-stage functionalization of amine C-H bonds. **M. Emmert**, C.J. Legacy, M. Frenette, F. Greenaway

**11:15 384.** Catalyst development for the decarboxylative functionalization of (hetero)arenes. **J.J. Topczewski**, R. Daley, E. Liu

Section F

Marriott Marquis San Diego  
Marina  
Marriott Grand Ballroom Section 8  
**Surface Chemistry & Structure  
in Ligand Protected  
Nanoparticles**

C. J. Johnson, B. Lear, *Organizers*  
A. Cirri, *Presiding*

**8:30 385.** How many organic molecules are there on gold nanocrystals? Results from both imaging and NMR. **C.J. Murphy**

**9:15 386.** Visualizing dynamic reorganization of surface-bound ligands on gold nanorods. **K.A. Willets**

**10:00** Intermission.

**10:10 387.** Ligand control of the electronic structure near the Fermi energy in metallic nanoparticles. **B.J. Lear**

**10:40 388.** Elucidating the role of ligand functionality in phosphine-protected gold clusters using mass spectrometry. **G.E. Johnson**, J. Laskin, H. Hernandez

**11:10** Intermission.

**11:20 389.** Dimensionality in surface functionalization. D.P. Goronzy, T. Base, K.N. Houk, **P.S. Weiss**

Section G

Marriott Marquis San Diego  
Marina  
Marina Ballroom Salon G

**Charge & Substrate Transport in  
3D Electrocatalytic Materials**

Cosponsored by CATL and ENFL  
A. Hall, V. Thoi, *Organizers*  
C. C. McCrory, *Organizer*, *Presiding*

**8:30 390.** Using polymer encapsulation to influence the mechanism, activity, and selectivity of electrocatalytic CO<sub>2</sub> reduction by molecular catalysts. **C.C. McCrory**

**8:55 391.** Developing materials to promote substrate channeling of intermediates in electrocatalytic cascades. **S.D. Minteer**

**9:20 392.** Ultrathin oxide overlayers for tunable electrocatalysis. **D. Esposito**

**9:45 393.** Exploiting transport limitations to enhance CO<sub>2</sub>-to-fuels selectivity. A. Wuttig, Y. Yoon, M. Schreier, S. Hall, **Y. Surendranath**  
**10:10** Intermission.

**10:25 394.** Making porous MOFs electrically conductive. **J.T. Hupp**, S. Goswami

**10:50 395.** Bridging homogeneous and heterogeneous catalysis with pincerMOFs. **C.R. Wade**, A. Kassie, B. Reiner

**11:15 396.** Redox hopping electron and ion transport in metal-organic framework materials. **A.J. Morris**, P. Celis Salazar, M. Cai

Section H

Marriott Marquis San Diego  
Marina  
Cardiff

**Inorganic Catalysts**

S. A. Koch, *Organizer*

**8:30 397.** Development of molecular electrocatalyst for CO<sub>2</sub> reduction based on polypyridyl and nitrogen-based macrocyclic ligands. **L. Lieske**, A.L. Rheingold, C.W. Machan

**8:50 398.** Electrocatalytic reduction of dioxygen to hydrogen peroxide by a molecular manganese complex with a bipyridine-containing Schiff base ligand. **S.L. Hooe**, A.L. Rheingold, C.W. Machan, D. Dickie

**9:10 399.** Effect of s-block metal ion on redox properties of Mn(V) salen-crown ether complexes: Methane activation. **A. Najafian**, T. Cundari

**9:30 400.** Synthetic [2Fe<sub>2</sub>S] biomimetics in metallopolymers as hydrogen evolution electrocatalysts. **K. Clary**, M. Karayilan, R.S. Glass, J. Pyun, D.L. Lichtenberger

**9:50 401.** Systematic study of proton-coupled electron transfer in tris(triazolyl)borate mid-late 3d, 4d-transition metals complexes: Computational study. **A. Nazemi**, T.R. Cundari

**10:10 402.** Turning off hydrogen evolution: Effects of secondary sphere electrostatic interactions on catalyst product selectivity. **J. Barlow**, J.Y. Yang

**10:30** Intermission.

**10:40 403.** Ionic strength of large polyions. **D.L. Collins-Wildman**, Y.V. Geletii, C.L. Hill

**11:00 404.** Pincer supported iron complexes for dinitrogen activation. **A.M. Lugosan**, D. Dickie, M. Zeller, W. Lee

**11:20 405.** Mechanism of photoreduction of CO<sub>2</sub> to CH<sub>4</sub> with iron-porphyrin catalyst. **L. Dang**, Z. Lu

**11:40 406.** Pd Single atom catalyst for small molecule transformations under practical conditions. G. Ding, **Q. Zhang**

**12:00 407.** Weaker interaction between second sphere and proton donor leads to increased selectivity and activity in Fe(III) Schiff base complexes for CO<sub>2</sub> reduction to formate. **A. Nichols**, S. Hooe, C.W. Machan

**12:20 408.** Electrocatalysis with Ni(P<sub>2</sub>N<sub>2</sub>)<sub>2</sub> complexes attached to the electrode through the phosphine

moiety. **F.M. Brunner**, C.P. Kubiak

<section>

**Future Insights into Syngas Conversion Catalysis: Symposium in honor of Burtron H. Davis**

Sponsored by CATL, Cosponsored by ENFL, ENVR, INOR and PHYS

<section>

**Advances in Catalysis with Ceria & Other Reducible Oxides Reactions and Other Metal Oxides**

Sponsored by CATL, Cosponsored by ENFL, ENVR, INOR and PHYS

**TUESDAY AFTERNOON**

Section A

Marriott Marquis San Diego Marina  
Marina Ballroom Salon F  
**Chemistry of Materials: Synthesis & Properties**

C. G. Lugmair, *Organizer*  
K. R. Kittilstved, C. E. Knapp, *Presiding*

**1:30 409.** Phenylalanine-based metallo-hydrogels with photo-switchable arylazopyrazole ligands. **K.Y. Ghebreyessus**, A. Sallee

**1:50 410.** Synthesis and optoelectronic properties of complex metal oxide A<sub>2</sub>M<sub>2</sub>O<sub>7</sub> nanoparticles. **Y. Mao**

**2:10 411.** Trigonal bisdithiazolyl radicals as building blocks towards three-dimensional magnetic exchange networks. **N.J. Yutronkie**, D. Bates, P. Dube, S. Winter, C.M. Robertson, R.T. Oakley, J. Brusso

**2:30 412.** Revealing the speciation of dopant ions in metal thiophenolate clusters. F. Kato, **K.R. Kittilstved**

**2:50 413.** From molecules to materials: Effect of precursor design on functional device synthesis. **C.E. Knapp**, H.R. Tinker, Y. Zhou, M.A. Bhide, S.P. Douglas, K.L. Mears

**3:10** Intermission.

**3:25 414.** Tunable cyclic Si-N hybrid materials. **C.P. Folster**, P.N. Nguyen, M.A. Siegler, R.S. Klausen

**3:45 415.** Tunable optical and magnetic properties in redox-

switchable all-inorganic polyoxometalate frameworks. **C. Lemmon**, A.M. Schimpf

**4:05 416.** Tunable polyoxometalate-based frameworks: Synthesis, structural characterization, and modulation of optical and electronic properties. **L. Chen**, **M. Turo**, K. San, J. Wang, M. Gembicky, A.M. Schimpf

**4:25 417.** Synthesis of high-quality, single-crystalline polyoxovanadate-based frameworks. **K.A. San**, A.M. Schimpf

**4:45 418.** Sustainable synthesis of high purity silicon carbide with carbon fiber production residual and a sandstone. **K. Sun**, X. He, T. Wang, W. Lu, M. Fan

**5:05 419.** Electrochemically switchable zwitterionic metal-organic frameworks. **J. Varghese**, F. Dix, K. Duell, D. Aulakh, M. Ciobanu, M. Wriedt

Section B

Marriott Marquis San Diego Marina  
Solana

**Learning from Nature: Earth-Abundant Metals for Oxidation Catalysis**

T. A. Jackson, A. Mukherjee, *Organizers*  
S. S. David, *Organizer, Presiding*

**1:30 420.** Gas phase tackling of the oxo-wall. **J. Roithova**

**2:00 421.** Oxidation of hydrocarbons by high-valent metal-halide complexes. **A.R. McDonald**

**2:25 422.** Small molecule activation at transition metal centers: Structure-function correlations. **K. Ray**

**2:50** Intermission.  
**3:00 423.** Scope and mechanism of C-H bond activation by bio-inspired copper complexes and peroxides. **A. Mukherjee**, N. Singh, N. Botcha

**3:25 424.** Spectroscopic investigations of metal binding and oxygen activation in the heterobimetallic Mn/Fe R2lox proteins. **H.S. Shafaat**, E. Miller, C. Ghosh, J.M. Hazel, Z.R. Smith, N. Trivelas

**3:50 425.** Proton-coupled electron transfer mechanisms in copper-oxygen chemistry. **W.B. Tolman**

**4:20 426.** Adventures in exploring the high-valent nonheme iron-oxo landscape. **L. Que**

Marriott Marquis San Diego Marina  
Marina Ballroom Salon D

**Chemistry of Materials: Metal Organic Frameworks**

C. G. Lugmair, *Organizer*  
B. R. Barnett, D. C. Powers, *Presiding*

**1:30 427.** Influence of metal substitution on the pressure-induced phase change in flexible zeolitic imidazolate frameworks. **C. McGuirk**

**1:50 428.** Structural control of metal-organic framework bearing N-heterocyclic carbene precursor and immobilization of NHC-metal complexes. **H. Kim**, E. Lee

**2:10 429.** De novo synthesis of homo and heterometallic titanium organic frameworks with high-throughput methodologies. J. Castells-Gil, N. Padial, N. Almora-Barrios, **C. Marti-Gastaldo**

**2:30 430.** Particle size and defect control in nanoparticulate UiO-66 via modulator-free synthetic conditions. **G.E. Decker**, Z. Stillman, C.A. Fromen, E.D. Bloch

**2:50 431.** Responsive metal-organic frameworks incorporating redox-active Mo<sub>2</sub>(INA)<sub>4</sub> molecular building units. **F.J. Claire**, M.A. Solomos, T. Kempa

**3:10** Intermission.

**3:25 432.** Ultrathin films of layered coordination polymers: Charge transport and spin crossover at the nanoscale. V. Rubio-Giménez, G. Escorcia-Ariza, N. Almora-Barrios, M. Galbiati, C. Bartual-Murgui, **S. Tatay**, C. Marti-Gastaldo

**3:45 433.** Probing substrate diffusion in interstitial MOF chemistry with kinetic isotope effects. **D.C. Powers**

**4:05 434.** Leveraging π-basicity in metal-organic frameworks for ambient temperature hydrogen storage: Structural, thermodynamic and kinetic insights. **B.R. Barnett**, J.R. Long

**4:25 435.** Fabrication and characterization of a defect-free mixed matrix membrane by facile mixing PPSU with ZIF-8 core-shell microspheres for solvent-resistant nanofiltration. **J. Dai**, S. Li, L. Wang, J. Lei

**4:45 436.** Harnessing metal-metal interactions in metal organic

framework based catalysts. **S. Desai**, J. Ye, T. Webber, T. Islamoglu, O.K. Farha, D.G. Truhlar, R. Penn, C.C. Lu

Section D

Marriott Marquis San Diego Marina  
Marriott Grand Ballroom Section 9  
**Emerging Research in Molecular Synthesis**

A. C. Brewer, J. M. Hoover, J. Y. Yang, *Organizers*  
V. A. Schmidt, *Organizer, Presiding*

**1:30 437.** Carbenes as powerful transition metal surrogates. **G. Bertrand**

**2:00 438.** Accessing ambiphilic phosphine boronates by phosphine-directed C–H borylation. **T.B. Clark**, S.E. Wright, S. Richardson-Solorzano, K.C. Morris, W. Schumacher, T.N. Stewart

**2:30 439.** Manipulation of main group element fragments with transition metal isocyanides. **J.S. Figueroa**

**3:00** Intermission.

**3:15 440.** Playing with charges: Electrostatically tethered reactive ion pairs. **V. Lavallo**

**3:45 441.** Main group-mediated olefin functionalization reactions. **A.E. Wendlandt**

Section E

Marriott Marquis San Diego Marina  
Santa Rosa  
**Surface Chemistry & Structure in Ligand Protected Nanoparticles**

B. Lear, *Organizer*  
C. J. Johnson, *Organizer, Presiding*

**1:30 442.** Synthetic and postsynthetic chemistry of silver monolayer-protected clusters. **T.P. Bigioni**

**2:00 443.** Switchable surfactants for the preparation of monodisperse nanoparticles. **S.R. Saunders**, K. Bryant

**2:30 444.** Laser synthesis and spectroscopy of ligand-coated nanoclusters and nanomaterials. **M.A. Duncan**

**3:00** Intermission.

**3:10 445.** Precise synthesis of platinum and alloy clusters and

elucidation of their structures. **Y. Negishi**

**3:55 446.** Monitoring nanoparticle-driven chemistry with ultrafast surface-enhanced Raman spectroscopy. **R.R. Frontiera**

**4:40** Intermission.

**4:50 447.** Surface chemistry and image dipoles in PbS quantum dots during resonant relaxation of excited intraband states. **J.B. Asbury**

**5:20** Concluding Remarks.

Section F

Marriott Marquis San Diego Marina  
Marriott Grand Ballroom Section 8  
**Charge & Substrate Transport in 3D Electrocatalytic Materials**  
Cosponsored by CATL and ENFL  
C. C. McCrory, V. Thoi, *Organizers*  
A. Hall, *Organizer, Presiding*

**1:30 448.** Enhancing the real-time detection of phase changes in lithium–graphite intercalated compounds through derivative *operando* (dOp) NMR cyclic voltammetry. **A. Co**, J. Lorie Lopez, P. Grandinetti

**1:55 449.** Accessing catalytically active ordered intermetallics electrochemically driven non-equilibrium phase transformations. **A. Hall**

**2:20 450.** Bicarbonate electroreduction in a flow cell. **C.P. Berlinguette**

**2:45 451.** Control over H<sup>+</sup>/OH<sup>-</sup> recombination in bipolar ion-exchange membranes enables extremely low overpotential reactivity for water dissociation or efficient light-driven ion pumping. W. White, R. Kautz, L. Schulte, S. Luo, R. Bhide, J. Glancy, L. Renna, **S. Ardo**

**3:10** Intermission.

**3:25 452.** 3D design in electrocatalysis. N. Becknell, P. Papa Lopes, D. Jung, D. Strmcnik, N. Markovic, **V. Stamenkovic**

**3:50 453.** Understanding lithium-mediated ammonia synthesis. **K. Manthiram**, N. Lazouski, Z. Schiffer, K. Williams

**4:15 454.** Assembly of Au nanoparticles on Cu nanowires to tune CO<sub>2</sub> reduction product from CO, C<sub>2</sub>H<sub>4</sub> to CH<sub>3</sub>CHO. **S. Sun**

Section G

Marriott Marquis San Diego Marina  
Marina Ballroom Salon G  
**Coordination Chemistry: Characterization & Applications**

A. Larsen, *Organizer*  
F. N. Castellano, C. J. Stein, *Presiding*

**1:30 455.** Photochemical upconversion with metal-to-ligand charge transfer sensitizers. **F.N. Castellano**

**1:50 456.** Water-soluble lanthanide (Eu, Tb, Sm) bioprobes combining a pycnen or TACN framework and conjugated antennas for two-photon imaging. **J. Shaya**, N. Hamon, R. Tripier, O. Maury  
**2:10 457.** Investigation of AlCl<sub>3</sub>-XCl (X = Cu, Ag) solutions in aromatics by <sup>27</sup>Al NMR spectroscopy. **W. Luo**, Z. Liu, X. Meng, R. Zhang, H. Liu, C. Xu

**2:30 458.** Mimicking thiol gold nanoparticles with atomically-precise tunable organometallic equivalents. **J. Stauber**, E.A. Qian, J. Logan, D. Fujita, Y. Han, P. Kral, A.M. Spokoiny  
**2:50 459.** Indium(III) complex of N, N'-bis(salicylidene) ethylenediamine as chemo-sensor for selective recognition of HSO<sub>4</sub><sup>-</sup> and hemolytic toxicity (red blood cells) studies. **T. Pandiyan**, C.A. Huerta-Aguilar, S. Huerta-Jose  
**3:10** Intermission.

**3:30 460.** Copper-benzoquinoid coordination polymer as electrode material for lithium-ion batteries. **C. Chang**, T. Chen

**3:50 461.** Synthesis and reactivity of cobalt N-heterocyclic phosphonium/phosphido complexes. **A. Poitras**, C.M. Thomas

**4:10 462.** Orbital entanglement analysis of exchange-coupled transition-metal complexes. **C.J. Stein**, V. Krewald, D.A. Pantazis

Section H

Marriott Marquis San Diego Marina  
Cardiff

**Organometallic Chemistry: Synthesis & Characterization: Late Transition Metals**

N. S. Radu, *Organizer*

**1:30 463.** Introducing the +1 oxidation state for derivatized 3d metallocene monoanions. C.

Goodwin, M. Vonci, H. Nicholas, S. Greer, N. Chilton, **D. Mills**  
**1:50 464.** Extrusion of dicobalt silicide cores via activation of all bonds at RSiH<sub>3</sub> (R = H, Ph) by [(*tris*-Phosphinoborate)CoI]<sup>-</sup>. **R.C. Handford**, P. Smith, T. Tilley  
**2:10 465.** Synthesis and reactivity of a rare Ni(I) methyl complex. **R. Witzke**, T. Tilley

**2:30 466.** Synthesis and characterization and reactivity of nickel(II)-calix[n]arene (n=4-6) complexes. **J.A. Carter**, B.A. Martinez Ortega

**2:50 467.** Formation of a Ni-C four-membered metallacycle and its reactivity toward X-Y bond activation. **X. Xing**, N.C. Tomson

**3:10 468.** Synthesis of cyclic (amino)(aryl)carbene copper(I) complexes. **J. Lorkowski**, U. Radius, C. Pietraszuk

**3:30 469.** Designing N-heterocycle functionalized phosphinoferrrocene ligands. **A. Sarbajna**, B.E. Silva, A.L. Rheingold, D. Grotjahn

**3:50 470.** Coordination of diatomic boron monofluoride to iron. **M.J. Drance**, J.S. Figueroa

**4:10 471.** Structure and Reactivity of Group IX Three-Coordinate Monoanions. **M.L. Neville**, C. Chan, J.S. Figueroa

**4:30 472.** Low valent cobalt isocyanides: Exploration of cobalt phosphide cluster building blocks. **C. Chan**, J.S. Figueroa

**4:50 473.** Readily accessible cyclic (alkyl)(amino)carbenes (CAACs). **L.C. Oliveira**, R. Jazzar, G. Bertrand

**5:10 474.** Synthesis and reactivity of a well-defined mixed-valent copper (0)/(I) nanocluster. **J.L. Peltier**, R.F. Jazzar, G. Bertrand

<section>

**Future Insights into Syngas Conversion Catalysis: Symposium in honor of Burtron H. Davis**

Sponsored by CATL, Cosponsored by ENFL, ENVR, INOR and PHYS

**TUESDAY EVENING**

Section A

Placeholder

**Coordination Chemistry: Characterization & Applications**

A. Larsen, *Organizer*

5:30 - 7:30

**475.** Synthesis, characterization, and antibacterial studies of Fe(III) complex of 3-nitro-N'-((3-hydroxy-5-(hydroxymethyl)-2-methylpyridin-4-yl)

methylene)benzohydrazide. **V. Chittireddy**

**476.** Rhenium(I) supramolecular rectangles for ion-sensing applications. **S.A. Dhanpat, A. Kumar**

**477.** Ligand-assisted dissolution of gold in organic solvents. **E. Heliövaara, M. Räsänen, T. Repo**

**478.** Polypyridine bridged ruthenium dimers as inner-sphere ketone transfer hydrogenation catalysts. **C.H. Weeks, E.P. Kelson**

**479.** Electrochemical and spectroelectrochemical studies of electrodes modified with ruthenium nitrosyl complexes. **S.B. Ritter, M.J. Shaw**

Section B

Placeholder

### Coordination Chemistry: Synthesis & Characterization

A. Larsen, *Organizer*

5:30 - 7:30

**480.** Some MOFs with substituted biphenyldicarboxylic acid to show novel topologies. **X. He, S. Zhang, D. Zhu**

**481.** Preparation of mixed-metal thiocyanate of SnCu(SCN) for opto/electronic applications. **C. Wechwithayakhlung, S. Horike, P. Pattanasattayavong**

**482.** Synthesis and characterization of palladium mononuclear complexes with electron donor (N,O) species. **C. Jimenez, J. Aviña, R. Guzmán-Mejía, R. Herrera, J. González-campos**

**483.** Perfect C<sub>3</sub> symmetric sulfate complex with a urea-based hexafunctional synthetic receptor. **A. Hossain, B. Portis, C.R. Johnson, M. Emami Khansari, A. Jahan, D.R. Powell**

**484.** Effect of a coordinating pyridine moiety on the SAP and TSAP isomer proportions of bimodal Ln(III) complexes. **M. Poveda, Z. Steinberg, O. Evbuomwan**

**485.** Supramolecular architectures and coordination polymers based on metallacrown complexes: Magnetic and sorption properties. **A.V. Pavlishchuk, M. Zeller, L.**

Carella, E. Rentschler, L.K. Thompson, **A.W. Addison**

**486.** Synthesis of fluorinated cobalt oxo cubanes: Catalysts for water oxidation. **A. Rahman, T. Tilley**

**487.** Synthesis of substituted bipyridylphosphine oxides via palladium(II) cross-coupling: Method development and application to coordination chemistry. **T. Grutza, M. Bezpalko, W.S. Kassel**

**488.** Synthesis of lanthanide molybdates via reaction of molybdenum(VI) oxide with aqueous acetate salts. **K. Alrashidi**

**489.** Synthesis, characterization, and electrochemistry of a ruthenium saloph nitrosyl complex. **K. Shrestha, M.J. Shaw**

**490.** Synthesis and characterization of a series of 5-methoxypyridyl-substituted phosphines and associated metal complexes. **L. Warring, W.S. Kassel, M. Bezpalko**

**491.** Synthesis and characterization of tris(2-pyridyl)phosphine oxide (OPPy<sub>3</sub>) complexes of select lanthanide(III) nitrates with potential application in molecular sensing. **C. Cox, M. Bezpalko, W.S. Kassel**

**492.** Anilino-pyridine ligand framework: Steric and electronic effects on the coordination chemistry to late transition metals. **M. Bezpalko, W.S. Kassel**

**493.** Systematic study of steric and electronic effects in substituted trispyridylphosphine ligands using molybdenum carbonyl complexes. **J. Leonard, M. Bezpalko, W.S. Kassel**

Section C

Placeholder

### Environmental & Energy-Related Inorganic Chemistry

S. A. Koch, *Organizer*

5:30 - 7:30

**494.** Tetraphenylphosphonium metal halide perovskites synthesis and crystal structures. **S.A. Althobaiti**

**495.** Electrocatalytic reduction of carbon dioxide at a 2D rhenium covalent organic framework. **M. Rahman**

**496.** Electrocatalytic alcohol oxidation by Co(3-*x*)M<sub>x</sub>O<sub>4</sub> catalysts. **M. Riehs, S.E. Michaud, C.C. McCrory**

**497.** Time dependence of iron-binding compound production in marine microorganisms under competitive growth conditions. **J.D. Martin, S. Littlejohn, K. Brown**

**498.** Tin polyesters: Polyimide blends as a dielectric material for energy storage application. **A.A. Deshmukh, S. Nasreen, M. Baczkowski, G.M. Treich, M. Tefferi, C. Anastasia, Y. Cao, G. Sotzing**

Section D

Placeholder

### Main Group Chemistry

T. Hudnall, *Organizer*

5:30 - 7:30

**499.** Synthesis and their characteristics of 1,1-disubstituted-2,5-bis{(trimethylsilyl)ethynyl}-3,4-diphenyl-siloles. **J.W. Lim, Y.T. Park**

**500.** Binary zinc borates and their industrial use. **D.M. Schubert, M.B. Jacobs**

**501.** Full-color luminescent dimethylamino-substituted difluoroboron β-diketonate complexes as environment-sensitive probes. **F. Wang, S. Chung, C.A. DeRosa, D. Song, C.L. Fraser**

**502.** Antibacterial performance and mechanism of inorganic salt cations. **Z. Ding, X. Zhao, Y. Zhang**

**503.** 1,8-Naphthalenediol derived boronic esters and inclusion properties of the 4,4'-bipyridine based Lewis acid-base complexes with different aromatic guest molecules. **C. Manankandayalage, C. Krempner**

Section E

Placeholder

### Lanthanide & Actinide Chemistry

A. De Bettencourt Dias, *Organizer*

5:30 - 7:30

**504.** Synchrotron and electron microscopy microstructural characterization of PuO<sub>2</sub>. **M.A. DeVore, J.L. Venzie, B.A. Powell, L.C. Shuller-Nickles, J. Fortner, M. Newville**

**505.** Understanding the effect of ligand environment on the

tunability europium(II)-containing visible-light photocatalysts. **R. Barraza, M.J. Allen**

**506.** Lanthanide extraction from fly ash using coordination chemistry. **J. Hovey, M. Dardona, T.M. Dittrich, M.J. Allen**

**507.** Slow magnetic relaxation in mono- and multinuclear uranium metallocene complexes. **D. Lussier, M. Boreen, K. Chakarawet, J. Arnold, D.K. Shuh, J.R. Long**

**508.** Lanthanide- and Ln doped bismuth- organic complexes: Structural motifs, visible excitation, and luminescence color tuning via dual emission pathways. **R.L. Ayscue, C. Verwiel, K.E. Knope**

**509.** F-element Fagan-Nugent coupling chemistry. **J.K. Pagano, K.A. Erickson, J.L. Kiplinger**

**510.** Organoactinide complexes of uranium and neptunium. **A. Myers, J.R. Walensky**

**511.** Comparative insertion reactivity of small molecules into thorium-nitrogen and thorium-phosphorus bonds. **M. Tarlton, J.R. Walensky**

**512.** Functionalization of cyclooctatetraene aimed to improve erbium single molecule magnet behavior. **A. Butts**

Section F

Placeholder

### Nanoscience

B. G. Trewyn, *Organizer*

5:30 - 7:30

**513.** Garlic based two photon nanoprobes for targeted triple-negative breast cancer imaging. **S. Begum, A. Pramanik, K. Gates, Y. Gao, P.C. Ray**

**514.** Continuous growth of iron-oxo clusters to iron oxide nanoparticles: Insights on iron oxide nanoparticle formation at the early stage. **H. Chang, T. Hyeon**

**515.** Holey graphene noble metal nanoparticle composites via crystalline polymer templated etching. **D. White, S. Burkert, S. Hwang, A. Star**

**516.** Microwave-assisted synthesis of Mn- and rare earth ion-doped CsPbX<sub>3</sub> (X = Br, Cl) perovskite nanocrystals. **K.Y. Ghebreyessus, L. Flagg, U. Hommerich**

**517.** Controlling nanocomposite magnetism through magnetic

orientation within a polymeric matrix. **T. Zand**

**518.** Magnetic characterization of iron-doped polydopamine nanoparticles. **K.S. Cay**, J.D. Rinehart, P.C. Bunting, Y. Xie

**519.** High-performance superparamagnetic Co-Mn-Zn ferrite nanoparticles for magnetic hyperthermia therapy of cancer. **J. Pan**, P. Hu, J. Shi, Q. Wu

**520.** Fe- and Sn-doped titania nanoparticles for metal-ion battery applications. B.D. Fahlman, **M.K. Islam**

**521.** Microwave-assisted flow synthesis of titania nanotubes. **Y. Luo**, **M. Calzado Delgado**, K. Yeung

**522.** Investigation of the influence of sonochemical parameters and initial temperature study on (ZnxAg<sub>y</sub>In<sub>z</sub>)S<sub>2</sub> synthesis mechanism. **H. Jung**, S. Sul, J. Jung, J. Park

**523.** Engineering pseudo spin valve magnetoresistance in colloiddally prepared nanoparticle films. **B. Zhou**, J.D. Rinehart

**524.** Synthesis of barium ferrite nanoparticles for new magnetic materials. **K.M. Kirkpatrick**, P.C. Bunting, J.D. Rinehart

Section G

Placeholder

**Organometallic Chemistry: New Ligand Platforms**

N. S. Radu, *Organizer*

**5:30 - 7:30**

**525.** Dipyrityldimethane derivatives as ligands for highly efficient iridium catalyzed sp<sup>3</sup> C-H borylation. **M.R. Jones**, N.D. Schley

**526.** Synthesis and characterization of terpyridine intermediate and derivatives for metal coordination. **M. Moghadasnia**

**527.** Strong magnetic exchange in dinuclear transition metal-Me<sub>6</sub>tren single-molecule magnets facilitated by a radical bridging ligand. **K. Chakarawet**, J.R. Long

Section H

Placeholder

**Organometallic Chemistry: Synthesis & Characterization: Late Transition Metals**

N. S. Radu, *Organizer*

**5:30 - 7:30**

**528.** Ferrocene-based heteroscorpionate nickel complexes for atom transfer radical polymerization. **S. Li**, P. Diaconescu

**529.** Evidence of carbon dioxide insertion into palladium-phenyl complex. **K. Zhang**, **W. Williams**, **D. Dickie**, **D.H. Ess**, **T.B. Gunnoe**

**530.** Use of silyl-calixarene derivative compound as precursor for the synthesis of transition metallo-calixarene complexes. **B.M. Olivo**, B.A. Martinez Ortega

**531.** Synthesis, reactivity, and magnetism of carbene-cobalt complexes. **A. Mantanona**, K.S. Cay, J.D. Rinehart

**532.** Synthesis, characterization, and photophysical properties of platinum(II) complexes with thiophene and halide ligands. C. Mastrocinque, M. Greenberg, **C.M. Anderson**, J. Tanski

Section I

Placeholder

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

N. S. Radu, *Organizer*

**5:30 - 7:30**

**533.** Aromatic substituent effects modulate catalytic activity of synthetic [NiFe]-Hydrogenase mimics. **C.R. Forbes**, L. Gan, N.S. Herringer, T.L. Groy, P. Tarakeshwar, A.K. Jones

**534.** Tantalafuran supported by a linked cyclopentadienyl-carboranyl ligand: Synthesis and structure. **J. Yang**, Z. Xie

**535.** Synthesis and characterization of precursors for the electrochemical deposition of refractory metals out of ionic liquids. **C. Egger**, R. Reich, O. Schneider, F.E. Kuehn

**536.** Synthesis and structures of thermolabile organotitanium monoalkyl phosphates: Solvent effect on nuclearity, utility as epoxidation catalysts and single-source molecular precursors for TiP<sub>2</sub>O<sub>7</sub>. **S. Verma**, G. Bhat, R. Murugavel

**537.** Experimental and computational mechanistic and

structural studies on substituted bis(cyclopentadienyl)tantalum(v) trihydrides for hydrocarbon activation. **S. Rehbein**

Section J

Placeholder

**Solid-State Inorganic Chemistry**

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

**5:30 - 7:30**

**538.** Establishing the complex crystal chemistry of the coinage metals through synthesis, computation, and data-driven analysis. **S. Lotfi**, A. Mansouri Tehrani, J. Brgoch

**539.** Synthesis of ternary metal tetrel-pnictides using arc-melted precursors. **G. Akopov**, J. Mark, B. McBride, K. Kovnir

**540.** Tuning the thermoelectric properties of 2D layered GeAs. **S. Lee**, B. Owens-Baird, K. Kovnir

**541.** New ternary transition metal selenide Na<sub>2</sub>MoSe<sub>4</sub>: Computational and experimental study. **E.I. Palos**, R.I. Hernández Lima, J. Guerrero Sánchez, G. Alonso Nuñez, A. Reyes Serrato

**542.** Flexible and hierarchical structured MnO<sub>2</sub>@ZrO<sub>2</sub> nanofibrous membranes with high catalytic performance. **X. Zhang**, X. Wang, J. Yu, B. Ding

**WEDNESDAY MORNING**

Section A

Marriott Marquis San Diego Marina  
Marina Ballroom Salon F

**Environmental & Energy-Related Inorganic Chemistry**

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

**8:30 543.** Electrocatalytic water oxidation by a trinuclear copper complex. **A. Geer**, X. Jia, B.A. McKeown, R.J. Nielsen, W.A. Goddard, T.B. Gunnoe

**8:50 544.** Electrocatalytic CO<sub>2</sub> reduction by cobalt nis(pyridylmonoimine) complexes: Effects of ligand structure on catalytic activity. **W. Nie**, C.C. McCrory

**9:10 545.** Effects of surface modification of p-type silicon on

the photoelectrochemical reduction of CO<sub>2</sub> with group VII catalysts. **C. Miller**, S. Okuno, P. Cheung, C.P. Kubiak

**9:30 546.** Molecular control over excited-state supramolecular assembly. **M. Turlington**, L. Troian-Gautier, R. Sampaio, E.E. Beauvilliers, G.J. Meyer

**9:50 547.** Sustainable simplified process for production of vanadium oxides (V<sub>2</sub>O<sub>5</sub>, VO<sub>2</sub>, and V<sub>2</sub>O<sub>3</sub>).

**H.S. Devi**, A. Mishra, M.S. Reza, M. Singh

**10:10** Intermission.

**10:15 548.** Mixed-valency across supramolecular systems:

Stabilizing soft interactions with electron delocalization. **J.M.**

**Palasz**, F.M. Brunner, C.P. Kubiak

**10:35 549.** Enhancing Si(111) photocathode performance with surface dipoles and surface density of states. **M.J. Rose**, D. Boucher

**10:55 550.** Copper-dioxygen chemistry using novel tren-based, tris(phosphinimine) ligands. **A. Weberg**, N.C. Tomson, S. McCollom

**11:15 551.** Design and studies of novel iron-based complexes for hydrogen photo-evolution. **A. Aydogan**, O. Schott, G. Hanan, M. Singleton, B. Elias

**11:35 552.** Taming a high valent tetra-nickel cluster for PCET of small molecules. **S. Jacob**, G. Menard

**11:55 553.** High nuclearity Co/Mn oxo clusters: Potential water oxidation catalysts. **P. Mahalay**, G. Maayan, K.A. Abboud, G. Christou

Section B

Marriott Marquis San Diego Marina  
Solana

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

S. A. Koch, *Organizer*  
T. Karabencheva-Christova, *Presiding*

**8:30 554.** Structural and spectroscopic insights into the reaction mechanism of carotenoid cleaving oxygenases. P. Kiser, **E.R. Farquhar**

**8:50 555.** Spectroscopic insights into the unusually high reactivity of the S = 1 [Fe<sup>IV</sup>(O)(Me<sub>3</sub>NTB)]<sup>2+</sup> complex that shed light on the oxidation mechanism of ferryl complexes. **S. Banerjee**, W. Rasheed, L. Que

**9:10 556.** Cu-dependent hydroxylation combined with 6-membered intramolecular cyclization under benign reaction conditions. **R. Trammell**, I. Garcia-Bosch, A. Cordova, P. Polunin, B. Blackmore

**9:30 557.** Genomic analysis of siderophore Fe(II)/ $\alpha$ -ketoglutarate-dependent Aminoacyl  $\beta$ -Hydroxylases reveals functional subtypes. **Z.L. Reitz**, A. Butler

**9:50 558.** Mechanistic investigation of stereoselective olefin cyclopropanation catalyzed by an engineered carbene transferase. **A. Tinoco**, R. Fasan

**10:10** Intermission.

**10:30 559.** Modeling copper active sites in biology: Synthesis and reactivity of bioinspired mononuclear copper(II) complexes. **T. Jones**, A. Mukherjee

**10:50 560.** Solvation dynamics at a surface loop of lipoyxygenase and its relationship to catalytic proton-coupled electron transfer. **J. Zaragoza**, J. Klinman

**11:10 561.** Insights into the linkage between the catalytic reaction cycle and proton pumping in  $\text{ba}_3$  cytochrome c oxidase: combining DFT, electrostatics, molecular dynamics, and new X-ray structures. **L. Noodleman**, W. Han Du, Y. Chen, D. McRee, K. Hartfield, A.W. Goetz, T. Goh, T. Doukov, A. Cohen, V. Cherezov, M. Soltis, P. Padayatti

**11:30 562.** Selective removal of endogenous CO *in vitro* and *in vivo* by aqueous hemoprotein model complexes. **H. Kitagishi**

**11:50 563.** Synthesis and characterization of heterobimetallic Fe–O–Mn complexes: Modeling RNR 1c and R2lox. **P. Crossland**, A. Zhou, L. Que

**12:10 564.** Insights into non-heme iron and 2-oxoglutarate demethylases by QM/MM and MD methods. **T. Karabencheva-Christova**, S.O. Waheed, R. Rajeev, C. Christov

Section C

Marriott Marquis San Diego Marina  
Marina Ballroom Salon D

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

N. S. Radu, *Organizer*

**8:30 565.** Stable ethylene-carbon dioxide group 6 metal complexes. **P.J. Perez**, M. Alvarez

**8:50 566.** Tungsten-ligand bond strengths for 2p elements, a DFT and *ab initio* study. **C. Moulder**, K. Kafle, T. Cundari

**9:10 567.** Organomanganese phosphine-phenol(ate) complexes: Coordination chemistry, and catalysis. **K. Kadassery**, S.N. MacMillan, D.C. Lacy

**9:30 568.** Synthesis and characterization of mono(oxazoline)-substituted cyclopentadienyl zirconium complexes. **Y. Chu**, N. Eedugurala, A.D. Sadow

**9:50 569.** Organometallic complexes of early transition metals supported by bulky acetylacetonate ligands. **S.M. Krajewski**, M.P. Marshak

Section D

Marriott Marquis San Diego Marina  
San Diego Ballroom Salon C

**Chemistry of Materials: Metal Organic Frameworks**

C. G. Lugmair, *Organizer*  
E. D. Bloch, J. Rimsza, *Presiding*

**8:30 570.** Theoretical study of porphyrin-based MOF structure for storage, separation, and drug delivery applications. **R. Belosludov**

**9:10 571.** Gold nanoparticles in the NU-1000 metal organic framework: Structures and O<sub>2</sub> activation. **R.D. Senanayake**, R. Snurr, C.J. Cramer

**9:30 572.** Hierarchical self-assembly of supramolecular coordination polymers using giant metal-organic nanocapsules as building blocks. **C. Zhang**, F. Wang, R. Patil, C.L. Barnes, T. Li, J.L. Atwood

**9:50 573.** Liquid-phase separations of fluoroarenes in metal-organic frameworks. **P.J. Milner**, M. Gonzalez, J.R. Long

**10:10** Intermission.

**10:25 574.** Gas storage in porous coordination cages. **E.D. Bloch**

**10:45 575.** Low-valent coordination networks with *m*-terphenyl isocyanides based linkers. **A. Arroyave**

**11:05 576.** Probing metal-organic framework growth process with competitive nucleation. **M.C.**

**Wasson**, J. Lyu, T. Islamoglu, O.K. Farha

**11:25 577.** Acid gas adsorption and structural characterization of RE-DOBDC MOFs via density functional theory. D.J. Vogel, T.M. Nenoff, **J. Rimsza**

Section E

Marriott Marquis San Diego Marina  
Santa Rosa

**Chemistry of Materials: Nanomaterials**

C. G. Lugmair, *Organizer*  
S. Chen, Y. Mao, *Presiding*

**8:30 578.** Kinetically controlled sequential seeded growth as a route toward metal dendrimers. **J.D. Smith**, M.M. Scanlan, S.E. Skrabalak

**8:50 579.** Tunable library of aminophosphines provides mechanistic insights on InP nanocrystal nucleation and growth. **B. McMurtry**, J. De Roo, J.K. Teglassi, K. Qian, A. Swarnakar, J.S. Owen

**9:10 580.** Scalable solid-state synthesis of SnS<sub>2</sub>/graphene nanostructured hybrids for high performance supercapacitor applications. **S. Al Hassan**, S. Lonkar, V. Pillai

**9:30 581.** Synthesis and characterization of nanoscale europium barium titanate (Eu<sub>0.5</sub>Ba<sub>0.5</sub>TiO<sub>3</sub>). **N. Farahmand**, S. O'Brien, J. Lombardi, F.A. Pearsall, L. Yang, S.J. Billinge, Z. Gai

**9:50 582.** Crystallinity and size control of colloidal germanium nanoparticles from organogermanium halide reagents. **B. Pescara**, K. Mazzio, K. Lips, S. Raoux

**10:10 583.** Transformation of cuprous oxide microcrystals into hollow copper nanoshells by facet-selective extraction of photoexcited charges. **C. Qin**, B. Campbell, M. Shen, T. Zhao, B. Sadtler

**10:30** Intermission.

**10:35 584.** Mesoporous silica coated CuFe<sub>2</sub>O<sub>4</sub> nanoparticles: Synthesis, characterization and application in gas phase H<sub>2</sub>S removal. **G. BASINA**, D. Abdullah Ali Gaber, S. Abdullah Ali Gaber, V. Tzitzios, C. Gioti, A. Mourkas, I. Ismail, I. Panagiotopoulos, M.A. Karakassides, **Y. Fowad AlWahedi**

**10:55 585.** Enzyme immobilization with reduced confinement in metal-organic frameworks. **S. Chen**, W. Lo, L. Chou, F. Shieh, C. Tsung

**11:15 586.** Molten-salt synthesis of pyrochlore RE<sub>2</sub>Hf<sub>2</sub>O<sub>7</sub> nanoparticles. **Y. Mao**, M. Pokhrel, K. Wahid, S. Gupta

Section F

Marriott Marquis San Diego Marina  
Marina Ballroom Salon E

**Coordination Chemistry: Synthesis & Characterization**

A. Larsen, *Organizer*  
T. Betley, M. Stollenz, *Presiding*

**8:30 587.** Correlation of formal oxidation state with the N–N bond distance of chromium dinitrogen complexes. **F. Ahmadi Darani**, K.H. Theopold

**8:50 588.** Aromaticity in bis(imino)pyridine complexes. **T. Bass**, T.J. Sherbow, C.R. Carr, L.A. Berben

**9:10 589.** Interaction between bimetallic sites in bimetallic composite ionic liquids. **Y. Zhang**, X. Meng, R. Zhang, H. Liu, C. Xu, Z. Liu

**9:30 590.** Heteroleptic calladium(II) complexes of the redox-active propentdyopent scaffold supported by intramolecular hydrogen bonding. **C. Curtis**, E. Tomat

**10:10** Intermission.

**10:15 591.** To multiply bond or not. **T. Betley**

**10:35 592.** Investigation on the stability of a series of BODIPYs in acidic conditions: Experimental and computational study into the role of the substituents at boron. **M. Wang**, D.R. Mason, P.N. Bobadova-Parvanova, M. Vicente

**10:55 593.** Synthetic investigation of competing magnetic interactions in 2D metal-organic frameworks. **K. Collins**, M. Fataftah, D.E. Freedman

**11:15 594.** Lewis-acid-catalyzed BODIPY boron functionalization utilizing trimethylsilyl nucleophiles. **G. Zhang**, M. Wang, F.R. Fronczek, K.M. Smith, M. Vicente

Section G

Marriott Marquis San Diego Marina  
Marina Ballroom Salon G

**Inorganic Catalysts**

S. A. Koch, *Organizer*

**8:30 595.** New classes of homo- and heteroleptic Cu(I) metal-to-ligand charge transfer photosensitizers. **F.N. Castellano**

**8:50 596.** Real-time detection of large Abeta oligomers using photoluminescence anisotropy. **B. Jiang**, A. Aliyan, A. Smith, A. Marti, I. Gonzalez-Moreno

**9:10 597.** Delayed photoluminescence in metal-conjugated fluorophores. **M. Yang**, M. Zamkov, H.M. Mattoussi

**9:30 598.** Methane C–H activation via cyclic (alkyl)(amino)carbenes (CAACs) and CAAC-supported transition metal complexes: Computational study. **Z. Sun**, T.R. Cundari

**9:50 599.** Photoinitiated oxidation of halides to halogen using ruthenium trisbipyridyl complexes as catalysts. C. Chen, **I. Chang**

**10:10 600.** New approaches to hydrocarbon feedstock conversion: Bifunctional Pd complexes for tunable heterolytic C–H activation. **R. Tenney**, W. Christman, N. Arulsamy, E.B. Hulley

**10:30 601.** High-throughput screening of MOF catalysts. **J. Palomba**, S. Cohen, M. Kalaj

**10:50** Intermission.

**11:00 602.** Molecular cobalt complexes with pentadentate ligands for electro- and photocatalytic hydrogen generation in aqueous solution. **P. Wang**, G. Liang, E. Towles, D. Li, C. Boyd, K. Hill, B. Shaver, W. Grubbs, C.E. Webster, X. Zhao

**11:20 603.** Electrochemical and computational investigation of aromatically bridged [2Fe-2S] clusters for electrocatalytic hydrogen production. **M.O. Hamilton**, J.M. Kiselka, M. Karayilan, R.S. Glass, J. Pyun, D.L. Lichtenberger

**11:40 604.** Effect of hydrogen bonds on photocatalysis of CO<sub>2</sub> reduction. **P. Cheung**, T. Zeng, C.P. Kubiak

**12:00 605.** Chemically driven water oxidation by mononuclear Ru(II) complexes and deactivation pathway. **A. Kundu**, S. Mandal

**12:20 606.** Synthesis and reactivity studies of molybdenum(VI) and rhenium(V) oxo complexes as bioinspired oxo transfer catalysts. **M. Hossain**, J. Schachner, M.O.

Haukka, A. Lehtonen, N. Mösch-Zanetti, E. Nordlander

Marriott Marquis San Diego Marina  
Cardiff

### Nanoscience

B. G. Trewyn, *Organizer*

**8:30 607.** Revealing the peculiar solubility of some atomically-precise gold nanoclusters. **M.J. Cowan**, T. Higaki, R. Jin, G. Mpourmpakis

**8:50 608.** Nonthermal plasma-synthesized PB co-doped Si NCs: New approach to non-toxic NIR-emitters. **G. Pach**, R. Limpens, N.R. Neale

**9:10 609.** Structural identification and quality assessment of graphene derivatives by X-Ray diffraction. **I. Sengupta**, S. S S Sharat Kumar, S. Pal, S. Chakraborty

**9:30 610.** Capitalization on self-assembly for the preparation of rhenium carbonyl-based nanoparticles for theranostic applications. **K. Chan**

**9:50 611.** Probing the interior nanoscale heating mechanism of a magnetic core in mesoporous silica drug-delivery nanoparticles using fluorescence depolarization. **F. Lin**, J.I. Zink

**10:10 612.** Mosquito bite prevention through graphene barrier layers. **C. Castilho**, D. Li, M. Liu, Y. Liu, H. Gao, R. Hurt

<section>

### Future Insights into Syngas Conversion Catalysis: Symposium in honor of Burtron H. Davis

Sponsored by CATL, Cosponsored by ENFL, ENVR, INOR and PHYS

<section>

### Understanding the Role of Water in Solid Acid-Base Catalysis

Sponsored by CATL, Cosponsored by ENFL, INOR and PHYS

### WEDNESDAY AFTERNOON

Section A

Marriott Marquis San Diego Marina  
Marina Ballroom Salon F

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

S. A. Koch, *Organizer*

M. J. Rose, *Presiding*

**1:30 613.** Acid pK<sub>a</sub>-dependence O–O bond lysis of a nonheme Fe<sup>III</sup>–OOH species: Analogy to the formation of heme compound I. **S. Xu**, A. Darksharapu, W. Rasheed, L. Que

**1:50 614.** Investigating the mechanism of formation of a rare thiolate-ligated Fe(III)-sulfenate. **A. Downing**, M.N. Blakely, J. Kovacs

**2:10 615.** Functional hydride transfer in anthracene scaffold-based synthetic models of [Fe]-hydrogenase. **M.J. Rose**, S. Kerns, J. Seo

**2:30 616.** Investigation of the binding of nitrogen-based exogenous ligands in iron complexes within a C<sub>3</sub>-symmetrical phosphinic amide tripodal ligand. **C. Sun**, A. Borovik

**2:50 617.** From organometallic carbides to nitrogenase-inspired clusters: Sulfurization of Fe<sub>6</sub> and Fe<sub>5</sub>Mo carbides. **M.J. Rose**, C. Joseph

**3:10** Intermission.

**3:30 618.** Artificial iron proteins using biotin–streptavidin technology. **K. Miller**, A. Borovik

**3:50 619.** Tetranuclear Mn<sub>4</sub>O<sub>4</sub> complexes as models of the oxygen evolving complex of photosystem II. **A. Shiau**, H. Lee, P. Oyala, T. Agapie

**4:10 620.** Spectroscopic characterization of thiolate ligated iron-dioxygen and oxo-atom donor intermediates. **M. Dedushko**

**4:30 621.** Fluorescent probes for New Delhi metallo-β-lactamases to explore bacterial zinc homeostasis. **R. Mehta**, P. Thomas, W. Fast, E.L. Que

**4:50 622.** High valent non-heme iron-oxido and -hydroxido complexes. **J. Lee**, V. Oswald, S. Biswas, M.P. Hendrich, A. Borovik

**5:10 623.** Principles of metal selectivity bias and cluster assembly in metallothionein metal thiolate clusters. J.S. Calvo, N. York, B.S. Pierce, **G. Meloni**

Section B

Marriott Marquis San Diego Marina  
Solana

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

C. G. Lugmair, *Organizer*  
A. J. Karkamkar, R. M.

Kennedy, *Presiding*

**1:30 624.** Facile solvent free synthesis of iron porphyrin COFs for CO<sub>2</sub> reduction. **P. Cheung**, S. Lee, C.P. Kubiak

**1:50 625.** Covalent organic frameworks composed of rhenium bipyridine and metal porphyrins: Designing heterobimetallic frameworks with two distinct metal sites. **E. Johnson**, R.M. Haiges, S.C. Marinescu

**2:10 626.** Surface-immobilized conjugated polymers incorporating rhenium bipyridine motifs for electrocatalytic and photocatalytic CO<sub>2</sub> reduction. **N.M. Orchanian**, L.E. Hong, J. Skrainka, J. Esterhuizen, D. Popov, S.C. Marinescu

**2:30 627.** Electrocatalytic CO<sub>2</sub> reduction in water using Re complex catalyst with polymer ion gels electrode. **S. Sato**, B.J. McNicholas, R.H. Grubbs

**2:50** Intermission.

**3:05 628.** Catalytic hydrogenation of CO<sub>2</sub> to methanol using tandem catalysis involving encapsulated ruthenium complexes in the metal-organic framework UiO-66. **T. Rayder**, E.H. Adillon, C. Tsung, J.A. Byers

**3:25 629.** Catalytic upcycling of waste polymers by supported metal catalysts. **R.M. Kennedy**, G. Celik, R. Hackler, S.C. Ammal, M. Ferrandon, A.M. LaPointe, A.D. Sadow, A. Heyden, K.R. Poeppelmeier, M. Delferro

**3:45 630.** CO<sub>2</sub> reduction to CO by rhenium catalyst and various attachment strategies to carbon electrode surfaces. **A. Zhanaidarova**, C.P. Kubiak

**4:05 631.** Alternative ammonia storage materials for SCR of NO<sub>x</sub>. **A.J. Karkamkar**

**4:25 632.** Exploration of p-type delafossite CuMO<sub>2</sub> oxides as photocatalysts. **Y. Mao**

**4:45 633.** Electron localization and transport through ruthenium polypyridyl dye-sensitized core/shell SnO<sub>2</sub>/TiO<sub>2</sub> mesoporous thin films. **E. James**, M. Bennett, G.J. Meyer

Section C

Marriott Marquis San Diego Marina  
Marina Ballroom Salon D

### Chemistry of Materials: Metal Organic Frameworks

C. G. Lugmair, *Organizer*  
M. I. Gonzalez, M.  
Wriedt, *Presiding*

**1:30 634.** Metal-organic frameworks as templates for the controlled growth of catalytically active copper nanoparticles. **L. Redfern**, O.K. Farha

**1:50 635.** Controlled encapsulation of biomolecules into nanoporous materials. **C. Tsung**

**2:10 636.** Confinement of atomically-defined metal halide sheets in a metal-organic framework. **M.I. Gonzalez**, A. Turkiewicz, L.E. Darago, J. Oktawiec, K. Bustillo, F. Grandjean, G.J. Long, J.R. Long

**2:30 637.** Framework structure defines the excitonic properties of mo fs. **P. Deria**, J. Yu

**2:50 638.** Synthesis and enhanced performance of metal-organic framework hybrid materials. **Y. Liu**, S. Klein, K. Nelms, J. Sosa

**3:10 Intermission.**  
**3:25 639.** Old linkers new tricks: Evolution of 14-Connect Zr<sub>6</sub> secondary building units. M.J. Hurlock, **Q. Zhang**

**3:45 640.** Photodoping as a route to storing electrons in metal-organic frameworks. **C.H. Hendon**

**4:05 641.** Energy and charge transfer dynamics in porphyrin: MOF composite. **X. Li**, J. Yu, P. Deria

Section D

Marriott Marquis San Diego Marina  
San Diego Ballroom Salon C  
**Organometallic Chemistry: Catalysis - Late Transition Metals**

N. S. Radu, *Organizer*

**1:30 642.** Rhenium bipyridine catalysts with hydrogen bonding pendant amines for CO<sub>2</sub> reduction. **A. Hellman**, S.C. Marinescu, R.M. Haiges

**1:50 643.** Generation of active palladium(0) catalyst species from air-stable palladium(II) precatalysts and their application in cross-coupling reactions. **K.H. Shaughnessy**

**2:10 644.** Novel metal-catalyzed nitrene transfer reactions: Increasing molecular complexity. **P.J. Perez**, M. Diaz-Requejo, M.R. Rodríguez, A. Moreno

**2:30 645.** Optimizing ene-yne metathesis reactions: Understanding how optimal conditions shift with substrate. **K. Basemann**, B. Schmidt, T.L. Windus, A.D. Sadow

**2:50 646.** Chasing copper hydrides. J.L. Peltier, E.A. Romero, d. munz, **R.F. Jazsar**, G. Bertrand  
**3:10 647.** Co-catalytic effects in iron-mediated hydrogenation of electron-rich carbonyl compounds. U. Jayarathne, N. Hazari, **W.H. Bernskoetter**

**3:30 648.** Development of molecular electrocatalysts for energy-related transformations. **K.M. Waldie**, S. Katipamula, M. Zou, S. Warriar

**3:50 649.** Comparison of reactivity of iron alkoxide complexes towards azoarene synthesis. **D. Wannipurage**, S. Kurup, M. Yousif, S. Groysman, R.L. Lord

**4:10 650.** Development of group 9 transition metal based catalysts for the oxidative alkenylation of arenes. **W. Zhu**, J. Chen, X. Jia, D. Dickie, T.B. Gunnoe

Section E

Marriott Marquis San Diego Marina  
Santa Rosa  
**Chemistry of Materials: Nanomaterials**

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

**1:30 651.** Systematic tailoring of CdSe quantum dot-molecule composites for triplet energy transfer reactions. **D.T. Yonemoto**, F.N. Castellano

**1:50 652.** Conversion of InP clusters to nanomaterials and its role in the design of alloyed III-V nanomaterials for emissive applications. **M. Friedfeld**, J. Stein, D. Johnson, B. Cossairt

**2:10 653.** Nucleation kinetics and molecular mechanism in transition-metal nanoparticle formation: Intriguing, informative case of a bimetallic precursor,  $\{[(1,5\text{-COD})\text{Ir}^{\text{I}}(\text{HPO}_4)]_2\}^{2-}$ . **C. Whitehead**, R.G. Finke

**2:30 654.** Attaining tunability of colloidal copper phosphide nanocrystals through synthetic design and post-synthetic redox modulation. **A. Rachkov**, A.M. Schimpf

**2:50 655.** Functionalization of boron-nitride nanomaterials using

reductive conditions. C.A. de los Reyes, K. Hernandez, C. Martinez, A. Smith McWilliams, M. Pasquali, **A.A. Marti**

**3:10 Intermission.**  
**3:25 656.** Stitching quantum dots in formamide as an alternative route to make heterostructures. **P. Moroz**, M. Zamkov, J. Cassidy, D. Porotnikov

**3:45 657.** Synthesis and properties of ferroic and multiferroic transition/rare-earth metal oxide nanomaterials. J. Lombardi, F. Pearsall, N. Farahmand, L. Yang, J. Li, Z. Gai, S. Billinge, **S. O'Brien**

**4:05 658.** Applications of the nanoconfinement effect in explosive stabilization, chemical dosimeters, and water treatment. **A.W. Apblett**, N.F. Materer, E. Kadossov, R. Butt

**4:25 659.** Colloidal CuFeS<sub>2</sub> nanocrystals: Synthesis and insights into the intermediate Fe d-band that influences its optical properties. **S. Ghosh**, D.J. Milliron

Section F

Marriott Marquis San Diego Marina  
Marina Ballroom Salon E  
**Coordination Chemistry: Synthesis & Characterization**

A. Larsen, *Organizer*  
R. Hernandez Sanchez, *Presiding*

**1:30 660.** Some novel bioactive carboxylate metal complexes: Synthesis, structural elucidation and antimicrobial properties. **J.A. Obaleye**

**1:50 661.** Ruthenium-cobalt oxo cubane bearing a terminal Ru<sup>V</sup>-oxo. **J. Amtawong**, D. Balcells, J. Wilcoxon, N. Biggins, R. Britt, T. Tilley

**2:10 662.** Thermochromic properties of mixed anion crystals of bis(cyclohexyl isocyanide) gold(I) complexes. **P.M. Luong**, V. Moshayedi, M.M. Olmstead, A.L. Balch

**2:30 663.** Reaction of iron ions with 2-oximinocarboxylates: Kinetics of complex formation and the thermal conversion of the products to metal oxides. **W. Alamier**, A.W. Apblett

**2:50 664.** Atomically-defined nanoscale materials. **R. Hernandez Sanchez**

**3:10 Intermission.**

**3:30 665.** Questions of noninnocence and ease of azo

reduction in diruthenium frameworks. **F.F. Fatima Khan**, G.K. Lahiri

**3:50 666.** Accessing a new molecular scaffold for Fe(II) spin-state switching through post-synthetic modification. **B. Livesay**, M.P. Shores

**4:10 667.** Fe<sup>II</sup> spin-crossover complexes as temperature- and pH-responsive <sup>19</sup>F chemical shift magnetic resonance probes. **A.E. Thorarindottir**, A.I. Gaudette, D. Harris

**4:30 668.** NHC-, CAAC-, and CDC-alkaline earth metal complexes as reagents for bond activation. L.A. Freeman, J. Walley, G. Wang, G. Breiner, D. Dickie, **R.J. Gilliard**

Section G

Marriott Marquis San Diego Marina  
Marina Ballroom Salon G  
**Lanthanide & Actinide Chemistry**

A. De Bettencourt Dias, *Organizer*  
D. A. Penchhoff, D. Stamberga, *Presiding*

**1:30 669.** Predicting stability constants for terbium(III) complexes with 4-substituted dipicolinic acid analogues using density functional theory. **H. Chen**, R. Shi, H. Ow

**1:50 670.** High-throughput screening to achieve benchtop separations for selected rare earth elements. **J. Nelson**, T. Cheisson, H. Rugh, M. Gau, P. Carroll, E.J. Schelter

**2:10 671.** Ion coupled plasma mass spectrometry detection of the isotachophoretic separation of nonradioactive lanthanides in a capillary and a microfluidic device. **H.E. Lackey**, D. Bottenus, S.D. Branch, M. Liezers, S.D. Shen, A. Lines

**2:30 672.** Complexation of lanthanides and actinides: Theoretical perspective on predicting binding selectivity. **D.A. Penchhoff**, C. Peterson, G.K. Schweitzer, D.M. Jenkins, R. Harrison, H.L. Hall

**2:50 673.** Tetravalent cerium complexes and clusters. **J.N. Wacker**, A.S. Ditter, S.A. Kozimor, K.E. Knope

**3:10 674.** Crucial impact of cerium reduction on photoluminescence

properties. **R. GÁ©nois**, R. Gautier, F. Massuyeau, S. Jobic  
**3:30 675.** Isolation and assessment of the cytotoxicity of oligothiopyrene-based luminescent lanthanide complexes. **K. Johnson**, C.V. Rodrigues, M.O. Rodrigues, V.C. Lombardi, A. De Bettencourt Dias  
**3:50 676.** Separation of rare earth elements using novel diglycolamide ligands. **D. Stamberga**, C. Albißer, M.R. Healy, K.L. Lyon, I. Popovs, S. Jansone-Popova

**4:10 677.** Highly functional rare Earth starting materials. **R. Beattie**, J.K. Pagano, K.A. Erickson, S.K. Cope, B. Scott, D.E. Morris, J.L. Kiplinger

**4:30 678.** Peroxide-selective O<sub>2</sub> reduction via metal-coupled electron transfer with rare earth triflates. **M.J. Lueckheide**, M.Z. Ertem, J.R. Robinson

**4:50 679.** ErCOT: An anisotropic metal-ligand pair for targeted molecular magnet design. **M.G. Bernbeck**, J. Hilgar, J.D. Rinehart

Section H

Marriott Marquis San Diego  
Marina  
Cardiff

### Main Group Chemistry

T. Hudnall, *Organizer*  
R. J. Gilliard, C. E. Knapp, *Presiding*

**1:30 680.** Eclipsed digermynes as building blocks to construct catenated multinuclear germanium chains and rings. Y. Wey, G. Huang, J. Yu, Y. Tsai

**1:50 681.** Cyclodiphosphazanes in metal-organic frameworks. **M.S. Balakrishna**

**2:10 682.** Inorganic rings of group 13 and 14 elements as a platform for molecular hybrid materials. W. Yang, K.E. Krantz, D. Dickie, **R.J. Gilliard**

**2:30 683.** Iron, cobalt, and nickel complexes with silylene ligands. **C. Cui**, Y. Bai

**2:50** Intermission.

**3:00 684.** Investigations into the synthesis, reactivity, and thermolysis of heterobimetallic precursors. **K.L. Mears**, C.E. Knapp, C.J. Carmalt

**3:20 685.** Designer aluminium compounds for use as precursors in low temperature metal coatings. **S.P. Douglas**, C.E. Knapp

**3:40 686.** Synthesis and characterization of selenium and tellurium containing organic materials toward sensors and emitters. **G. Hoover**, B. Drummond, S. Jones, D. Credgington, D.S. Seferos

**4:00 687.** Precursor design, synthesis, and reactivity: Tuning molecules for low temperature conversion to functional materials. **C.E. Knapp**, H.R. Tinker, Y. ZHOU, M.A. Bhidé, S.P. Douglas, K.L. Mears

<section>

### Understanding the Role of Water in Solid Acid-Base Catalysis

Sponsored by CATL, Cosponsored by ENFL, INOR and PHYS

### THURSDAY MORNING

Section A

Marriott Marquis San Diego  
Marina  
Marina Ballroom Salon F

### Chemistry of Materials: Synthesis & Properties

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

**8:30 688.** Fabrication and thermal behavior of metal matrix composites containing NTE ZrW<sub>2</sub>O<sub>8</sub>. **Q. Zhang**

**8:50 689.** Lead-free all-inorganic Ag doped cesium bismuth iodide perovskite for resistive switching with ultra-low operating voltage and high on/off ratio by preconditioned metal conducting filament. **J. Han**

**9:30 690.** Designer gallium precursors towards functional materials. **K.L. Mears**, C.E. Knapp, C.J. Carmalt

**9:50 691.** Synthesis and structural characterization of nano coordinated Cd(II) complexes. **M. Raja**

**10:10** Intermission.

**10:25 692.** Ultrathin PdAg single-crystalline nanowires enhance ethanol oxidation electrocatalysis. **H. Lv**, Y. Wang, D. Xu, B. Liu

**10:45 693.** Accelerating the discovery of type II porous liquids using high-throughput automation. **R. Kearsey**, B.M. Alston, M.E. Briggs, R.L. Greenaway, A.I. Cooper

**11:05 694.** Synthesis and design of semiconductor-core crystalline

Bragg fibers. **A. Hendrickson**, M. Coco, J. Krug, C. Mathewson, S.C. Aro, S. McDaniel, J. Mauro, P. Sazio, G. Cook, V. Gopalan, J.V. Badding

**11:25 695.** *In silico* design of new functional materials. V.

Korolev, **A. Mitrofanov**, A. Eliseev, B. Sattarov, V. Tkachenko

**11:45 696.** Experimental screening for discovery of low dimensional metal halides with intense white-light emission. **R. Gautier**

Section B

Marriott Marquis San Diego  
Marina  
Solana

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

N. S. Radu, *Organizer*

**8:30 697.** ‘Super-bulky’ ligands: Coordination chemistry and application in ring-opening polymerization reactions. **C. Bakewell**

**8:50 698.** Mechanistic and kinetic studies of ring-opening metathesis polymerization with third-generation Grubbs catalysts. D. Walsh, M. Hyatt, **D. Guironnet**

**9:10 699.** Chemical mapping and optimization of redox switchable metal complexes for ring-opening polymerization. **A. Lai**, N. Fey, P. Diaconescu

**9:30 700.** Electrochemically controlled redox-switchable ring-opening polymerization. **Z. Hern**, C. Liu, P. Diaconescu

**9:50 701.** Increasing stereocontrol in lactide polymerization with flexible catalysts. P. Daneshmand, **F. Schaper**

**10:10 702.** Redox switchable (co)polymerization reactions with a zirconium compound. **R. Dai**, P. Diaconescu

**10:30 703.** CVD functionalization of graphene using transition metal carbonyls: Facile route to generate bandgaps. **K. Vinodgopal**, K. Robinson, X. You, J. Atkin, M. Terrones, D. Grasseschi, S.C. Sendlinger

**10:50 704.** Nickel-based bimetallic catalysts for Olefin polymerization. **S. Xiong**, T. Agapie

**11:10 705.** Introducing complexity to polysilanes using fused ring building blocks: Poly(siladecalin). **E. Marro**, R.S. Klausen

Section C

Marriott Marquis San Diego  
Marina  
Marina Ballroom Salon D

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

C. G. Lugmair, *Organizer*  
V. Doan-Nguyen, R. Mishra, *Presiding*

**8:30 706.** Oxide ion conductors in the hexagonal perovskite family. **A. Mclaughlin**, E. Wildman, S. Fop

**8:50 707.** MOF crystal branching: Novel solution to counteracting plasticization in MOF-polymer mixed-matrix membranes. **K. Zhang**, B.J. Sundell, D. Harrigan, S.C. Hayden, W. Chi, Z. Smith

**9:10 708.** Dual functions of water in stabilizing the metal-pentazolate hydrates [M(N<sub>5</sub>)<sub>2</sub>(H<sub>2</sub>O)<sub>4</sub>]·4H<sub>2</sub>O (M = Mn, Fe, Co, and Zn) high-energy density materials. **M. Cheng**

**9:30 709.** Quinone-based metal-organic materials for energy storage and gas separation. **T. Chen**

**9:50 710.** Nanoporous ceramic membranes for redox flow batteries. **S. Candelaria**, K.L. Corp, A. Salunkhe, G.M. Newbloom

**10:10** Intermission.

**10:25 711.** Generation of well-defined electrophilic surface sites on sulfated zirconium oxide. **M.P. Conley**

**10:45 712.** Structural evolution of transition metal trisulfide electrode materials. **V. Doan-Nguyen**

**11:05 713.** New look at an old compound: X-ray photocrystallography studies of potassium ferrioxalate upon photolysis in the solid state. **M. Nava**, M. Gonzalez, E.J. Johnson, D.G. Nocera

**11:25 714.** Storing solar energy: Photochemical oxygen capture and thermal release. **T. McCormick**, L. Lutkus

**11:45 715.** KBaTeBiO<sub>6</sub>: Lead-free, inorganic double-perovskite semiconductor for photovoltaic applications. A.S. Thind, S. Kavadiya, M. Kouhnavard, R. Wheelus, S.B. Cho, L. Lin, A.Y. Borisevich, G. Pilania, P. Biswas, **R. Mishra**

Section D

Marriott Marquis San Diego  
Marina  
San Diego Ballroom Salon C

## Nanoscience

B. G. Trewyn, *Organizer*

**8:30 716.** Prussian blue analogues for templated nanoparticle growth. **E.T. Nguyen**, D.A. Hardy, G.F. Strouse

**8:50 717.** Probing the electronic states of small metallic nanoparticles using conduction electron spin resonance. **S.S. Cruz**, B. Lear

**9:10 718.** Electrolyte-induced conformational change of alkanethiolate ligands on gold nanoparticles in organic solutions. **V. Tanygin**, B. Lear

**9:30 719.** Bottom-up design of metal oxide and peroxide nanoclusters using neural networks. **P. Miro**

**9:50 720.** Carbon capture with MgO(111). **R.M. Richards**

**10:10 721.** STEM-in-SEM methods for 2D material defect and reliability studies. **E. Mansfield**, J.D. Holm

**10:30 722.** Active plasmonics based devices using metal oxide nanocrystals: Fundamentals and applications. **A. Agrawal**, D.J. Milliron

Section E

Marriott Marquis San Diego  
Marina  
Santa Rosa

### Solid-State Inorganic Chemistry

C. G. Lugmair, V. Poltavets, *Organizers*  
R. Compton, T. Ortner, *Presiding*

**8:30 723.** Vacuum transport of transition metal-doped ZnSe fiber lasers. **A. Hendrickson**, J. Krug, C.J. Mathewson, M. Coco, S.C. Aro, S. McDaniel, P. Sazio, J. Mauro, G. Cook, V. Gopalan, J.V. Badding

**8:50 724.** New methods for measuring absolute optical constants using loose powders: Implementation, validation, and renewable energy applications. **P. Khalifah**, T. Glotch

**9:10 725.** Tuning the photoluminescence by controlling the oxidation states of dopants. **R. Gautier**

**9:30 726.** New additions to the cesium lithium chloride system: Cs<sub>3</sub>Li<sub>2</sub>Cl<sub>5</sub> and the hydrated Cs<sub>3</sub>LiCl<sub>4</sub> \* 4H<sub>2</sub>O. **T. Ortner**, J.P.

Scheifers, Y. Zhang, A. Iyer, J. Flores, B. Fokwa

**9:50 727.** Dimensional reduction of halide double perovskites. **B. Connor**, L. Leppert, M.D. Smith, J. Neaton, H. Karunadasa

**10:10 728.** Redox properties of dysprosium 3+/4+ in barium zirconate. **J.R. O'Brien**, S. Ricote, L. Krishna

**10:30** Intermission.

**10:45 729.** Structural and physical properties of CaLaMReO<sub>6</sub>. F. Yuan, **C.M. Thompson**

**11:05 730.** Geometrically frustrated magnetism in transition metal borides. **A. Iyer**, Y. Zhang, B. Fokwa

**11:25 731.** Varying the fermi level in gadolinium transition-metal aluminides. **G. Agbaworvi**, C. Thompson

**11:45 732.** Topotactic transformations of heterolayered borides. **L. Alameda**, R.E. Schaak

**12:00 733.** First-principles study of phase stabilities in Al<sub>1-x</sub>Fe<sub>x</sub>OOH and Al<sub>1-x</sub>Cr<sub>x</sub>OOH metal oxyhydroxides. **D. Pope**, A.E. Clark, M. Prange

**12:15 734.** Manipulating magnetic properties via chemical variations in TlFe<sub>3</sub>Te<sub>3</sub>. **R. Compton**, C.M. Thompson

Section F

Marriott Marquis San Diego  
Marina  
Marina Ballroom Salon E

### Organometallic Chemistry: Catalysis - Late Transition Metals

N. S. Radu, *Organizer*  
M. A. Bowring, *Presiding*

**8:30 735.** Mechanistic insights of the direct arylation of arylhalides: Density functional theory study. **R. Wei**, P. Miro

**8:50 736.** Modeling the reactivity of alkanes toward organometallic electrophiles. **P.J. Perez**, A. Caballero, G. Asensio, M. Etienne, F. Maseras, A. Olmos, R. Gava, M. Besora, K. Jacobs

**9:10 737.** Thermodynamic hydricity as a tool for designing catalysts for hydrogenation of ketones and esters. **E.S. Wiedner**, B. Neisen, J.C. Linehan, A.M. Appel

**9:30 738.** Highly active ruthenium metathesis catalysts at low temperatures: Unprecedented ring-

opening metathesis polymerization of cyclopentadiene. **S. Hong**

**9:50 739.** Robust Re(V) alkylidyne catalysts for alkyne metathesis reactions. **M. Cui**, W. Bai, H. Sung, I. Williams, Z. Lin, G. Jia

**10:10 740.** Strongly  $\sigma$ -donating ligands with pendant bases for water oxidation catalysis. **A.G. Nash**, B.D. Vincenzini, C.J.

Breyer, B.E. Silva, D.B. Grotjahn

**10:30 741.** Large isotope effects in organometallic reactions. **M.A.**

**Bowring**, P.T. Truong, E.D. Douma, M.P. Ahmad, Z. Mathe, J. Tsang

**10:50 742.** High variance of metal oxidation states in nickel catalysis. A. de Aguirre, I. Funes-Ardoiz, **F. Maseras**

**11:10 743.** Reversible CO<sub>2</sub>/formate conversion by a homogeneous platinum electrocatalyst. **D.W. Cunningham**, J.Y. Yang

Section G

Marriott Marquis San Diego  
Marina  
Marina Ballroom Salon G

### Main Group Chemistry

T. Hudnall, *Organizer*  
F. Jaekle, E. Lee, *Presiding*

**8:30 744.** Reactive phosphonium cations. **R. Dobrovetsky**

**8:50 745.** *N*-heterocyclic carbene-functionalized ferrocenes. **E. Lee**

**9:10 746.** Lewis pair functionalization of polycyclic aromatic hydrocarbons. K. Liu, M. Vanga, R. Lalancette, **F. Jaekle**

**9:30 747.** Lewis adduct formation of sulfones, sulfonate, and sulfate esters with arsenic and antimony pentafluoride. **T.H. Saal**, K.O. Christe, R.M. Haiges

**9:50** Intermission.

**10:00 748.** C<sub>6</sub>F<sub>5</sub>B-Binolate: Synthesis, structure, Lewis acid–base chemistry and catalytic activity. **S. Garg**, C. Krempner

**10:20 749.** Guanidine-based intramolecular frustrated Lewis pairs (FLPs): Synthesis, structure and small molecule activation. **C. Manankandayalage**, C. Krempner

**10:40 750.** Reductive elimination at a carbene center. **D.R.**

**Tolentino**, S. Neale, C. Isaac, S. Macgregor, M.K. Whittlesey, R. Jazzar, G. Bertrand

**11:00 751.** Carbenes and catalysis. **T. Ong**

##Next Division##