

INOR

Division of Inorganic Chemistry

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

OTHER SYMPOSIA OF INTEREST:

Homogeneous Catalysis for Applied Organic Synthesis (see *CATL*, Mon, Tue)

Innovative Chemistry & Materials for Electrochemical Energy Storage (see *ENFL*, Sun, Mon, Tue, Wed)

Carbon Dioxide Conversion & Artificial Photosynthesis (see *ENFL*, Sun, Mon, Tue)

Actinide Complexes & Nanoclusters (see *NUCL*, Sun, Mon, Tue)

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium (see *PROF*, Sun, Mon)

Radiopharmaceutical Chemistry (see *FLUO*, Tue, Wed, Thu)

SUNDAY MORNING

Section A

Ernest N. Morial Convention Center Room 345

Synthetic Chemistry Addressing Challenges in Energy & the Environment

Cosponsored by *CATL* and *WCC*
L. A. Berben, A. De Bettencourt Dias, A. L. Prieto, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 1. Synthesis and characterization of the Zintl phase $\text{Yb}_{2.4}\text{Eu}_x\text{CdSb}_2$ for direct thermal to electrical energy conversion. **S. Kauzlarich**

8:55 2. Mössbauer spectroscopic insights into the electronic structure and mechanism of bio-inspired iron complexes. **C.V. Popescu**, P. Ghosh, S. Ding, M.Y. Darenbourg, M.B. Hall

9:15 3. The synthesis and characterization of metal organic frameworks for CO_2 utilization. J. Zhu, P. Usov, **A.J. Morris**

9:35 Intermission.

9:45 4. Obtaining white light from layered perovskites. M.D. Smith, A. Jaffe, E. Dohner, A. Lindenberg, **H. Karunadasa**

10:05 5. Linear and star block copolymers derived from biorenewable resources as adsorbents for waste water remediation. **A.M. Balija**, K. Bernhardt, K. Moore

10:25 6. New trimetallic assemblies for solar energy conversion: combining new light absorbers with new catalysts. **C. Turro**, W.T. Kender, K.R. Dunbar

10:45 Intermission.

10:55 7. Developing a mild and modular route to chemically modified electrodes for photoelectrochemical cells. **J.Y. Yang**

11:15 8. Use of peptoids for molecular recognition of contaminants in water.

A.A. Fuller, K.M. Tenorio, J. Huber, K. Dowell, S. Hough

11:35 9. Re-wiring biological hydrogen production. **A. Parkin**

Section B

Ernest N. Morial Convention Center Room 344

Metal-Organic Frameworks: What Are Next?

W. Lin, H. Zhou, *Organizers*

S. Ma, *Organizer, Presiding*

B. Wang, *Presiding*

8:30 Introductory Remarks.

9:20 10. MOF design to applications: Impact of pore system control on gas separations and storage. **M. Eddaoudi**

9:50 11. polyMOFs: Bridging the polymer-MOF materials gap. **S. Cohen**, Z. Zhang, S. Ayala, G. Schukraft

10:20 Intermission.

10:30 12. The organic secondary building unit: π -Stacking interactions define topology in MOFs. **M. Dinca**, S. Park, L. Xie

11:00 13. Electrically conductive coordination networks. **H. Kitagawa**

11:30 14. Metal-organic frameworks applications in the face of increasing demand for novel electronic materials to advance special purpose technologies. **J. Ornstein**, R. Ozdemir

Section C

Ernest N. Morial Convention Center Room 343

ACS Award in Organometallic Chemistry: Symposium in honor of Clifford P. Kubiak

J. S. Figueroa, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 15. Role of uranium–arene bonding in H_2O reduction catalysis. **K. Meyer**

9:00 16. Excited states of new bimetallic complexes for solar energy applications. **C. Turro**, T.J. Whittimore, C. Xue, T.A. White, H.J. Sayre

9:25 17. Elucidating the mechanism of CO_2 reduction to CO by group 6 $\text{M}(\text{CO})_6$ species using infrared spectroelectrochemistry and quantum chemistry. **K.A. Grice**, C. Saucedo, M. Groenonboom, J. Nganga, A.M. Angeles Boza, J.A. Keith

9:50 18. Organic mixed valence compounds and Kekulé diradicaloids derived from CAACs. **G. Bertrand**

10:15 19. Polypyridyl electrocatalysts for the reduction of CO_2 . L. Lieske, **C.W. Machan**

10:40 Intermission.

11:00 20. Running the alphabet from A(-frames) to Z(-schemes) with hydrogen. **R. Eisenberg**

11:25 21. Second-sphere coordination assists metal-halogen bond photoactivation. **D.G. Nocera**, S. Hwang, D. Gyi

11:50 22. From ceiling to fluorine: Stable metal heptafluoroisopropyl complexes and transfer reagents. N.O. Andrella, K. Liu, M. Vasiliu, D.A. Dixon, **R. Baker**

Section D

Ernest N. Morial Convention Center Room 352

ACS Award in Inorganic Chemistry: Symposium in honor of James Moers Mayer

S. N. Brown, C. T. Saouma, *Organizers*
J. J. Warren, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 23. Interfacial proton-coupled electron transfer: Interplay between experiment and theory. **S. Hammes-Schiffer**

8:55 24. Identifying proton-coupled electron transfers that give rise to potential- pK_a relationships in catalysis. **J.L. Dempsey**, E. Rountree, B.D. McCarthy

9:15 25. Mechanisms and distance-dependence of proton-coupled electron transfer. **L. Hammarstrom**

9:35 26. Hydrogen atom transfer reactions of bis(iminosemiquinonato)palladium(II) and -platinum(II): Thermodynamic and kinetic coupling. **S.N. Brown**, K.M. Conner, A.C. Arostegui, D.D. Swanson

9:55 27. Investigating concerted proton-electron transfer with base-appended radical cations. E.A. Welker, D.J. Robinson, B.L. Tiley, C.M. Sasaran, M. Vettleson, N.T. Fretz, J.J. Geruntho, M.A. Zuchero, W. Tong, R.A. Richards, F.M. Simpson, S. Stoll, J. Wolbach, **I.J. Rhile**

10:15 Intermission.

10:25 28. Examining the effects of structural modifications on explosive sensitivity. **V. Manner**, M. Cawkwell, E. Kober, T. Myers, J. Yeager, G. Brown, H. Tian

10:45 29. Metal complexes of “two-story” calix[6]arene ligands: Structure and reactivity. **D.E. Over**, G. De Leener, N. Le Poul, F. Topić, K.T. Rissanen, Y.F. Le Mest, I. Jabin, O. Renaud

11:05 30. Sterically undemanding pincer ligands: Reactions of iridium complexes. **D.M. Heinekey**, T. Lekich, B. Gary, S.M. Bellows, T.R. Cundari

11:25 31. Sulfuric acid catalyzed cyclohexylbenzene hydroperoxide cleavage: effects of reaction medium and mechanistic implications. **K. Wang**, R. Garcia

Section E

Ernest N. Morial Convention Center Room 353

ACS Award in Pure Chemistry: Symposium in honor of Mircea Dinca

Y. Roman-Leshkov, *Organizer*

Y. Surendranath, *Organizer, Presiding*

8:00 Introductory Remarks.

8:10 32. Hydrocarbon separations in metal-organic frameworks. J. Bachman, M. Kapelewski, M.I. Gonzalez, D. Reed, E.D. Bloch, Z. Herm, J.A. Mason, **J.R. Long**

8:40 33. Advanced porous organic polymers for environmental remediation. **S. Ma**

9:10 34. Postsynthetic metal exchange in pincer MOFs. **C.R. Wade**, A.A. Kassie

9:40 35. Bioinspired sponges: Design principles for metal-organic frameworks-enzymes composite. **O.K. Farha**

10:10 Intermission.

10:30 36. Strategies for incorporating p-block element catalysts inside MOFs for reductions and oxidations.. B. Tahmouresilerd, P. Larson, **A.F. Cozzolino**

11:00 37. Metal-organic frameworks as flasks: Chromophore photophysics in a confined environment. **N.B. Shustova**, E. Dolgoplova, A.M. Rice

11:30 38. Withdrawn

Section F

Ernest N. Morial Convention Center Room 354

Alfred Bader Award in Bioinorganic or Bioorganic Chemistry: Symposium in honor of Alison Butler

Cosponsored by *WCC*

J. S. Martinez, *Organizer*

M. Haygood, *Presiding*

8:30 Introductory Remarks.

8:40 39. Siderophore production and quorum sensing in the marine bacterium *Vibrio Harveyi*. D.L. McRose, **F. Morel**

9:05 40. Iron recycling in marine systems: Of microbes and molecules. **K.A. Barbeau**

9:30 41. Alkane oxidizing enzymes in the marine environment: What we can learn from integrating biochemistry, microbiology, and omic databases. **R.N. Austin**

9:55 42. Siderophores in a symbiotic system. **M. Haygood**, H. Naka

10:20 Intermission.

10:40 43. Abundant mesopelagic metalloenzymes in the Pacific oxygen minimum zone. **M. Saito**, M.R. McIlvin, D.M. Moran, A. Santoro, C. Dupont, C. Lamborg, P. Rafter

11:05 44. Redox chemistry and mussel adhesion. **H. Waite**

11:30 45. Mechanistic investigations of manganese(IV) oxide biomineralization catalyzed by a multicopper oxidase complex. **B.M. Tebo**, C. Romano, A. Soldatova, M. Zhou, A.C. Dohnalkova, L. Kovarik, L. Tao, T.A. Stich, Y. Song, V.H. Wysocki, L. Pasa-Tolic, W.H. Casey, R. Britt, T.G. Spiro

11:55 46. Solution and (nano)particulate chemistry within the dynamic mixing zone of the first 2 meters of hydrothermal vent orifices. **G.W. Luther**, E.R. Estes, A. Findlay, M. Yucel, A. Gartman, R. Rosas, N.R.

Coffey, V.E. Oldham, T.J. Shaw, J. Ferry, M.c. Dias, B.M. Tebo

Section G

Ernest N. Morial Convention Center Room 210

Nitrogen Un-Fixation: Mechanisms & Models of Nitrification/ Denitrification Reactions

K. M. Lancaster, *Organizer*

N. Lehnert, *Organizer, Presiding*

8:30 47. Nitrite-ammonia expressway, with no stop at dinitrogen. **P.M. Kroneck**

9:00 48. Evolution and modularity of ammonia oxidation pathways. L.Y. Stein, **M.G. Klotz**

9:30 49. Evaluating the mechanism of NO reduction in a flavodiiron nitric oxide reductase model complex. **C. White**, N. Lehnert

9:50 50. Nitrous oxide reduction mediated by a nucleophilic nickel(II) sulfide. **T.W. Hayton**

10:20 Intermission.

10:30 51. Structure and function of particulate methane monooxygenase, an ammonia monooxygenase homolog. **A.C. Rosenzweig**

11:00 52. Synthetic copper-sulfide models of Cu₂ with activity towards N₂O and other small molecules. B. Johnson, S. Bagherzadeh, S. Rathnayaka, C. Hsu, **N.P. Mankad**

11:30 53. Revision by enzymology of bacterial ammonia oxidation. **J.D. Caranto**

11:50 54. Probing mechanisms of nitrous oxide generation in a denitrifying polyphosphate accumulating bacteria enrichment culture. H. Gao, Y. Mao, T. Zhang, **G. Wells**

Section H

Ernest N. Morial Convention Center Room 211

Undergraduate Research at the Frontiers of Inorganic Chemistry

C. Nataro, L. A. Watson, *Organizers*
K. L. Stone, *Presiding*

8:30 Introductory Remarks.

8:40 55. Schiff-base vanadium(V) catecholate complexes and their interactions with a model membrane interface. S.M. Petry, J.T. Koehn, C.M. Glover, A. Levina, P. Lay, **D.C. Crans**

9:00 56. Synthesis, characterization, and reactivity of platinum indazole complexes with potential anti-cancer activity. **R.E. Bachman**, K. Barwick, A.J. Bachman, K.A. Wheeler

9:20 57. Mixed fluorinated subphthalocyanines and subnaphthalocyanines: Tuning fluorescence by synthetic design. **K.J. McAuliffe**, L. Sejdarsi, E.R. Trivedi

9:40 58. Understanding the molecular basis of multiple mitochondrial dysfunctions syndrome 1: Impact of substitution on the structure and

function of the essential iron-sulfur protein NFU1. **N. Wesley**, J. Cowan

10:00 Intermission.

10:15 59. Intramolecular hydrogen bonding between peptide strands directed by a rigid, bimetallic ring system. **T.P. Curran**, J.L. Stewart, T.T. Nguyen, J. Frempong

10:35 60. Modeling coupled binuclear copper enzymes using *de novo* designed *Due Ferri* single chain (DFsc) proteins. **B. VanDyke**, A.J. Reig

10:55 61. The IONiC/VIPeR Grand Experiment in teaching inorganic chemistry: Come join us! **B.A. Reisner**, **J.L. Stewart**

11:15 Discussion.

Section I

Ernest N. Morial Convention Center Rooms 340/341

Bioinorganic Chemistry: Proteins & Enzymes & Model Systems

S. A. Koch, *Organizer*

P. J. Farmer, Y. Zhang, *Presiding*

8:30 62. Catalysis of superoxide degradation by a Zn(II) complex with a quinol-containing ligand. M.B. Ward, M. Yu, A. Scheitler, I. Ivanovic-Burmazovic, **C.R. Goldsmith**

8:50 63. Photoswitchable probes to reversibly control the activity of carbonic anhydrase in cancer cells. **K. Aggarwal**, E.L. Que

9:10 64. Copper guanidinoquinoline complexes as entatic state models of electron transfer proteins. **J. Stanek**, A. Hoffmann, S. Herres-Pawlis

9:30 65. Tyrosinase model systems with efficient catalytic activity. **P. Liebhäuser**, C. Wilfer, A. Hoffmann, S. Herres-Pawlis

9:50 66. Multiple-site, long-distance concerted proton electron transfer in biomimetic metallopeptides. **B. Koronkiewicz**, J. Swierk, C.A. Schmuttenmaer, J.M. Mayer

10:10 Intermission.
10:20 67. A computational investigation of some mechanistic effects of metal center on regulating reactivity of heme-copper oxidase. M. Michael, Y. Shi, **Y. Zhang**

10:40 68. Mechanism-guided design of efficient P450 catalysts for C-H amination via nitrene transfer. **V. Steck**, R. Fasan

11:00 69. Quantum chemical modeling of metal-dependent decarboxylases. **F. Himo**

11:20 70. Building copper active sites in artificial metalloproteins. **S.I. Mann**, T. Heinisch, T.R. Ward, A. Borovik

11:40 71. Photo-induced oxygenations of Ru(II) bisbipyridyl flavonolate complexes. **P.J. Farmer**, X. Han, M. Kumar, M.A. Omary, M. Ghimire

12:00 72. Engineering the facial triad of the alpha-ketoglutarate oxygenase FIH. **M. Knapp**

Section J

Ernest N. Morial Convention Center Room 212

Chemistry of Materials: Materials for Energy & Catalytic Applications

C. G. Lugmair, *Organizer*

P. Dongare, C. Schoettle, *Presiding*

8:30 73. 9,10-Dihydro-9,10-diboraanthracene salts as versatile catalysts. **E. von Grothuss**, M. Wagner

8:50 74. (Ag)Au concave cubes as experimental models of computationally predicted active sites for the oxygen-assisted coupling of alcohols. **D. Robertson**, M.E. King, M.L. Personick

9:10 75. Highly active and stable calixarene-protected clusters for hydrogenation catalysis. **C. Schoettle**, A. Okrut, A. Palermo, A. Solovoyov, A.S. Katz

9:30 76. Refinement of aerosol processes to generate highly dispersed catalytic centers for metathesis on silica supports. **B.S. Hanna**, M. Bukhovko, S.C. Hayden, S. Shaikh, M. Khokhar, S. Zhang, D.F. Consoli, Y. Roman-Leshkov, M. Ostraat

9:50 Intermission.

10:05 77. Synthesis of POSS based hybrid catalysts and their application in alkane oxidation. **A.J. Karkamkar**

10:25 78. Mechanistic investigation of alkyl benzene photooxidation by flavin photocatalyst. **P. Dongare**, I. MacKenzie, D.A. Nicewicz, T.J. Meyer

10:45 79. Characterization of and catalysis with lattice-confined reactive intermediates. **D. Powers**

11:05 80. Carbonate-promoted C-H carboxylation of aromatic hydrocarbons with CO₂. **D.J. Xiao**, A. Yau, M. Kanan

Section K

Ernest N. Morial Convention Center Room 335

Coordination Chemistry: Synthesis & Characterization

A. Larsen, *Organizer*

W. Lee, N. A. Piro, *Presiding*

8:30 81. From T-shaped to face-capping: A flexible bisguanidiny pyridine ligand for Fe to Zn. J.E. Allen, **N.A. Piro**

8:50 82. Allosteric regulation of a four-state WLA macrocycle. **A. d'Aquino**, H. Cheng, J. Barroso, Z. Kean, J.E. Mendez, C. McGuirk, C.A. Mirkin

9:10 83. Synthesis and structural characterization of copper(I) oxalate complexes. **A.T. Royappa**, A.D. Royappa, R.F. Moral, A.L. Rheingold, R.J. Papoular, D.M. Blum, T.Q. Duong, **J.R. Stepherson**, O.D. Vu, B. Chen, M.R. Suchomel, J.A. Golen, G. André, N. Kourkoumelis, A.D. Mercer, A.M. Pekarek, D.C. Kelly, C.L. Stern, P. Mueller

9:30 84. Crystal structure of zirconium tetrachloride revisited. **R. Borjas Nevarez**, S.M. Balasekaran, E. Kim, P. Weck, F. Poineau

9:50 85. Electronic coupling in cationic and anionic ligand-centered, mixed-valence complexes of nickel, palladium, and platinum. **C.P. Ramirez**, A.F. Heyduk

10:10 Intermission.

10:20 86. Synthesis and characterization of an iron complex bearing a hemilabile NNN-pincer for catalytic hydrosilylation of organic carbonyl compounds. H. Lin, M. Zeller, C. Chen, **W. Lee**

10:40 87. Synthesis and structural characterizations of fluorine substituted cobalt oxo-cubes. **A. Rahman**, A. Nicolay, P. Lee, R. Lavoire, T. Tilley

11:00 88. Structural and vibrational spectroscopic studies of hexafluororhenate (IV) salts. **J. Louis-Jean**, S. Mariappan Balasekaran, D. Smith, A. Salamat, C. Pham, F. Poineau

11:20 89. Counter ion influence based on the copper(II) methylbenzoic acid complex mixed with 2,2'-bipyridine: Synthesis, X-ray characterization and biological activity. **J.A. Obaleye**, A.A. Ajibola, V.B. Bernardus

Water, Water Everywhere But Not a Drop to Drink: Preserving, Protecting & Delivering Clean Water
Sponsored by PRES, Cosponsored by AGFD, BMGT, CATL, CEI, CELL, CHAS, CHED, COLL, CTA, ENVR, GEOC, I&EC, INOR, MPPG, SCHB and YCC

Fluid-Solid Interfacial Phenomena at the Nexus of Energy & Geochemistry Research: A Symposium in Honor of David J. Wesolowski

Sponsored by GEOC, Cosponsored by COLL, ENFL, ENVR and INOR

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Emerging Applications of Organic & Biochemistry: Soil Science, Biomaterials & Synthesis

Sponsored by PROF, Cosponsored by ANYL[‡], BIOL[‡], BIOT, CHED, CMA, COLL, COMP[‡], CWD, ENVR, INOR[‡], MEDI[‡], ORGN, PHYS[‡], PMSE[‡], POLY[‡], PRES[‡], WCC and YCC

Control of Zeolite Structure, Composition & Sites for Catalysis
Sponsored by CATL, Cosponsored by INOR

Activation of Light (C1-C4) Hydrocarbons: Theory & Experiments

Sponsored by CATL, Cosponsored by ENFL, INOR and PHYS

Innovative Chemistry & Materials for Electrochemical Energy Storage
Sponsored by ENFL, Cosponsored by CATL, INOR and PMSE

Challenge & Opportunity in Lignin Valorization

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

SUNDAY AFTERNOON

Section A

Ernest N. Morial Convention Center
Room 345

Synthetic Chemistry Addressing Challenges in Energy & the Environment

Cosponsored by CATL and WCC

L. A. Berben, A. De Bettencourt Dias, A. L. Prieto, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 90. Structural and thermochemical parameters influencing the PCET formation of a cobalt(III)-hydride. **J.L. Dempsey**, D. Kurtz, N. Elgrishi, W.C. Howland, B. Kandemir

1:55 91. Biosynthesis of the H-cluster of the [FeFe]-hydrogenase. **J.B. Broderick**

2:15 92. Surface-ligand induced stabilization of plasmonic behavior of copper sulfide nanoparticles. Z. Georgieva, M. Tomat, **K. Plass**, C. Kim
2:35 93. Aqueous chemistry of transition metal complexes of perfluoropinacolate ligands. J.E. Henebry, E.M. Laaker, **L.H. Doerr**
2:55 Intermission.

3:00 94. Mimicking nature by metal-organic frameworks: Perspective and applications. **N.B. Shustova**, E. Dolgoplova, A.M. Rice, B. Yarbrough
3:20 95. Bio-inspired dehalogenation: Developing first-row transition metal complexes to treat priority pollutants perchloroethylene and trichloroethylene. **K.M. Van Heuvelen**
3:40 96. Manipulating the thermoelectric properties of polymer semiconductors. J. Ogle, M. Teferi, C. Boehme, **L.L. Whittaker**
4:00 97. Elemental distribution and excited state dynamics in oxynitride nanocrystals. **G. Dukovic**

Section B

Ernest N. Morial Convention Center
Room 344

Metal-Organic Frameworks: What Are Next?

W. Lin, S. Ma, H. Zhou, *Organizers*
B. Chen, D. Jiang, *Presiding*

1:30 98. Toward forth generation porous coordination polymers/metal-organic frameworks. **S. Kitagawa**
2:15 99. Optimizing NIR-emitting MOFs through design and modulation of Ln-MOF platforms. **N.L. Rosi**, T. Luo, C. Liu, P. Muldoon
2:45 100. Metal-organic frameworks for programmable drug release. **H. Deng**
3:15 101. A novel application of Metal Organic Framework (MOF) as a smart fragrance delivery vehicle for consumer products. **L. Pan**
3:35 Intermission.

3:50 102. A toolkit for the modification of high valent carboxylate MOFs. **H. Zhou**, S. Yuan

4:20 103. Exchange of linkers and guests in MOFs. **A.J. Matzger**

4:50 104. Evolution of form in metal-organic frameworks. **W. Choe**

Section C

Ernest N. Morial Convention Center
Room 343

ACS Award in Organometallic Chemistry: Symposium in honor of Clifford P. Kubiak

J. S. Figueroa, *Organizer*
A. A. Barney, *Presiding*

1:30 105. Electrocatalytic alcohol oxidation with molecular catalysts. **R.M. Waymouth**, K.M. Waldie, E. McLoughlin, C.E. Chidsey

1:55 106. Structural and chemical aspects of metal-isocyanide network materials. **J.S. Figueroa**, D. Agnew, A. Arroyave

2:20 107. Phosphinidene chemistry stemming from anthracene-based reagents. W.J. Transue, A. Velian, M.B. Geeson, M. Nava, **C.C. Cummins**

2:45 108. Bifunctional metalloligands in $Mn_2S_2 \bullet Re/Mn(CO)_3X$ complexes designed for CO_2 reduction catalysts. A.M. Lunsford, N. Arnet, S. Ding, M.B. Hall, **M.Y. Darensbourg**

3:10 Intermission.

3:30 109. Capturing intermediates of molecular catalyst/semiconductor systems by transient mid-IR spectroscopy. **L. Hammarstrom**, M. Abdellah, M. Gilbert Gatty

3:55 110. Electrochemically-promoted catalytic asymmetric hydrogenation using chiral organorhodium complexes. **B.T. Donovan-Merkert**

4:20 111. Organometallic species at the heart of small molecule reduction catalysis. **J.C. Peters**

4:45 112. Catalytic C-H borylation: New catalysts with high regioselectivities for challenging substrates. **M.R. Smith**

Section D

Ernest N. Morial Convention Center
Room 352

ACS Award in Inorganic Chemistry: Symposium in honor of James Moers Mayer

C. T. Saouma, J. J. Warren, *Organizers*
S. N. Brown, *Organizer, Presiding*

1:30 113. Mechanistic studies on iron-catalyzed alkene coupling reactions. D. Kim, **P.L. Holland**, W. Rahaman, R. Poli

1:50 114. The role of amines in CO_2 reduction. **C.T. Saouma**

2:10 115. Mechanistic studies of the insertion of carbon dioxide into late transition metal element sigma bonds. **N. Hazari**, J. Heimann

2:30 116. Proton relays in CO_2 reduction catalysts: Is one enough? **J.J. Warren**, S. Sinha, S. Hanson

2:50 117. Metal-oxido and metal-hydroxido complexes in biology. **A. Borovik**

3:10 Intermission.

3:20 118. Proton-electron promoted reductive O-O cleavage within synthetic heme- O_2 -copper assemblies. **K.D. Karlin**, S.M. Adam, G.B. Wijeratne, P.J. Rogler, S. Sharma, I. Garcia-Bosch

3:40 119. Radical reactions at metal-oxo complexes: Revisiting old questions about metal-oxo " π radicals". **J.D. Soper**

4:00 120. Mechanisms of dinitrogen cleavage and nitride reduction to ammonia at pincer complexes. **A.J. Miller**, S. Schneider, I. Siewert, F. Hasanayn, B.M. Lindley, R.S. van Alten, Q.J. Bruch

4:20 121. Adding or removing protons and electrons in metal-mediated reduction of N_2 and oxidation of NH_3 . **R. Bullock**, D. Prokopchuk, A.J. Kendall, P. Bhattacharya, E.S. Wiedner, M.T. Mock

Section E

Ernest N. Morial Convention Center
Room 353

ACS Award in Pure Chemistry: Symposium in honor of Mircea Dinca

Y. Roman-Leshkov, *Organizer*
Y. Surendranath, *Organizer, Presiding*

1:30 Introductory Remarks.

1:40 122. MOF-templated metallic clusters as catalysts and electrocatalysts. C. Kung, Z. Li, A. Atilgan, O. Farha, **J.T. Hupp**

2:10 123. Electrically conductive metal-organic frameworks: Insights from theory. **C.H. Hendon**

2:40 124. Metal-semiquinoid magnets: From molecules to materials. I. Jeon, J. DeGayner, L. Liu, **D. Harris**

3:10 Intermission.

3:30 125. Strategies and results for controlled activation of small-molecule zinc sensors in cells. J.M. Goldberg, **S.J. Lippard**

4:00 126. Transition metal signaling in the brain and beyond. **C.J. Chang**

4:30 127. Bioinorganic explorations of the competition for nutrient metal ions at the host/microbe interface. **E.M. Nolan**

5:00 128. Carbon-fixation pathway of the bionic leaf. C. Liu, S. Nangle, P. Silver, **D.G. Nocera**

Section F

Ernest N. Morial Convention Center
Room 354

Alfred Bader Award in Bioinorganic or Biorganic Chemistry: Symposium in honor of Alison Butler

Cosponsored by WCC

J. S. Martinez, *Organizer*
V. L. Pecoraro, *Presiding*

1:30 Introductory Remarks.

1:40 129. New biology revealed by tracking mobile zinc in the brain. **S.J. Lippard**

2:05 130. Metals, drugs and disease.

K.J. Franz

2:30 131. Investigations of siderophore-mediated antibiotic delivery to Gram-negative bacteria. **E.M. Nolan**

2:55 132. Biosynthesis of methanobactin. **A.C. Rosenzweig**

3:20 Intermission.

3:40 133. In sickness and in health: Relationships between plasma metal ions and the development of infectious diseases. **P.L. Carver**

4:05 134. Seeing red: The role of heme in *Pseudomonas aeruginosa* virulence and pathogenesis. **A. Wilks**, S. Mourifio, W. Huang, A.T. Dent

4:30 135. Immunotherapy is enhanced by vanadium compounds. **D.C. Crans**, M. Selman, J. Diallo

4:55 136. A bioinorganic-inspired approach for developing inhibitors of influenza endonuclease. **S. Cohen**, C.V. Credille, B. Dick, C. Morrison

Section G

Ernest N. Morial Convention Center
Room 210

Nitrogen Un-Fixation: Mechanisms & Models of Nitrification/Denitrification Reactions

K. M. Lancaster, N. Lehnert,
Organizers

J. D. Caranto, *Presiding*

1:30 137. Bioinorganic aspects of nitrogen monoxide (NO) oxidation or reduction chemistry mediated at copper or heme centers. **K.D. Karlin**, J.J. Liu, G.B. Wijeratne, R. Cao, S. Sharma
2:00 138. A missing link from nitric oxide to nitrite in ammonia oxidizing bacteria. **K.M. Lancaster**, M. Smith, J.D. Caranto

2:30 139. Investigation of enzymatic N_2O production through isotopic analysis and engineered enzymes. **C. Finders**, E.L. Hegg, J. Haslun, N. Ostrom

2:50 140. Modeling key intermediates in Cytochrome P450 Nitric Oxide Reductase: Electronic structure and reactivity. **N. Lehnert**

3:20 Intermission.
3:30 141. A metalloprotein functional mimic of cytochrome *c* nitrite reductase. **K. Bren**, Y. Guo, B. Kandemir, J. Stroka

4:00 142. Probing the mechanism of microbial N_2O production. **E.L. Hegg**, C. Finders, J. Haslun, N. Ostrom, N. Lehnert

4:30 143. Influences of the heme-lysine crosslink in Cytochrome P460 over redox catalysis and nitric oxide sensitivity. **A.C. Vilbert**, K.M. Lancaster

4:50 144. Rebalancing the nitrogen cycle: Earth-abundant metal reduction of nitrate with purpose-designed ligands. **K.G. Caulton**, A. Cabelof, D.M. Beagan, J. Seo, S. braley, A.V. Polezhaev, C. Chen

Section H

Ernest N. Morial Convention Center
Room 211

Undergraduate Research at the Frontiers of Inorganic Chemistry Catalysis, Coordination Chemistry & Materials

C. Nataro, L. A. Watson, *Organizers*
B. Fox, *Presiding*

1:30 145. Synthesis, separation, and characterization of two-dimensional tin (II) sulfide nanosheets. E. Juarez-Diaz, E.S. Aydil, **J.D. Dwyer**

1:50 146. Bio-derived building blocks for various drop in fuels and value added chemicals. **O. Staples, C. Moore, R. Jenkins, T. Semelsberger, W. Kubic, A.D. Sutton**

2:10 147. Synthesis and spectroscopic studies of rhodium pincer hydride complexes. **A. Talosig, O. Ozerov, B. Morse, A. Larsen**

2:30 Intermission.

2:45 148. Synthetic, spectroscopic, and computational study of SNS copper(I) pincer complexes based on bis-imidazole and bis-triazole precursors: Impact of ligand design and solvent coordination on conformer interconversion. **J.R. Miecznikowski, M. Lynn, J. Jasinski, E. Reinheimer**

3:05 149. High throughput synthesis of thermoelectric nanocrystals: Investigation of the lithium, zinc, antimony phase space. **K. Baumler, A. White, A. Medina-Gonzalez, J. Vela**

3:25 150. Synthesis and structural characterization of $RE_6Cd_{23}T$ ($RE = La-Gd$; $T =$ late group 14, 15, or 16 element). **G.J. Desroches, S.S. Bobev**
3:45 151. Tuning cation exchange of copper chalcogenide nanoparticles. **A. Unruh, B. Li, H. Le, K. Plass**

Section I

Ernest N. Morial Convention Center
Rooms 340/341

Organometallic Chemistry: Synthesis & Characterization-Early Transition Metals

N. S. Radu, *Organizer*

C. Camp, J. A. Telsler, *Presiding*

1:30 152. Paramagnetic resonance spectroscopy of catalytically relevant organochromium(III) complexes. **J.A. Telsler, H. Hansen, J. Krzystek, M. Enders**

1:50 153. Influence of tetradentate macrocyclic ligand sterics on the conformational flexibility and photoluminescent properties of copper(I) complexes. **P. Patil, J. Khusnutdinova**

2:10 154. Synthesis, characterization and reactivity of chromium(VI) alkylidene complexes. **P. Wu, K.H. Theopold, G.P. Yap**

2:30 155. Zirconocene-amine intermolecular frustrated Lewis pairs. **H. Hamilton, A.M. King, O. Metters, D. Wass**

2:50 156. Light-dependent, zirconium-catalyzed hydrophosphination. **C. Bange, R. Waterman**

3:10 157. Towards tantalum-based early-late heterobimetallic complexes. **C. Camp**

3:30 158. Synthesis and characterisation of cyclopalladated with C^N ligand complexes for catalytic carbon hydrogen bond activation. **N.P. Yahaya**

3:50 159. Exploring Shrock cycle intermediates: Synthesis of CCC-NHC Ta bis imido complexes and their reactivity with hydrazine derivatives. **T.R. Helgert, T.K. Hollis, C.E. Webster, J. Denny, G. Liang, B. Donnadieu**

Section J

Ernest N. Morial Convention Center
Room 212

Environmental & Energy-Related Inorganic Chemistry

S. A. Koch, *Organizer*

B. L. Davis, T. M. Nenoff, *Presiding*

1:30 160. Progress toward high voltage, high cycle life non-aqueous flow cells for grid scale energy storage. **T. Chu, S. Maurya, I.A. Popov, N. Mehio, E.R. Batista, P. Yang, B.L. Davis**

1:50 161. Ligand exchange reactions of copper bipyridyl redox couples used in dye sensitized solar cells. **Y. Wang, T. Hamann**

2:10 162. Heterometallic molecular precursor for the preparation of low-temperature Li-Mn oxide. **H. Han, A.M. Abakumov, E. Dikarev**

2:30 163. N-heterocyclic carbene catalytic platforms for solar fuel conversions. **O. Luca, A.M. Lilio**

2:50 164. Capture of carbon dioxide via electrochemical concentration. **S.A. Chabolla, J.Y. Yang**

3:10 Intermission.
3:20 165. Curved carbon-rich materials for energy storage applications. **M.A. Petrukhina**

3:40 166. Structure-function trends in immobilized molecular catalysis of CO₂ reduction. **K. Prather, J.D. Blakemore**

4:00 167. Selective silica separations from waste water using ion-exchange media. **T.M. Nenoff, K. Sasan, P.V. Brady, J. Krumhansl**

4:20 168. The impact of surface chemistry and texture on the CO₂ uptake capacity of graphene oxide. **A.S. Alazmi, O. El Tall, M. Hedhili, P. Costa**

4:40 169. Stranded and shut-in gas provides a stop-gap measure for electrical demand. **S. Tedesco**

5:00 170. Nano-pyrite as a highly efficient reagent for remediation of chromate. **A.W. Apblett, A. Bergeson, T. Reed, J. Stephens**

Section K

Ernest N. Morial Convention Center
Room 335

Chemistry of Materials: Nanomaterials

C. G. Lugmair, *Organizer*
L. Wheeler, *Presiding*

1:30 171. On the use of carboxylic acid groups to graft photosensitizers on Ru nanoparticles for water splitting catalysis: Experimental and theoretical characterization of the surface composition. **R. Gonzalez Gomez, R. Poteau, K. Philippot, C. Amiens, I. Del Rosal, L. Cusinato**

1:50 172. Sequential cationic and anionic ligand exchange chemistry on cesium lead halide perovskite quantum dots for high-efficiency photovoltaics. **L. Wheeler, A. Marshall, E. Sanehira, P. Schulz, M. Suri, N.C. Anderson, J. Berry, L. Lin, J. Luther**

2:10 173. Molecular clusters as precursors for battery electrodes. **A. Pinkard**

2:30 174. Exploring the effect of nanoscale architecture on thermal conductivity of nanoporous SiO₂ films. **Y. Yan, M. Li, S. King, J. Kang, T. Galy, Y. Hu, S.H. Tolbert**

2:50 175. Low fluence multiphoton imaging with alloyed lanthanide nanocrystals. **B. Tian, A. Fernandez-Bravo, E. Chan, P. Schuck, B.E. Cohen**

3:10 176. *In vivo* X-ray imaging of transport of renal clearable gold nanoparticles in the kidneys. **J. Xu, M. Yu, J. Zheng**

3:30 Intermission.
3:45 177. PEI or GSH coated gold nanoparticles conjugated to cullin-5 DNA and heat shock protein 90 inhibitor, tanespimycin, for breast cancer therapy. **S. Talamantez-Lyburn, E. Ehrlich, M. Devadas**

4:05 178. Synthesis of core/shell nanoparticles and their impact on cytotoxicity of A549 lung cells. **W.C. Corbin, A.A. McBride, K.S. Butler, B.A. Hernandez-Sanchez**

4:25 179. Blood biocompatible conjugate of super robust and water-soluble gold-aryl functional nanoparticles with bovine serum albumin. **A. Mohamed, M. Karuthaka, M. Naggar, I.A. Shehadi, B. Workie**

4:45 180. Manganese and iron oxo-clusters as a substitute for gadolinium in MRI contrast. **V. Dahanayake, S.L. Stoll**

5:05 181. Photo/chemo/immunotherapy of primary tumor and remission of metastasis by using cascade upconversion nanoparticles

J. Chen

Actinide Complexes & Nanoclusters
Sponsored by NUCL, Cosponsored by INOR

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Experimental & Computational Frontiers in Inorganic & Materials Chemistry

Sponsored by PROF, Cosponsored by ANYL[‡], BIOL[‡], BIOT, CHED, CMA, COLL, COMP[‡], CWD, ENVR, INOR[‡], MEDI[‡], ORGN, PHYS[‡], PMSE[‡], POLY[‡], PRES[‡], WCC and YCC

Fluid-Solid Interfacial Phenomena at the Nexus of Energy & Geochemistry Research: A Symposium in Honor of David J. Wesolowski

Sponsored by GEOC, Cosponsored by COLL, ENFL, ENVR and INOR

Science Cafes & Engaging the Public: Techniques for Hosting Successful Events

Sponsored by PRES, Cosponsored by CATL, CELL, CHAS, CHED, COLL, CPRC, CTA, ENVR, I&EC, INOR, MPPG, SCHB and YCC

Control of Zeolite Structure, Composition & Sites for Catalysis

Sponsored by CATL, Cosponsored by INOR

Magnetically Recoverable Catalysts

Sponsored by CATL, Cosponsored by COLL, ENFL and INOR

Challenge & Opportunity in Lignin Valorization

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

Innovative Chemistry & Materials for Electrochemical Energy Storage

Sponsored by ENFL, Cosponsored by CATL, INOR and PMSE

SUNDAY EVENING

Section A

Ernest N. Morial Convention Center
Hall D

Undergraduate Research at the Frontiers of Inorganic Chemistry General

C. Nataro, L. A. Watson, *Organizers*
5:30 - 7:30

182. IONiC VIPER: Slithering to the next stage of improving the teaching and learning of inorganic chemistry. **L.A. Watson, C. Nataro, A.K. Bentley, H.J. Eppley, E.R. Jamieson, A.R. Johnson, J.R. Raker, B.A. Reisner, S.R. Smith, J.L. Stewart, N. Williams**

Section B

Ernest N. Morial Convention Center
Hall D

Undergraduate Research at the Frontiers of Inorganic Chemistry Bioinorganic Chemistry

C. Nataro, L. A. Watson, *Organizers*
5:30 - 7:30

183. Synthesis of a nickel iron phosphine complex: Structural mimic of carbon monoxide dehydrogenase

(CODH). **N. Sutthirat**, Z. Thammavongsy, J.Y. Yang
184. Ni²⁺ and Co²⁺ biomimetic structural analogues of the enzyme active site of acireductone dioxygenase (ARD). **A. Sanchez**, S.A. Toledo, V. Lynch
185. Investigating dechlorination abilities of bio-inspired nickel compounds. **R. Griffin-Hare**, C. Ye, B. Wada, K. Van Heuvelen
186. Cancer selective ruthenium prodrugs have been studied to show that pH can influence the distribution coefficient and uptake. **S. Altman**, A.R. Hairston, J. Gray, F. Qu, E.T. Papish
187. Peptides linked via a methyleneamine linker to a rigid, bimetallic ring system as a formation model system for β -sheet formation. T.P. Curran, J.L. Stewart, **P.R. Handali**, **J.P. Sanderson-Brown**
188. Synthesis and conformational analysis of peptides linked to a rigid, bimetallic ring system using aromatic spacers. T.P. Curran, J.L. Stewart, L.M. Davidson, N. Pokharel, **J. Frempong**, **M.L. Phillip**, **C.B. Gober**
189. Synthesis of new tridentate ligands to model the active sites of zinc metalloproteases. **S. Bradley**
190. Altering the *de novo* *Due Ferri* single chain protein to mimic the structure and reactivity of coupled binuclear copper enzymes. **S. Worthington-Kirsch**, B. VanDyke, A.J. Reig
191. Exploring the electronic structure of sulfite oxidase utilizing a metal complex bearing a selenium scorpionate ligand. **S. Nichols**
192. Ru(II)-diimine complexes for cross-linking P450 enzyme aggregates. **M. Do**, **M. Kato**, **L.E. Cheruzel**
193. Investigation of ⁸⁹Zr⁴⁺ chelation for positron emission tomography. **A. Chung**, M. Abdalrahman, B. Barron, R.P. Planalp

Section C

Ernest N. Morial Convention Center Hall D
Alfred Bader Award in Bioinorganic or Bioorganic Chemistry: Symposium in honor of Alison Butler
 Cosponsored by WCC
 J. S. Martinez, *Organizer*
5:30 - 7:30
194. Iron and gold nanoparticles, where do they go? Bioanalytical techniques to measure metal content by ICP-MS. **H.M. Neu**, K. Ok, S.A. Alexishin, M.A. Kane, J.E. Polli, S. Teymorian, M.H. Griep, S.L. Michel
195. Mechanistic investigations of thioesterase domain in siderophore biosynthesis. **A. Jelowicki**, Z.L. Reitz, A. Butler
196. A photoreactive marine siderophore from an *Alcanivorax* species with unique iron binding capabilities. **C.D. Hardy**, A. Butler

197. A suite of asymmetric siderophores produced by a marine *Shewanella* species. **J. Carmichael**, A. Butler
198. Genomics-based expansion of a natural combinatoric library of siderophores. **Z.L. Reitz**, K. Dulaney, A. Butler

Section D

Ernest N. Morial Convention Center Hall D
Nitrogen Un-Fixation: Mechanisms & Models of Nitrification/Denitrification Reactions

K. M. Lancaster, N. Lehnert, *Organizers*
5:30 - 7:30
199. Synthesis and characterization of cytochrome P460 active site model complexes. **R.E. Coleman**, K.M. Lancaster
200. Withdrawn
201. Role of redox non-innocence in a Co-based nitrate reduction electrocatalyst. **G.R. Ware**, D.C. Ashley, E. Jakubikova
202. Elucidating the role of nitrosocyanin in ammonia-oxidizing bacteria. **M. Smith**, J.D. Caranto, K.M. Lancaster
203. Investigating the mechanism of cytochrome P460 from the methanotroph *Methylococcus capsulatus* (Bath). **S.H. Majer**, K.M. Lancaster
204. A mechanistic view of Cytochrome *c* nitrite reductase (ccNiR)-catalyzed reduction of nitrite to nitric oxide- a partial reduction of six-electron reduction of nitrite to ammonia (ammonification)- by weak reducing agent. **M. Ali**
205. New synthetic model that relevant to NO reduction by flavodiiron NO reductases. **H. Dong**, C.J. White, N. Lehnert
206. Spectroscopic analysis of *Nitrosomonas europaea* cytochrome C₅₅₄ mutant F156H. **D.P. Koltermann**

Section E

Ernest N. Morial Convention Center Hall D
F. Albert Cotton Award in Synthetic Inorganic Chemistry: Symposium in honor of Andrew S. Borovik
 D. C. Lacy, C. G. Riordan, J. Y. Yang, *Organizers*
5:30 - 7:30
207. Remotely operated systems for primary recovery of ⁹⁹Mo from accelerator-driven sub-critical fission of LEU. **J.F. Krebs**, A. Youker, J. Byrnes, K. Quigley, S. Chemerisov, G. Vandegrift
208. Coordination chemistry of organomanganese phenolic-pincer complexes. **K. Kadassery**, S.N. MacMillan, D.C. Lacy
209. Synthesis and characterization of a high-spin Fe-NO enzyme model

complex with H-bond donors. **B. Burke**, M. Martin, G.P. Yap, R.C. Scarrow
210. Quantification of non-idealized hapticity in aza-heterocyclic adducts of Manganocene. **A.F. Cannella**, S. Dey, S.N. MacMillan, D.C. Lacy
211. Investigation of a peroxomanganese(III) species supported by a diazacycloalkane-based tetradentate ligand. **M. Denler**, T.A. Jackson, G.B. Wijeratne
212. Modulating the catalytic activity of first-row transition metal catalysts supported by redox-active ligands. **C.B. Kovel**, O. Villanueva, J.K. Elinburg, C.E. MacBeth
213. Nickel(II) catalyzed aziridination reactions. **D. Liu**, J. Bacsa, C.E. MacBeth
214. New (μ -Hydroxo)(μ -peroxo)diiron(III) complex: Structure, magnetism, Mössbauer spectra, and reactivity. **A. Kumar**
215. Catalytic aerobic oxidation of alcohols by copper complexes bearing redox-active ligands with tunable H-bonding groups. **K. Rajabimoghadam**, I. Garcia-Bosch
216. Ligand-based reductions in iron pyridinediimine complexes with protonated secondary coordination spheres. **P. Cheung**, J.D. Gilbertson
217. Effect of the second coordination sphere on reactivity of monomeric manganese complexes with terminal oxido and hydroxido ligands. **C. Sun**, S. Barman, J.R. Jones, A. Borovik
218. Mechanistic studies of cobalt-mediated C-H activation of aminoquinoline-directed biaryl coupling reactions. **E.E. Liu**, C.E. MacBeth, J. Bacsa
219. Biosynthetic inorganic chemistry: Artificial metalloproteins. **K.R. Miller**, S.I. Mann, D. Brazzolotto, L. Olshansky, A. Borovik
220. Biosynthetic inorganic chemistry. **V. Oswald**, J.L. Lee, C. Sun, D.L. Ross, J.A. Bogart, J.L. Kneebone, S.K. Barman, A. Borovik
221. Symmetric azulene-based π -linkers asymmetrically functionalized with isocyanide and mercapto junctions. **J. Applegate**, N.R. Erickson, N. Gerasimchuk, M.V. Barybin
222. Polyelectrochromism of diisocyanide-terminated, linear bi- and terazulenic platforms. **N.R. Erickson**, A.D. Spaeth, D.M. McGinnis, M.V. Barybin
223. Syntheses and structural comparison of [Co(DIG₃tren)X]BPh₄ complexes (X = halide). **D. Suryavanshi Magar**, R.C. Scarrow, G.P. Yap, M. Martin
224. Enticing anion reduction with Lewis acids in the secondary coordination sphere of iron (II) pyridinediimine complexes. **K.T. Burns**, J.D. Gilbertson
225. Exerting extreme π -acidity of isocyanoazulene ligands through

cyanation of the azulenic scaffold. **Z.A. Wood**, M.D. Hart, J.J. Meyers, N. Gerasimchuk, M.V. Barybin
226. Functional diversity in gentisate 1,2 dioxygenases: A spectroscopic study. **R. Gupta**, E. Eppinger, J. Gröning, A. Stolz

Section F

Ernest N. Morial Convention Center Hall D
Undergraduate Research at the Frontiers of Inorganic Chemistry, Organometallic Chemistry, Coordination Chemistry & Catalysis

C. Nataro, L. A. Watson, *Organizers*
5:30 - 7:30
227. Synthesis of dimeric zinc complexes for use as ring opening polymerization catalysts. **K.D. Brooks**, D.B. Green, A.L. Rheingold, J.M. Fritsch
228. Synthesis of chiral tridentate ligands for titanium and tantalum catalyzed asymmetric hydroamination. **A.R. Johnson**, **B.S. Mitchell**
229. Tuning hydrosilylation of hydrocarbons with substituted alpha-diamine iron(II) bromide precatalysts. **C.C. Cody**, C.E. Schulz, H.M. Hoyt
230. Synthesis of alkali and alkaline earth metal-NNN pincer complexes. **D. Haugh**, B. Wilson, A.Y. O'Brien, M.M. Gillett-Kunnath, K. Ruhlandt-Senge
231. Catalytic ring closing reactions of gold compounds containing bis(phosphino)ferrocene ligands. **T.A. Michaels**, C. Nataro
232. Synthesis, spectroscopy properties, structural and electrochemistry characterization of two novel heterometallic pentanuclear complexes. **K. Gutierrez**, D. Pinero
233. Progress toward development of Ni/Zn phosphineoxide catecholate bimetallic olefin polymerization catalysts. **Y. Nguyen**, T. Tran, L. Do
234. Tris(diphenylphosphinomethyl)phenylborates with electron donating and withdrawing groups at the bridgehead boron phenyl substituent. **S. Senthil**, J.T. Stephan, M. Swift, E.T. Chan, P.J. Fischer
235. An investigation of distant inductive effects on donation into group VI metals in tris(diphenylphosphinomethyl)phenylborate complexes. **J.T. Stephan**, S. Senthil, M. Swift, E.T. Chan, M.V. Vollmer, V.G. Young, Jr., P.J. Fischer
236. Design and synthesis of polymetallic coordination compounds. **J. Tami**, J.R. Jiménez, R. Plamont, R. Lescouëzec
237. Mixed-valent copper-based electrocatalysts for the oxygen evolution reaction. **B.H. Torda**, J.K. Nagle
238. Electronic and spectroscopic properties of [Ru(tpy)(tpyph(OH))][PF₆]₂ and [Ru(tpyph(OH))₂][PF₆]₂ (tpy =

- 2,2':6',2''-terpyridine; tpyph(OH) = 4'-(4-hydroxyphenyl)-2,2':6',2''-terpyridine). **C.L. Montgomery, C.N. Teahan, S.L. Shepherd, T. Dudley, D.P. Harrison, J.J. Paul**
- 239.** Synthesis of transition-metal catalysts with diverse potential reactivity. **A.A. DeLucia, K. Omolo, J.P. Sadighi, L.G. Habgood**
- 240.** Mechanochemical synthesis of chiral and achiral diphosphine dioxide manganese(II) complexes: Polymorphs and solid-state photoluminescence. **N. Rabaey, M. Stamp, D.E. Janzen**
- 241.** Synthesis of heavy donor antimony ligands coordinated to 3D metals for structural and electronic studies. **S. Shubert, L. Taylor, M.J. Rose**
- 242.** Reaction of quinolinethiols with Fe₃(CO)₁₂. **B. Simkhada, C.A. Mebi**
- 243.** Iron carbonyl complexes with mercaptopyrindines. **J. DeArmond, S. McLendon, E. Boraj, F. Oliver, C.A. Mebi**
- 244.** Synthesis of copper complexes with 3-hydroxyimidazole-1-oxide as potential single molecule magnets. **C.C. Taylor, P. Baran**
- 245.** Gold(III) complexes for intramolecular functionalization of strong, sp³-hybridized C-H bonds. **G.R. Donalson, B. Probsdorfer, K.M. Gilmore, J.E. Thompson, M. Sleck, D. Ohlson, N.A. Curry, H.R. Murphy, O.A. Rodriguez, K. Saucedo Chavez, A.L. Rheingold, D.R. Weinberg**
- 246.** CO₂ bond scission via a [P₂Si]Rh silylene intermediate. **P.O. Peterson, T.M. Donnell, M.T. Whited**
- 247.** Acceptorless dehydrogenation of alcohols using Cp*Ir(pyridinesulfonamide)Cl complexes. **E. Schreiber, A.R. O'Connor**
- 248.** Rare earth complexes with sulfonamidoquinoline ligands: Synthesis and applications. **S.M. Rumrill, N. Sequeira, A. Morillo, B.C. Chan**
- 249.** Copper(II) dimer liquid crystals: Effects of axial ligation with caprolactam. **R. Katz, B.W. Mussleman, K.A. Wheeler, T.W. Clayton**
- 250.** Synthesis of cyclopentadienyl-Co(III) *N*-heterocyclic carbene or phosphite complexes as a starting point to explore cobalt mediated C-H bond cleavage. **C.W. Frye, J.P. Lee**
- 251.** Tosylimido transfer reactions with copper complexes of 2,6-bis-(*tb*)pyridine. **J.E. Allen, N.A. Piro**
- 252.** Catalytic activity of dioxovanadium(V) salicylaldehyde semicarbazone complexes in oxidation reactions: effect of electron directing groups. **O.Q. Conover, M.A. Bernard, G.J. Mason, V.P. McCaffrey**
- 253.** Utilizing molybdenum complexes bearing oxygen-donating scorpionate ligands as sulfite oxidase biomimetic models. **N. Fitzpatrick**
- 254.** Metallation of [O,O,N,O] ligands obtained from amino acid precursors for applications in polymerization. **C.M. Laux, A. Anderson-Wile**
- 255.** Water soluble phosphate Schiff-base complexes as detectors for selenate in water. **E. Gier, L. Jefferies**
- 256.** Catalytic activity of dioxovanadium(V) salicylaldehyde semicarbazone complexes in oxidation reactions: Scope of reaction. **M.A. Bernard, O.Q. Conover, G.J. Mason, V.P. McCaffrey**
- 257.** Computational investigation of sulfonyl fluoride activation using bidentate NHC ligands and nickel. **N.J. Chan, M. Ogba, D.J. O'Leary, N.D. Ball**
- 258.** Synthesis and characterization of indium (III) redox active ligand complexes. **K.E. Camacho, A. Arnold, N. Phan, L.A. Berben**
- 259.** Sensitizing lanthanide luminescence with CMPO-based ligands. **A.T. Henry, A.K. Mulville, E.K. Connor, S.M. Biros, E.J. Werner**
- 260.** Variation of extraction conditions for selective lanthanide chelation utilizing tripodal CMPO ligands. **E.K. Connor, A.K. Mulville, E.J. Werner, A.T. Henry, S.M. Biros**
- 261.** Photocatalytic water oxidation by dicopper-dihydroxo complex. **K. Loveridge, P. VanNatta, M.T. Kieber-Emmons**
- 262.** Homogeneous catalysts for the conversion of epoxides to alcohols. **A.N. Rainsberry, J.G. Sage, M.L. Scheuermann**
- 263.** Mechanistic investigations of reductive elimination from Pt(IV) systems. **C. Roleder, E. Stephens, E. Zepeda, N. Williams**
- 264.** Progress towards heteroleptic alkaline earth metal silyl amides. **M. Cousins, M.M. Gillett-Kunnath, K. Ruhlandt-Senge**
- Section G
- Ernest N. Morial Convention Center Hall D
- ACS Award for Distinguished Service in the Advancement of Inorganic Chemistry: Symposium in honor of Thomas B. Rauchfuss**
- Z. M. Heiden, L. F. Szczepura, *Organizers*
5:30 - 7:30
- 265.** Synthesis of novel rhenium selenide clusters containing Fischer carbene ligands. **C.P. Chin, D.N. Huh, W. Wilson, L.F. Szczepura**
- 266.** Exploring the chemistry of Re and Mo based octahedral hexanuclear clusters. **L.F. Szczepura**
- 267.** Green syntheses using BASIL technique. **P.F. Brandt**
- 268.** Atom-economical homogeneous catalytic reduction of CO₂ to commodity chemicals. **W. Chu, K.I. Goldberg**
- 269.** Electrochemical H₂ oxidation enabled by metal-to-metal hydrogen atom transfer. **G. Chambers, E.S. Wiedner, R. Bullock**
- 270.** Metallodithiolate ligands as pendant base in [Fe^{II}Fe^I], [Fe^I[Fe(NO)]^{II}] and [(μ-H)Fe^{II}Fe^{II}] systems. **K. Kariyavasam Pathirana, P. Ghosh, C. Hsieh, N. Bhuvanesh, M.Y. Darenbourg**
- 271.** Probing photochemical processes of [FeFe]-hydrogenase model compounds by combined spectroscopic/computational study. **S. Niu, A. Nelson, P.M. De La Torre, C.F. Works, M.B. Hall**
- 272.** Synthesis of secondary phosphines by copper-catalyzed P-C cross-coupling reaction. **M. Frik, A.L. Haber, E.B. Schiff, J.M. Camara**
- 273.** Synthesis and reactivity of molecular fluorescent pincer complexes. **J.L. Fernandez, Z.M. Heiden**
- 274.** Beyond common bonding, ferrocene-transition metal interactions. **M. Ringenberg**
- 275.** Synthesis and characterization of hydrophobic [(η⁶-arene)Ru(L)Cl₂] complexes. **A.L. Eckermann, L.A. Miller, C. Chamberlain, V. Drust, C. Davenport**
- Section H
- Ernest N. Morial Convention Center Hall D
- ACS Award in Inorganic Chemistry: Symposium in honor of James Moers Mayer**
- S. N. Brown, C. T. Saouma, J. J. Warren, *Organizers*
5:30 - 7:30
- 276.** Mapping the variable reactivity of oleate-capped cerium dioxide nanoparticles. **R. Agarwal, D. Damatov, J.M. Mayer**
- 277.** Tuning the electronics of *p*-substituted tris(amidophenoxide) molybdenum complexes. **A.N. Erickson, S.N. Brown**
- 278.** Exploring differences in bonding between group 10 bis(iminosemiquinone) complexes. **K. Conner, S.N. Brown**
- 279.** Marcus inverted region in photo-induced proton coupled electron transfer. **G.A. Parada, S. Kolmar, B. Petterson, L. Hammarstrom, J.M. Mayer**
- Section I
- Ernest N. Morial Convention Center Hall D
- Undergraduate Research at the Frontiers of Inorganic Chemistry Main Group Chemistry**
- C. Nataro, L. A. Watson, *Organizers*
5:30 - 7:30
- 280.** Systematic computational studies of ene reactions between (F₃C)₂B=N(CH₃)₂ and substituted alkenes. **S.E. Hammer, J.M. Lafferty, K.R. Lawson, J.R. Gustafson, A.L. Gille, B.C. Dutmer, T.M. Gilbert**
- 281.** Preparation of (alkylaminomethylene)indoles and their corresponding main group complexes. **N.R. Wills, S. Sabbagh, N.B. Kingsley**
- 282.** Synthesis and analysis of major pentavalent thioarsenicals. **R. Rivera, C. Fan, Y. Cai**
- Section J
- Ernest N. Morial Convention Center Hall D
- Undergraduate Research at the Frontiers of Inorganic Chemistry Materials, MOFs & Solid-State Chemistry**
- C. Nataro, L. A. Watson, *Organizers*
5:30 - 7:30
- 283.** Nanocasting – Introducing secondary supports into metal-organic frameworks to increase thermal stability of the nodes. **J. Duan, C. Malonzo, S.P. Desai, T. Webber, Z. Li, O.K. Farha, J.T. Hupp, C. Lu, R. Penn, A. Stein**
- 284.** Actinide aqueous hydrolysis reactions: Initial steps in actinide aggregation. **D. Xia, A. Gomez, M. Vasiliiu, D.A. Dixon**
- 285.** Synthesis of MOF-templated mixed-metal oxides for catalytic carbon monoxide oxidation. **J. Bence, C.W. Abney**
- 286.** Growth kinetics and cytotoxicity effects of surface modified zinc oxide quantum dots. **J.K. Davis-Gunn, D.M. McCall-Butler, D. Francis, P.P. Benz, A. Schrock, P. Cavnar, K. Molek, A. Mena, B. Colon**
- 287.** Synthesis, characterization, and catalytic activity of hollow Mn₃O₄ nanoparticles for cyclohexene oxidation. **C.M. Karkk, J.D. Hoefelmeyer**
- 288.** Decorating carbon electrodes with gold nanoparticles to study the kinetics of redox reactions. **G.E. Kamm, T. Le, E.M. Ness, J.C. Lytle, J.F. Parker, D.R. Rolison, J.W. Long**
- 289.** Application of the underlying chemistry in PbTiO₃ for the design of new polar perovskites. **A. Kandel, G. Laurita-Plankis**
- 290.** Immobilization of earth abundant metals coordinated in heterobimetallic ligand scaffolds on metal organic frameworks. **K. Riley, S.P. Desai, J. Vitillo, C. Lu**
- 291.** Precursor development of iron nanopowders for nanoink Aerosol Jet 3D printing. **D. Perales, T.J. Boyle, N.S. Bell, A.W. Cook, L.J. Treadwell, D. Reinholtz**
- 292.** Kinetic investigation into the mechanism for H₂ activation on supported Au nanoparticles. **C. Peterson, S. Kumar, T.N. Whittaker, C. Pursell, L. Grabow, B. Chandler**
- 293.** Host:Guest chemistry inside a series of zirconium-based metal-organic frameworks. **C. Sparrow, G.J. McManus**
- 294.** Solving gold-containing intermetallic compounds using an

- automated inorganic crystal structure refinement tool. **G. Viswanathan**, A. Oliynyk, E. Antono, J. Ling, B. Meredig, J. Brgoch
- 295.** Experimental and computational studies of anisotropic hardness in NiP₂. **A. Lim**, J. Brgoch, A. Mansouri
- 296.** Structural and optical properties of Ba₃Y₂B₆O₁₅:Ce³⁺: A cubic borate with extremely narrow, high efficiency photon emission. **S. Hariyani**, A.C. Duke, J. Brgoch
- 297.** New transition metal and alkali metal complexes containing the hydrotris(3,5-dimethyl-1,2,4-triazolyl)borate ligand. **B.A. Reisner**, B.C. Chan, E.T. Roberts, E.C. Krist, T. Hain, A.R. Losquadro
- 298.** Synthesis and analysis of liquid crystals based on copper (II) tetramers. **A.M. Iradukunda**, T.R. Helgren, T.W. Clayton
- 299.** Encapsulation of fluorescent probes within the pores of a metal-organic framework. **L. Lamos**, G.J. McManus
- 300.** Probing surface recombination at functionalized silicon(111) surfaces. **J. Speller**, D. Boucher, M.J. Rose
- 301.** Modification of the metal coordination sites on 1D coordination polymers. **B.J. Johnson**, N. Ibrahim, W.A. Stubbs
- 302.** Encapsulation of molecules in metal-organic frameworks. **B.J. Johnson**, **S. Smith**, **D. Moe**
- 303.** Synthesis and characterization of liquid crystalline properties of heteroleptic copper(II) dimers using 2-propyl valerate ligands. **Y.F. Wittmer**, C. Oscar, T.W. Clayton
- 304.** Surface chemistry of protein-capped gold nanoparticles. **Z.A. Schonrock**, **A.K. Bentley**
- 305.** Synthesis and characterization of two-dimensional SnS nanoparticles. **E. Juarez Diaz**, J.D. Dwyer, E.S. Aydil
- 306.** High room temperature separation of CO₂ vs. C₂H₂ and N₂ in Mn(II) acetylenic phosphine-based metal organic framework. **K.M. Walsh**, J. Reynolds, B. Li, B. Chen, S.M. Humphrey
- 307.** Designing flexible ligands for the synthesis of breathable metal-organic frameworks. **N. Giorgi**, G.J. McManus
- 308.** Cholesteric liquid crystalline porphyrin VOC sensors. **M.E. Zick**, M.R. Ramsey, J.E. Winklerek, A.L. Dorfner, J.C. Kranick, L.J. Tucker, J.L. O'Donnell
- 309.** Synthesis and characterization of novel phosphine coordination materials (PCMs) implementing a tetrahedral phosphonium ligand with M(III) ions. **D. Kristek**, J. Reynolds, S.M. Humphrey, A. Bohnsack
- 310.** Synthesis and structural characterization of Ba₂SrGaO₄F. **R. Green**, **V. Pierre**
- 311.** Determination of inorganic water contaminants via quantum dot doped MOFs using fluorescence spectroscopy. **K. Parson**, K.T. Jackson
- Section K
- Ernest N. Morial Convention Center Hall D
- Main Group Chemistry**
- T. W. Hudnall, *Organizer*
5:30 - 7:30
- 312.** Structures and rotational dynamics of (triarylmethyl)germane propellers. **M.C. Franke**, S.J. Stoudt
- 313.** Structural studies of alkaline earth and rare metal *trans*-azobenzene complexes. **A.G. Goos**, D. Weissmann, J. Pichler, J. Binder, D. Allis, **S. Vonn Dyke**, M.M. Gillett-Kunnath, K. Ruhlandt-Senge
- 314.** Synthesis and reactivity studies of cationic diborane compounds. **H. Liu**, **W. Yen**, C. Chiu
- 315.** Synthesis and reactivity studies of metallylenes. **T. Lin**, **I.F. Yu**, C. Chiu
- 316.** Synthesis and characterization of functionalized organosilicate systems. **M.A. Boucher**, K.M. Specht, L.S. Dake
- 317.** Photochemistry of main group / late transition metal complexes. **E.S. Tabei**, S. Sen, F.P. Gabbai
- 318.** Luminescent 1*H*-1,3-benzazaphosphole derivatives. **S. Evariste**, A.L. Rheingold, C. Moore, J. Heinicke, J.D. Protasiewicz
- 319.** Structure function analysis: The role of metal-fluorine interactions in controlling coordination chemistry in alkaline earth metal compounds. **Y. Takahashi**, B. Wilson, **A.Y. O'Brien**, D. Allis, M.M. Gillett-Kunnath, K. Ruhlandt-Senge
- 320.** H[Al(OTeF₅)₄] – Synthesis and application of a Brønsted superacid. **A. Wiesner**, T.W. Gries, S. Riedel
- Section L
- Ernest N. Morial Convention Center Hall D
- ACS Award in Pure Chemistry: Symposium in honor of Mircea Dinca**
- Y. Roman-Leshkov, Y. Surendranath, *Organizers*
5:30 - 7:30
- 321.** Non-planar multidentate metal-linker in metal-organic framework: Synthesis and catalytic performance. **C. Sun**, M. Dinca
- 322.** Lithium-ion conductivity in oligoethylene oxide functionalized covalent organic frameworks. **D.A. Vazquez-Molina**, G. Pope, A. Ezazi, F.J. Uribe-Romo
- 323.** Investigation of electronic structures of two dimensional conductive metal organic frameworks. **L. Yang**, M. Dinca
- 324.** Conductive metal-organic frameworks for gas sensing. **Y. Ge**, M. Dinca
- Section M
- Ernest N. Morial Convention Center Hall D
- Harry Gray Award for Creative Work in Inorganic Chemistry by a Young Investigator: Symposium in honor of Dwight S. Seferos**
- M. R. Jones, A. M. Spokoyny, *Organizers*
5:30 - 7:30
- 325.** Ring expansion as a route to unique boron heteroarenes. **S. Yruegas**, C. Martin
- 326.** Exploring Diels-Alder chemistry of boroles. **J.J. Baker**, C. Martin
- Section N
- Ernest N. Morial Convention Center Hall D
- ACS Award in Organometallic Chemistry: Symposium in honor of Clifford P. Kubiak**
- J. S. Figueroa, *Organizer*
5:30 - 7:30
- 327.** Ultra thin layer of iron porphyrin COFs for CO₂ reduction in water. **P.L. Cheung**, S. Lee, S. Masaoka, C.P. Kubiak
- 328.** Covalent attachment of [Ni(alkynyl-cyclam)]²⁺ catalysts to the glassy carbon electrode. **A. Zhanaidarova**, C.P. Kubiak
- 329.** Revealing and predicting the stability of Pt^{II}-containing molecular gyroscope isomers. **A. Ehnbohm**, H. Joshi, S. Kharel, L.M. Pérez, M.B. Hall, J.A. Gladysz
- 330.** Rh(I) diisocyanide coordination polymers for electrochemical catalyst heterogenization and semiconductor material applications. **G. Lee**, C.P. Kubiak
- 331.** Mechanistic insight of M(N₂S₂) metalloligand in Re-based electrocatalysts for CO₂ reduction. **S. Ding**, **Y. Tong**, M.Y. Darensbourg, M.B. Hall
- 332.** Dynamic exchange on the ultrafast timescale. **T.M. Porter**, C.P. Kubiak
- 333.** Electron exchange between redox non-innocent bridging ligands in mixed-valent hydrogen bonded Ru₃O clusters. **G.P. Heim**, T.M. Porter, C.P. Kubiak
- 334.** Photoelectrochemical reduction of CO₂ through the attachment of Re(bpy)(CO)₃Cl derivatives to p-type Si. **C. Miller**, C.P. Kubiak
- 335.** New synthetic routes to functionalized P₂N₂ ligands. **F.M. Brunner**, C.P. Kubiak
- 336.** Thermodynamic insights for the development of nickel-based CO₂ reduction catalysts. **A.L. Ostericher**, C.P. Kubiak
- 337.** Altering the electronic structure of nanoparticles through external stimuli. **L.M. Mawby**, B.J. Lear
- 338.** Hydricity and other thermodynamic considerations for CO₂ reduction. **K.M. Waldie**, C.P. Kubiak
- Section O
- Ernest N. Morial Convention Center Hall D
- Electrochemistry**
- B. L. Lucht, *Organizer*
5:30 - 7:30
- 339.** Novel confined PFSA/Pt-zeolite composite membrane for self-humidifying PEMFC. **R. Deng**, **J. Song**, W. Han, K. Yeung
- 340.** Electrochemical analysis of Ru(II) complexes with redox non-innocent S₂N₂ ligands and their applications in the reduction of CO₂. **J.A. Luna**, G. Durgaprasad, K.D. Spielvogel, C. Haas, S.K. Shaw, S.R. Daly
- 341.** Electrocatalytic methods for O-atom transfer reactions. **T.A. Stinson**, T. Donadt, C.G. Martin, O.R. Luca
- 342.** Porous silicon composites for high-capacity metal-ion batteries. **M.L. Anger**, B.D. Fahlman
- 343.** Selenium redox chemistry: From surface reactivity to biological applications. **M. Diagne**, **G. Nemeth**, **E. Wiita**, M.C. Buzzeo
- 344.** Test-bed for detecting WSNs in Labview via unmanned vehicles. **D. Burks**
- 345.** Cyclic voltammetric studies of *Sulfobacillus thermosulfidooxidans* using a pyrite working electrode. **R. Blake**, Z. Huang, R. Painter, Z. Wang
- Section P
- Ernest N. Morial Convention Center Hall D
- Environmental & Energy-Related Inorganic Chemistry**
- S. A. Koch, *Organizer*
5:30 - 7:30
- 346.** Ionic conductivities and ion dissociation in silyl nitrile electrolytes with LiPF₆ and LiTFSI salts for applications in lithium-ion batteries. **S. Beecher**, **T. Derrah**, L.J. Lyons
- 347.** Testing the viability of nitroxide radicals as redox shuttles in quantum dot sensitized solar cells. **C.C. Riley**, C. Mi, R. Beaulac
- 348.** Photosensitization behavior of supramolecular Ir(III)-carborane complex in application to photocatalytic hydrogen production: Efficient visible light-driven charge separation and mediation. **S. Kim**, Y. Cho, B. Yun, C. Kim, S. Kang, H. Son
- 349.** Photocatalytic reduction of CO₂ to CO through a mixed hybrid system with cationic iridium(III) complexes and Re(I)-complex-anchored TiO₂ catalytic particles. **H. Cheong**, S. Kim, Y. Cho, S. Choi, C. Kim, D. Cho, C. Pac, S. Kang, H. Son
- 350.** Development of lower-energy photosensitizer for photocatalytic CO₂ reduction: Modification of porphyrin dye in hybrid catalyst system. **S. Choi**, H. Cheong, C. Kim, C. Pac, S. Kang, H. Son
- 351.** Understanding the natural mechanisms for chromium mobilization in groundwater. **M. Houlihan**, A. Lopez, S.E. Fendorf
- 352.** Synthesis of group 6 carbonyl complexes containing phosphine

- ligands for CO₂ reduction. **N. Walker, B.J. Bellott**
- 353.** New moisture harvesting material from superhydrophilic Titania nanotubes. **Y. Luo, J. Song, K. Yeung**
- 354.** Platinum@hexaniobate nanopeapods: Sensitized composite architectures for photocatalytic hydrogen evolution under visible light irradiation. **C. Davis-Wheeler Chin, P.R. Fontenot, R.H. Schmehl, J.B. Wiley**
- 355.** NMR measurements of ion and solvent transport for organosilicon nitrile electrolytes. **J. Zhu, L.J. Lyons**
- 356.** NMR diffusion studies of LiTFSI/organosilyl electrolytes. **E. Cunningham, L.J. Lyons**
- 357.** Activation of carbon dioxide through thiolate-bridged heterobimetallic complexes. **N. Arnet, A.M. Lunsford, X. Yang, M.Y. Darensbourg**
- 358.** Copper-based redox shuttles supported by rigid tetradentate ligands for dye-sensitized solar cells. **J. Lee, J.W. Jurss, L. Chen, R.R. Rodrigues, J.H. Delcamp**
- 359.** Cobalt schiff base complex using a pyridinediimine backbone for hydrogen production. **P. Hutchison, M. Kiker, C. Tinker, W.T. Eckenhoff**
- 360.** Hydrogen production using Mo(O)₃(tpa) complex. **C. Tinker, W. Eckenhoff**
- 361.** Nickel Schiff base complexes for light driven H₂ production. **M. Kiker, A. Graves, W. Eckenhoff**
- 362.** Nickel complexes with N₂S₂ ligands for electrocatalytic and light-driven production of hydrogen. **J. Dewar, W. Eckenhoff**
- 363.** Substituent effects on the fixation of carbon dioxide to oxalate by a binuclear copper complex. **F. Khamespanah, F.R. Fronczek, A.W. Maverick**
- 364.** Iridium dioxide nanocrystals synthesized by molten-salt method for oxygen and hydrogen evolution reactions. **S. Mohan, Y. Mao**
- 365.** Dose measurements of stray radiation inside the first optical enclosure of beamline 8-ID-A at the national synchrotron light source-II. **K. Kelly, J. Zapata, M. Harvey**
- 366.** Effects of promoters on increasing methane hydrate formation via gas-liquid interface alteration. **P. Rangsunvigit, A. Seangsai, K. Inking**
- 367.** Sidewalk development and research. **A. Plumber**
- 368.** Aerobic respiration on soluble iron is expressed constitutively by *Metallosphaera sedula*. **N. Pham, O. Griswold, R. Blake**
- 369.** Aerobic respiration on soluble iron is expressed constitutively in *Sulfobacillus thermosulfidooxidans*. **O. Griswold, N. Pham, R. Blake**
- 370.** Synthesis and characterization of organic-inorganic conjugate dyes designed for solar energy harvesting. **R.E. Bachman, B.C. Bierman, S. Parks**
- Section Q
- Ernest N. Morial Convention Center Hall D
- Inorganic Catalysts**
- S. A. Koch, *Organizer*
5:30 - 7:30
- 371.** Hollow dendritic Ag/Pt nanoparticles for enhanced methanol oxidation efficiency. **N. Sui, L. Wang, Q. Bai, W. Yu**
- 372.** Synthesis and characterization of pentadentate ligands for the formation of binuclear complexes. **A.C. Doner, S. Striegler**
- 373.** Mechanism of the electrocatalytic hydrogen evolution and oxidation with rhenium tris(thiolate) complexes. **H. Tang, E.N. Brothers, M.B. Hall**
- 374.** Computational study of the N₂ activation and N≡N bond cleavage by a family of group 6 dinuclear [M(II), M(II)] μ-N₂ complexes (M = Mo, W) supported by the cyclopentadienyl, amidinate (CPAM) ligand environment. **J.K. Kirkland, L.M. Duman, L.R. Sita, K.D. Vogiatzis**
- 375.** Layered, ternary water oxidation catalyst prepared by in-layer cobalt doping, and interlayer iron-oxo cluster intercalation in Mn-O-based birnessite. **L. Mohamad, I.G. McKendry, M. Zdilla**
- 376.** Silver (Ag) enhanced poly(3,4-ethylenedioxythiophene) (PEDOT) infused TiO₂ nanofibers for improved photocatalytic degradation of chemical pollutants. **D. Dwyer, J. Kinsley, J. DeCoste, W.E. Bernier, W. Jones**
- 377.** Synthesis, characterization, and catalytic activities of nickel(II) monoamido-tetradentate complex: Evidence for Ni^{III}-Oxo and Ni^{IV}-Oxo species. **H. Jeong, H. Ahn, H. So, H. Lee, C. Kim**
- 378.** Synthesis, characterization, and efficient catalytic activities of a nickel(II) porphyrin: Remarkable solvent and substrate effects on participation of multiple active oxidants. **A. Kim, D. Zhang, M. Kim, H. Jang, P. Kim, C. Kim**
- 379.** Synthesis of microporous vanadosilicate AM-6 for shape-selective photocatalytic applications. **J. Mastrandea, M. Ismail**
- 380.** Electrocatalytic CO₂ reduction with *cis* and *trans* conformers of a rigid dinuclear rhenium complex: Comparing the isolated monometallic and cooperative bimetallic pathways. **W. Yang, S. Sinha Roy, W.C. Pitts, R. Nelson, F.R. Fronczek, J.W. Jurss**
- 381.** Durable and highly reactive iron-oxo catalyst for hydrocarbon C-H bond functionalization. **L. Chen, X. Su, J.W. Jurss**
- 382.** Metallothiolates as S-donor ligands to palladium and their function as C-C cross coupling catalysts. **Z. Martinez, P. Ghosh, M. Quiroz, M.Y. Darensbourg**
- 383.** Computational study for the mechanism of CO₂ reduction using imidazolium-functionalized Rhenium electrocatalysts. **X. Li, S. Sung, M. Nippe, J. Panetier**
- 384.** DFT investigation on the catalytic reduction mechanisms of N₂ to NH₃ by Fe complexes. **S. Yu**
- 385.** Polymers from bio-derived resources: Synthesis of poly(silylether)s from Furan derivatives catalyzed by a high valent salen-Mn(N) complex. **S. Vijamarri**
- 386.** Development of bifunctional catalysts containing hydride-relay ligands for CO₂ hydrogenation. **N. Devi**
- 387.** Bioinspired manganese complexes with tetradentate pyridine-appended piperidine ligands catalyze olefin epoxidation. **F. Zhu, G. Yang, A.J. Zoll, S.A. Thompson, J. Jackson, P. Milne, E.V. Rybak-Akimova**
- 388.** Synthesis, characterization, and structure of non-heme copper(II) complexes: An efficient atom transfer catalyst. **H.U. Valle, K. Riley, D.E. Russell, D.K. Wolgemuth, S.L. Redd, S.L. Stokes, J.P. Emerson**
- 389.** Novel 5-coordinate and 6-coordinate low-valent molybdenum(VI)-dioxo complexes exhibiting deoxydehydration activity. **R. Tran, S.M. Kilyanek**
- 390.** Syntheses and characterization of molecular cobalt complexes with pentadentate ligands for electro- and photocatalytic hydrogen production. **P. Wang, S. Lei, M. Sow, M. Long, R. Reddy, G. Liang, C.E. Webster, X. Zhao**
- 391.** Low valent homogeneous catalysis using metal organic frameworks. **A.M. Rabon, M.C. Young**
- 392.** Activation of benzylic and allylic C-H Bonds catalyzed by a low-spin Co(II) complex. **A.D. Bell-Taylor, C. Goldsmith, J.D. Gordon**
- 393.** Incorporation of molecular rectifiers into homogeneous photocatalysts. **D.J. Boston, I. Bhowmick**
- 394.** Computational investigation of the mechanism of metal-oxo catalyzed deoxydehydration. **K.A. DeNike, S.M. Kilyanek**
- 395.** Electrocatalytic hydrogen production by bridged butterfly [2Fe-2S] catalysts. **M.O. Talbot, D.H. Evans, R.S. Glass, D.L. Lichtenberger**
- 396.** Investigation on the electrocatalytic water splitting performance of molten salt synthesized La_{1-x}Sr_xCoO₃. **S. Mohan, Y. Mao**
- 397.** Rational design and synthesis of substituted chiral BINAM ligands to improve enantioselectivity. **S. Murru, R. Bista, M. Kim, A. Hancock**
- 398.** Transition metal doped TiO₂/reduced graphene oxide composites for highly efficient dye adsorption. **W.R. Thalaspitiya, S.L. Suib**
- 399.** Mesoporous Cu Al mixed metal oxides for one pot synthesis of imines. **D. Dissanayake, S.L. Suib**
- 400.** Mesoporous manganese oxide catalyzed heterogeneous aerobic oxidation of primary amines to nitriles. **D. Rathnayake, S.L. Suib**
- 401.** Highly efficient photochromic mesoporous tungsten oxide hexagonal tunnels for catalytic coupling of alkenes. **T.M. Premalal, S.L. Suib**
- 402.** Computational chemistry: Active metal catalysts for the synthesis of urea. **T. Fitzpatrick**
- Section R
- Ernest N. Morial Convention Center Hall D
- Inorganic Spectroscopy**
- C. V. Popescu, *Organizer*
5:30 - 7:30
- 403.** Sensitization of lanthanides by graphene quantum dots: an exception to Kasha-Vavilov rule? **M. McDowell, A. Metzger, J.M. Tour, A.A. Marti**
- 404.** Photooxidation of Amyloid beta fibrils by a rhenium complex. **B. Jiang, A.A. Marti**
- 405.** Electronic structure and bonding in 1st row hetero-bimetallic complexes probed via multi-edge X-ray absorption spectroscopy. **S. Chatterjee, J. Moore, P. Dunn, I. Tonks, C. Lu, K.M. Lancaster**
- 406.** Bridging Ni electronic structure and reactivity: A spectroscopic and theoretical approach. **I. DiMucci, K.M. Lancaster, M.S. Sanford**
- 407.** Speciation of zinc in the weathered MSWI bottom ash by XAFS. **H. Zhang**
- 408.** TD DFT studies on phosphorescent cyclometalated alkynyl and phenylplatinum(II) complexes based on tridentate C^NN-coordinating ligands. **E. Warden, E. Javed, L. Yumin, S. Huo**
- 409.** "Intervalence-like" charge transfer in polypyridyl ruthenium complexes of 4-dimethylaminopyridine. **S.L. Guertin**
- 410.** Pt-Pt interactions occur in solution lead to aggregation and polymorphism of bipyridine platinum(II) complexes. **R.E. Bachman, J.L. Zahn, M.H. Hudson**
- Section A
- Ernest N. Morial Convention Center Great Hall A
- ACS Awards in Inorganic Chemistry: Plenary Session**
- S. A. Koch, N. S. Radu, *Organizers*
B. T. Donovan-Merkert, *Organizer, Presiding*
8:15 411. Award Address (ACS Award for Distinguished Service in the Advancement of Inorganic Chemistry sponsored by Strem Chemicals, Inc.). Metal hydrides in nature: Hydrogenase

chemistry with models and the proteins.

T.B. Rauchfuss

8:50 412. Award Address (Harry Gray Award for Creative Work in Inorganic Chemistry by a Young Investigator sponsored by the Gray Award Endowment). Electronically delocalized molecules and polymers that contain selenium and tellurium. **D.S. Seferos**

9:20 413. Award Address (ACS Award in Inorganic Chemistry sponsored by the Aldrich Chemical Company, LLC). Proton-coupled electron transfer from molecules to materials. **J.M. Mayer**

9:55 Intermission.

10:05 414. Award Address (ACS Award in Organometallic Chemistry sponsored by The Dow Chemical Company Foundation). The organometallic chemistry of CO₂ reduction. **C.P. Kubiak**

10:35 415. Award Address (Alfred Bader Award in Bioinorganic or Bioorganic Chemistry sponsored by the Alfred R. Bader Fund). Elements of marine bioinorganic chemistry: From microbes to mussels. **A. Butler**

11:05 416. Award Address (ACS Award in Pure Chemistry sponsored by the Alpha Chi Sigma Fraternity and the Alpha Chi Sigma Educational Foundation). Taking MOFs to the extreme: Water, ammonia, and halogen capture and release with azolate-based materials. **M. Dinca**

11:35 417. Award Address (F. Albert Cotton Award in Synthetic Inorganic Chemistry sponsored by the F. Albert Cotton Endowment Fund). Molecular complexity and inorganic chemistry: Utilizing non-covalent interactions to control function. **A. Borovik**

Actinide Complexes & Nanoclusters

Sponsored by NUCL, Cosponsored by INOR

Fluid-Solid Interfacial Phenomena at the Nexus of Energy & Geochemistry Research: A Symposium in Honor of David J. Wesolowski

Sponsored by GEOC, Cosponsored by COLL, ENFL, ENVR and INOR

Challenge & Opportunity in Lignin Valorization

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

Innovative Chemistry & Materials for Electrochemical Energy Storage

Sponsored by ENFL, Cosponsored by CATL, INOR and PMSE

Activation of Light (C1-C4) Hydrocarbons: Theory & Experiments

Sponsored by CATL, Cosponsored by ENFL, INOR and PHYS

MONDAY AFTERNOON

Section A

Ernest N. Morial Convention Center
Room 345

Lanthanide & Actinide Chemistry

A. De Bettencourt Dias, *Organizer*
K. Johnson, E. J. Werner, *Presiding*
1:30 418. On the difference in luminescence properties of red emitting La₂Zr₂O₇:Eu³⁺ and La₂Hf₂O₇:Eu³⁺ nanoparticles. **S. Gupta**, J. Zuniga, Y. Mao

1:50 419. Gd-based pH-sensitive MRI contrast agents. **N.N. Paranawithana**, A.F. Martins, P. Zhao, G. Kiefer, D. Sherry

2:10 420. Lanthanide luminescence and anion binding properties of tripodal iminopyridine complexes. **E.J. Werner**, S.M. Polzin, K.H. Felix

2:30 Intermission.
2:40 421. Electrochemical studies of surface-immobilized molecular lanthanide complexes. **K.J. Johnson**, D. Lionetti, J.D. Blakemore

3:00 422. Luminescent rare-earth complexes as sensitizers of singlet oxygen. **K. Johnson**, A. De Bettencourt Dias

3:20 423. Radical-bridged dinuclear and metallacyclic trinuclear lanthanide complexes. **B.S. Dolinar**, D.I. Alexandropoulos, V. Kuduva Radhakrishnan, T. James, K.R. Dunbar

3:40 Intermission.
3:50 424. Acquisition of upconversion luminescence images exciting with LEDs: A paradigm shift in upconversion imaging. **A. Baride**, J.M. Meruga, W.M. Cross, J.J. Kellar, S. May

4:10 425. BODIPY-functionalized 1,10-phenanthroline for near-infrared emitting ytterbium (III) complex. **H. He**

4:30 426. Lanthanide and actinide thiocyanate complexes. **R. Wilson**, T.J. Carter

Section B

Ernest N. Morial Convention Center
Room 344

Metal-Organic Frameworks: What Are Next?

W. Lin, S. Ma, H. Zhou, *Organizers*
W. Choe, N. L. Rosi, *Presiding*

1:30 427. Switchability phenomena in metal-organic frameworks: From fundamentals to functions? **S. Kaskel**

2:15 428. Recent progress on porous metal-organic frameworks for gas separation. **B. Chen**
2:45 429. Pore space partitioning and engineering of metal-organic framework materials. **P. Feng**, X. Bu
3:15 430. Crystal engineering of hybrid ultramicroporous materials for gas separation applications. **D.G. Madden**, M.J. Zaworotko

3:35 Intermission.

3:50 431. Engineering MOF porosity and functionality for highly effective gas separation and capture. H. Wang, B. Li, **J. Li**

4:20 432. Rapid hydrogen–deuterium exchange in metal-organic frameworks. **V. Stavila**, T.C. Wang, D. Cowgill, M. Allendorf

4:50 433. Ultrahigh and selective SO₂ uptake in inorganic anion-pillared hybrid porous materials. X. Cui, **Q. Yang**, R. Krishna, H. Wu, W. Zhou, B. Chen, H. Xing

Section C

Ernest N. Morial Convention Center
Room 343

ACS Award in Organometallic Chemistry: Symposium in honor of Clifford P. Kubiak

J. S. Figueroa, *Organizer*
C. W. Machan, *Presiding*

1:30 434. Cooperative effects between metals in chemical transformations. **T. Tilley**

1:55 435. Bringing inorganic insight to ligand design for metallic nanoparticles. **B.J. Lear**

2:20 436. Hydricity matters: From formate oxidation to CO₂ reduction. **J.Y. Yang**, C. Tsay, B. Ceballos, D.W. Cunningham, T.R. Cundari, C.L. Pitman

2:45 437. Thermodynamic hydricity as a tool for understanding transition metal hydride reactivity in water and acetonitrile. **A.J. Miller**, K.R. Brereton, T.R. Cundari, C.L. Pitman

3:10 Intermission.
3:30 438. Transition metal catalyzed hydrogenation of CO₂ and carbonyl compounds. W. Chu, Z. Culakova, **K.I. Goldberg**

3:55 439. Applications of tris[(1-isopropylbenzimidazol-2-yl)dimethylsilyl]methyl and related ligands to main group and transition metal chemistry. S. Ruccolo, M. Rauch, **G. Parkin**

4:20 440. Redox non-innocence in first row transition metal chemistry. **P.T. Wolczanski**, S.P. Heins, B. Zhang, B.P. Jacobs, D. Pokhriyal, T.R. Cundari

4:45 Concluding Remarks.
Section D
Ernest N. Morial Convention Center
Room 352
ACS Award in Inorganic Chemistry: Symposium in honor of James Moers Mayer

S. N. Brown, J. J. Warren, *Organizers*
C. T. Saouma, *Organizer, Presiding*

1:30 441. Reaction of an iridium(III) hydride with oxygen: experimental and computational studies of the mechanism. A.M. Wright, D. Pahls, B. Gary, T. Warner, J. Williams, S. Knapp, K. Allen, C.R. Landis, T.R. Cundari, **K.I. Goldberg**

1:50 442. Asset or achilles heel? The role of the pendent base in metal-ligand

cooperative dehydrogenation catalysis.

J.M. Blacquire, J.M. Stubbs, B.J. Bridge, E. El-Zouki

2:10 443. Olefin trimerization and ethylene tandem conversion to linear low density polyethylene. **J.E. Bercaw**

2:30 444. Predictive model for the rates of decarboxylation of silver benzoate complexes relevant to catalytic decarboxylative coupling reactions.

J.M. Hoover, R.A. Crovak, S. Ciccone, A.P. Honeycutt

2:50 445. Mechanistic insights into the catalytic synthesis of polyesters from biorenewable feedstocks. **W.B. Tolman**

3:10 Intermission.
3:20 446. Electrocatalytic oxygen reduction with molecular catalysts and mediators. **S.S. Stahl**

3:40 447. Multiredox chemistry with 2,2'-Bipyridine Equipped with a Disulfide/Dithiol Switch. Synthesis, electrochemistry and complexes. **M. Cattaneo**, C.E. Schiewer, A. Schober, S. Dechert, I. Siewert, F. Meyer

4:00 448. Electron flow through multicopper oxidases. **H.B. Gray**

4:20 449. Transition metal phosphide nanoparticles: Novel (pre)catalysts for water splitting. **S. Mutinda**, D. Li, R. Liyanage, **S. Brock**

4:40 Concluding Remarks.
Section E

Ernest N. Morial Convention Center
Room 353

ACS Award in Pure Chemistry: Symposium in honor of Mircea Dinca

Y. Surendranath, *Organizer*
Y. Roman-Leshkov, *Organizer, Presiding*

1:30 Introductory Remarks.
1:40 450. Synthesis of materials with emergent properties. S.M. Clarke, J.P. Walsh, A. Tamerius, R.A. Klein, **D.E. Freedman**

2:10 451. Porous molecular crystals based on fluorinated aromatics and cyclobenzoin. **O. Miljanic**

2:40 452. Redox-active tunable inorganic frameworks. **A.M. Schimpf**

3:10 453. Molecular approaches to heterogeneous electrocatalysis. **Y. Surendranath**, M. Jackson, S. Oh, C.J. Kaminsky, S. Chu

3:40 Intermission.
4:00 454. Design principles for core-shell catalysts: Transition metal carbides as ideal hosts for noble metal thin films. **Y. Roman-Leshkov**

4:30 455. Correlation of electronic structure to function: Reactivity and magnetism. **T. Betley**

5:00 456. Vibronic coherence as a mechanistic probe for ultrafast dynamics in transition metal-based chromophores. B. Paulus, E.D. Foszcz, **J.K. McCusker**

Section F

Ernest N. Morial Convention Center
Room 354

Alfred Bader Award in Bioinorganic or Bioorganic Chemistry: Symposium in honor of Alison Butler

Cosponsored by WCC

J. S. Martinez, *Organizer*

A. Butler, *Presiding*

1:30 Introductory Remarks.

1:40 457. Strategies for photo-uncaging small molecule bioregulators. **P.C. Ford**

2:05 458. Synthesis and characterization of organometallic copper nanoclusters. **T.W. Hayton**

2:30 459. Renewable polymers and ligands derived from lignin. **M.M. Abu-Omar**, S. Zhao, A. Whelton, X. Huang

2:55 460. Indoleamine 2,3-dioxygenase, the immune response and cancer. **J.T. Groves**, M.T. Nelp, P.A. Kates

3:20 Intermission.

3:40 461. Inorganic systems and interfaces for controlling bioprocesses: Hemostasis example. **G.D. Stucky**

4:05 462. Assemblies of gold, platinum and silver nanoclusters: Photophysics and catalysis. **J.S. Martinez**

4:30 463. Engineering bioinorganic functions through metal-directed protein self-assembly. **F.A. Tezcan**, L. Churchfield, J. Rittle, L. Williamson

4:55 464. Making oxygen for space travel. **H.B. Gray**

Section G

Ernest N. Morial Convention Center Room 210

Nitrogen Un-Fixation: Mechanisms & Models of Nitrification/Denitrification Reactions

N. Lehnert, *Organizer*

K. M. Lancaster, *Organizer, Presiding*

1:30 465. Using biosynthetic models of nitric oxide reductase (NOR) in myoglobin to elucidate structural features responsible for NOR activity and its reaction mechanism. A. Bhagi-Damodaran, J. Reed, **Y. Lu**

2:00 466. Cytochrome c nitrite reductase (ccNiR)-catalyzed reduction of nitrite to nitric oxide by ferrocyanide: Insights into the mechanism of ccNiR-catalyzed ammonification. **A. Pacheco**

2:30 467. Nucleophilic attack at the bound NO of stable ferric nitrosyl porphyrins. E.G. Abucayon, **G.B. Richter-Addo**

2:50 468. Ruthenium homogeneous catalysts for electrocatalytic oxidation of ammonia to dinitrogen at ambient temperatures. F. Habib-Zadeh, S.L. Miller, T. Hamann, **M.R. Smith**

3:20 Intermission.

3:30 469. Advances in electrocatalytic ammonia production by cytochrome c Nitrite reductases. **S.J. Elliott**

4:00 470. Homogeneous ammonia oxidation: Mechanistic investigation and catalyst development. **G. Menard**, M. Keener, C. Hunt

4:30 471. Nitrate binding and reduction by a cobalt-based electrocatalyst: the

unique properties of DIM ligand. **E. Jakubikova**

4:50 472. Mechanistic studies of denitrifying heme-nonheme nitric oxide reductases. **P. Moenne Loocz**

Section H

Ernest N. Morial Convention Center Room 211

Undergraduate Research at the Frontiers of Inorganic Chemistry Organometallic & Coordination Chemistry

C. Nataro, L. A. Watson, *Organizers*
S. Poland, *Presiding*

1:30 473. Coinage metal complexes of new N-heterocyclic thiones and selenes. **D. Rabinovich**

1:50 474. Protonation state effects on the electronic properties of [Ru(neo)₂(4,4'bpy(OH)₂)₂]²⁺ (neo = neocuproine; 4,4'bpy(OH)₂ = 4,4'-dihydroxy-2,2'-bipyridine). **A.M. Arcidiacono**, E.T. Papish, T. Dudley, J.J. Paul

2:10 475. Prospects for tuning Tris(diphenylphosphinomethyl)phenylborate donation via introduction of organic and organometallic substituents at the bridgehead boron phenyl group. **P.J. Fischer**, J.T. Stephan, S. Senthil, M. Swift, E.T. Chan, M.V. Vollmer, V.G. Young, Jr.

2:30 Intermission.

2:45 476. Selective catalytic reductions using Cp* iridium catalysts in formic acid/triethylamine. **J. Steets**, A.R. O'Connor

3:05 477. Catalytic asymmetric hydroamination using chiral early metal complexes of bi- and tridentate ligands. **A.R. Johnson**, C. Abelson, B.S. Mitchell, R. Karina, F. Sha, H.S. Slocumb

3:25 478. Catalytic coupling of epoxides and dry ice under mild conditions: Working toward an undergraduate laboratory experiment. **S. Poland**, T. Downs, J.B. McLemore

3:45 479. Synthesis and reactivity of palladium compounds with κ³-bis(phosphino)ferrocene ligands. **N.E. Wamser**, **R. Bal**, C. Nataro

4:05 Concluding Remarks.

Section I

Ernest N. Morial Convention Center Rooms 340/341

Organometallic Chemistry: Catalysis-Early Transition Metals

N. S. Radu, *Organizer*

D. Ess, S. Groysman, *Presiding*

1:30 480. Computational design and experimental realization of chromium catalysts with control of ethylene trimerization and tetramerization. **D. Ess**, S.M. Bischof, D. Kwon, U.J. Kilgore, J.T. Fuller, O.L. Sydora

1:50 481. Cyclopropanations via heme carbenes: Basic mechanism and effects of carbene substituent, porphyrin

substituent, and protein axial ligand. **Y. Wei**, **Y. Zhang**

2:10 482. Dinuclear pathways for the activation of strained three-membered rings. **H. Rounds**, C. Uyeda

2:30 483. Exploring nitrene sources for the titanium-catalyzed [2+2+1] formation of pyrroles. **A. Pearce**, I. Tonks

2:50 484. Earth-abundant metal catalysts for hydrogenation, hydrofunctionalization and dehydrogenative coupling reactions. **G. Zhang**, J. Aquilina, J. Cheng

3:10 485. Oxidative amination of alkene by extreme π-loading pincer N-heterocyclic carbene Tantalum bis(imido) complex. **G. Liang**, T.K. Hollis, C.E. Webster

3:30 486. Ring-opening oxidative amination of methylenecyclopropanes with diazenes via Ti^{II}/Ti^{IV} redox catalysis. **E. Beaumier**

3:50 487. Chiral ansa-zirconocenes bearing N-azolyl and related fragments: Synthesis, structure and performance in propene polymerization. **V.V. Izmer**, A.Y. Lebedev, I.S. Borisov, G.P. Goryunov, D.V. Uborsky, J.M. Canich, **A.Z. Voskoboynikov**

4:10 488. Heterobimetallic homogeneous catalysts for CO oxidation. **S. Groysman**, T. Hollingsworth

4:30 489. Organolanthanides and their surface organometallic catalysis for hydroboration of esters and epoxides. **S. Patnaik**, Z. Wang, J. Manzano, I.I. Slowing, M. Pruski, A.D. Sadow

4:50 490. Influence of neodymium coordination environment in ternary catalysts Nd(RCOO)₃-AlR₃-R₂AlCl on the activity in 1,3-butadiene polymerization: Titration of the active sites with a poisoning agent. **D.V. Uborsky**, V.A. Kudakina, A.Z. Voskoboynikov, H. Kloppenburg, T. Gross

Section J

Ernest N. Morial Convention Center Room 212

Coordination Chemistry: Characterization & Applications

A. Larsen, *Organizer*

L. M. Berreau, T. K. Hollis, *Presiding*

1:30 491. Anion effects on Cu/O₂-mediated oxidative aliphatic carbon-carbon bond cleavage reactions. **L.M. Berreau**

1:50 492. Tetradentate polypyridine transition metal complexes as water splitting catalysts. **L.M. Lifshits**, L. Kohler, L. Wickramasinghe, R.P. Thummel

2:10 493. Fluorinated copper scaffolds for ¹⁹F MR-based detection of hypoxia. **D. Xie**, E.L. Que

2:30 494. Ultrafast dynamic exchange in five-coordinate complexes of ruthenium. **T.M. Porter**, C.P. Kubiak

2:50 495. Cooperative ligand-centered reactivity in transition metal complexes

with triaminoborane-bridged diphosphines: Protonation turns on borane Lewis acidity. **K. Lee**, C.M. Donahue, S.R. Daly

3:10 Intermission.

3:20 496. NHC pincer complex donor ability? PtEP (Platinum (Pt) electronic parameter): A donicity scale incorporating strictly meridional, tridentate ligands. **T.K. Hollis**, C.E. Webster, M. Zhang, E.V. Dornshuld, V. Dixet, J. Camacho-Bunquin, M. Delferro

3:40 497. Photochemical dyads and triads built on rotaxane architectures. A. Ogawa, M. Bechtold, M. Wolf, J. Wytko, K. Oohora, T. Hayashi, D. Guldi, S. Campidelli, **J. Weiss**

4:00 498. Molecular underground chemical tracers for monitoring underground fluid flows. **J.M. Sears**, T.J. Boyle, R.A. Kemp, J.A. Greathouse, R.F. Hess, L.J. Treadwell

4:20 499. First row transition metal Mabiq complexes for photocatalysis. **C. Hess**

Section K

Ernest N. Morial Convention Center Room 335

Inorganic Catalysts

S. A. Koch, *Organizer*

J. Panetier, X. Zhao, *Presiding*

1:30 500. Toward a mechanistic understanding of selective olefin upgrading in metal-organic framework catalysts. **R.J. Comito**, E. Metzger, M. Dinca, Z. Wu, G. Zhang, J.T. Miller

1:50 501. Computational modeling of molecular electrocatalysts featuring N-heterocyclic carbenes for carbon dioxide reduction. **J. Panetier**, X. Li, K. McCardle, X. Su, J.W. Jurss, S. Sung, M. Nippe

2:10 502. Artificial photochemical reactions by metal complexes: Cofactor regeneration and CO₂ reduction. **J. Kim**, Y. Jeon, S. Kim, T. Anjong

2:30 503. Computational characterization of a visible light sensitized tellurorhodamine catalyst for thiol oxidation. **H. Irving**

2:50 504. Theoretical analysis of C-H activation of Cp^{*}Ir(PPh₃). **X. Yang**

3:10 505. Enhanced sulfide oxidation activity via tuning site environment of Zr cluster nodes in UiO-66 MOF: A synergistic experimental and computational study. **R. Limvorapitux**, H. Chen, M. Mendonca, R. Snurr, S.T. Nguyen

3:30 Intermission.

3:45 506. Water oxidation catalysis-the rate determining step? **A. Poater**

4:05 507. Performance of density functional theory for predicting hydrogenation and dimerization of ethylene using transition metal hydride catalysts supported on zeolites. **N.K. Dandu**, S.O. Odoh

4:25 508. Evidence for the photo-activation from a [Mo₅S₇(S₂CNR₂)₃]⁺ pre-catalyst to a Mo₅S₄ core complex as

a hydrogen evolution catalyst in alkaline media. **P.R. Fontenot**, B. Shan, B. Wang, S. Simpson, A.F. Greene, L.A. Hunt, N. Hammer, C.E. Webster, J.T. Mague, R.H. Schmehl, J.P. Donahue

4:45 509. Computational studies of earth-abundant macrocycle-like electrocatalysts for CO₂ reduction. **K. McCardle**, X. Su, J.W. Jurss, J. Panetier

5:05 510. Electronic and steric effects on hydrogen production catalyzed by molecular Co complexes with pentadentate ligands in aqueous solution. **X. Zhao**, P. Wang, P. Li, C. Mokry, S. Lei, M. Sow, C. Odero, G. Liang, C.E. Webster

5:25 511. Density functional theory insights into rhodium-catalyzed addition of arylboronic acids to ketones. **P. Miro**, R. Recio, I. Fernandez
5:45 512. Chromium complexes in photoredox catalysis. **M.P. Shores**, R.I. Portillo, R. Higgins, D.J. Boston, A.K. Rappe

Actinide Complexes & Nanoclusters
Sponsored by NUCL, Cosponsored by INOR

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Sponsored by PROF, Cosponsored by ANYL, BIOL, BIOT, CHED, CMA, COLL, COMP, CWD, ENVR, INOR, MEDI, ORGN, PHYS, PMSE, POLY, WCC and YCC

Homogeneous Catalysis for Applied Organic Synthesis

Sponsored by CATL, Cosponsored by INOR and ORGN[‡]

Innovative Chemistry & Materials for Electrochemical Energy Storage

Sponsored by ENFL, Cosponsored by CATL, INOR and PMSE

Magnetically Recoverable Catalysts

Sponsored by CATL, Cosponsored by COLL, ENFL and INOR

Activation of Light (C1-C4) Hydrocarbons: Theory & Experiments

Sponsored by CATL, Cosponsored by ENFL, INOR and PHYS

Undergraduate Research Posters Inorganic Chemistry

Sponsored by CHED, Cosponsored by INOR and SOCED

MONDAY EVENING

Section A

Ernest N. Morial Convention Center Halls D/E

Sci-Mix

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

8:00 - 10:00

38, 42, 53, 61, 155, 189, 194, 201-202, 205, 208, 216, 230-232, 235, 257, 271-273, 275, 286, 293, 325-326, 334-335, 342, 345-347, 357-358, 364-365, 373, 380-385, 388-390, 452. See previous listings.

574, 663, 713-717, 732-734, 742-744, 746, 751, 755-757, 790, 800, 802-803, 807, 811, 813, 816-817, 823-825, 831, 834-839, 841-844, 849-850, 856-857, 863, 867, 879, 891, 897, 904, 907-908, 939-940, 942-943, 959-962, 968-970, 988-990, 993-996, 1100, 1111, 1126, 1130, 1296, 1303, 1306, 1351, 1405, 1409, 1411. See subsequent listings.

TUESDAY MORNING

Section A

Ernest N. Morial Convention Center Room 345

ACS Award for Distinguished Service in the Advancement of Inorganic Chemistry: Symposium in honor of Thomas B. Rauchfuss

L. F. Szczepura, *Organizer*

Z. M. Heiden, *Organizer, Presiding*

J. van der Vlugt, *Presiding*

8:00 Introductory Remarks.

8:05 513. How nitrosyls soften first row transition metals for hydrogenase-inspired HER electrocatalysis: Mechanistic and computational studies. S. Ding, P. Ghosh, M.B. Hall, M.Y. Darenbourg

8:30 514. Iron thiolate catalysts for photo- electrochemical hydrogen production. **F. Gloaguen**

8:55 515. Some aspects of electrochemical and photoelectrochemical conversion of small molecules at iron sulfur clusters, diiron dithiolate and other centres.. **C.J. Pickett**

9:20 516. H₂ evolution and uptake: From biomimetic approaches to technologically relevant materials. **V. Artero**

9:45 Intermission.

9:55 517. The mechanism of nitrogen fixation by nitrogenase. **B.M. Hoffman**

10:20 518. Organometallic chemistry in the radical SAM superfamily. **J.B. Broderick**

10:45 519. Vibrational spectroscopy of hydrogen-processing enzymes using Mössbauer photons: Why the fuss about little bumps and squiggles? **S.P. Cramer**

11:10 520. Computational modeling of NiFe-hydrogenase and its biomimetic complexes. **M.B. Hall**, H. Tang, S. Niu
11:35 521. Hydrogen-evolving molecular electrocatalysts: Interplay between experiment and theory. **S. Hammes-Schiffer**

Section B

Ernest N. Morial Convention Center Room 344

Metal-Organic Frameworks: What Are Next?

W. Lin, S. Ma, H. Zhou, *Organizers*
S. M. Humphrey, N. B. Shustova, *Presiding*

8:30 522. AIM-ing for catalyst synthesis with single-atom precision. Z. Li, A. Peters, J. Liu, M. Rimoldi, I. Kim, K. Otake, A. Platero-Prats, K.W. Chapman, N. Schweitzer, D.G. Truhlar, L. Gagliardi, C.J. Cramer, A.B. Martinson, O.K. Farha, **J.T. Hupp**

9:15 523. Metal-organic framework encapsulated with Lewis pair as a new paradigm for heterogeneous catalysis. **S. Ma**, Z. Niu, W. Gunatilleke

9:45 524. Unraveling the machinery of CO₂ photoreduction and water stability in titanium metal-organic frameworks. **F.J. Uribe-Romo**

10:15 525. New catalytic applications and methods of analysis of MOFs. **S. Madrahimov**

10:35 Intermission.

10:50 526. Modeling C-H Bond activation on bimetallic two-atom Co-M oxide clusters deposited on Zr-based MOF nodes. **L. Gagliardi**

11:20 527. Design strategies to coupling chemistries in dual/multi-function MOF arrays. W.A. Maza, S. Lin, **A.J. Morris**

11:50 528. Catalysis in MOFs: The characterization challenge and opportunities. **K.W. Chapman**

Section C

Ernest N. Morial Convention Center Room 343

F. Albert Cotton Award in Synthetic Inorganic Chemistry: Symposium in honor of Andrew S. Borovik

D. C. Lacy, C. G. Riordan, J. Y. Yang, *Organizers*
C. E. MacBeth, *Presiding*

8:00 Introductory Remarks.

8:05 529. Amazing nonheme high-valent iron-oxo landscape. **L. Que**

8:30 530. Primary copper(I)-dioxygen adduct formation, stabilization and substrate oxidative reactivity. **K.D. Karlin**, D.E. Diaz Romero, D.A. Quist, M. Bhadra, R. Cao

8:55 531. Mechanism of energy transfer in high quantum yield time-resolved lanthanide complexes. **K.N. Raymond**

9:20 532. Proton-coupled electron transfer. An overview. **T.J. Meyer**, P. Dongare

9:45 533. Living with oxos. **H.B. Gray**

10:10 Intermission.

10:20 534. Enhanced electron transport via material design: Impact on electrochemistry. **E.S. Takeuchi**, K.J. Takeuchi, A.C. Marschilok

10:45 535. Structure, spectroscopy and activity studies of copper-containing *Lytic Polysaccharide Monoxygenases*. **P. Walton**, G. Davies

11:10 536. Metal ligand design: Diverging approaches. W. Keown, L. Chiang, J. Gary, E.C. Wasinger, **T.D. Stack**

11:35 537. Ligand effects on the properties of formally Cu(III) complexes. **W.B. Tolman**

Section D

Ernest N. Morial Convention Center Room 352

Molecular Confinement Effects in Inorganic & Organic Containers

M. Fujita, B. C. Gibb, J. L. Sessler, *Organizers*

K. Bowman-James, P. Lusby, *Presiding*

8:00 Introductory Remarks.

8:15 538. Molecular containers and logic devices based on calixpyrroles. **J.L. Sessler**

8:45 539. Molecular confinement from multiple vantage points. **K. Bowman-James**

9:15 540. Cu^{II} paddle wheel-mediated dimeric capsules based on tetra-arylextended calix[4]pyrrole ligands. **P. Ballester**

9:45 Intermission.

10:00 541. Recent developments in coordination driven self-assembly. **P.J. Stang**

10:30 542. Supramolecular recognition enhanced by hetero radical pairing interactions. **H. Li**

11:00 543. Turning capsule catalysis inside out: Novel approaches utilizing innately-polarized Pd₂L₄ scaffolds. **P. Lushby**

11:30 544. Supramolecular assemblies based on pillar-shaped macrocyclic compounds "pillar[n]arenes". **T. Ogoshi**

Section E

Ernest N. Morial Convention Center Room 353

ACS Award in Pure Chemistry: Symposium in honor of Mircea Dinca

Y. Surendranath, *Organizer*

Y. Roman-Leshkov, *Organizer, Presiding*

8:30 Introductory Remarks.

8:40 545. Recent advances in olefin metathesis by molybdenum or tungsten catalysts. **R.R. Schrock**

9:10 546. Redox switchable catalysis applied to ring opening polymerization. **P. Diaconescu**

9:40 547. Biphilic organophosphorus catalysis. **A.T. Radosevich**

10:10 Intermission.

10:30 548. Exploring dinuclear redox chemistry with silver. **M.G. Campbell**

11:00 549. Late transition metal complexes supported by "double-pincer" tetradentate ligands. **L.M. Mirica**

11:30 550. Metaphosphates: Avenues enabled by new reagents and starting materials. K. Chakarawet, **C.C. Cummins**, M.B. Geeson, Y. Jiang, S. Shepard, J. Stauber, M. Tan, W. To, Q. Wan

12:00 Concluding Remarks.

Section F

Ernest N. Morial Convention Center
Room 354

Harry Gray Award for Creative Work in Inorganic Chemistry by a Young Investigator: Symposium in honor of Dwight S. Seferos

M. R. Jones, *Organizer*

A. M. Spokoyny, *Organizer, Presiding*
C. W. Machan, *Presiding*

8:30 Introductory Remarks.

8:35 551. Frustrated Lewis pair chemistry: An avenue to synthesis and catalysis. **D.W. Stephan**

9:00 552. Investigation of new photoreactivity of organoboron compounds. **S. Wang**, K. Yuan, S. Mellerup, D. Yang
9:25 553. Resolving orbital pathways for charge transfer at the interface. **C.P. Berlinguette**, C.W. Kellett, F.G. Parlane, G.J. Meyer, W. Swords, M.D. Turlington

9:50 554. Earth-abundant molecular electrocatalysts for the reduction of CO₂ and O₂. A. Nichols, S. Chatterjee, S. Hooe, **C.W. Machan**

10:15 Intermission.

10:25 555. Light-driven redox chemistry of antimony compounds. **F.P. Gabbai**

10:50 556. Catalytic and self-assembly routes to functional molecules and materials. **I. Manners**

11:15 557. Organoboron compounds in cross coupling chemistry and as catalysts for FLP reductions. **C.M. Crudden**

11:40 558. Boron clusters as dopants for solid-state and polymer materials. **A.M. Spokoyny**

12:05 Concluding Remarks.

Section G

Ernest N. Morial Convention Center
Room 210

PCET PhotoCatalysis with Inorganic Molecules & Materials

Cosponsored by PHYS
J. L. Dempsey, C. Heyer, E. Leon,
Organizers

G.J. Meyer, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 559. Proton-coupled electron transfer in artificial photosynthesis and photoreduced nanoparticles. **S. Hammes-Schiffer**

8:30 560. New synthetic methods and aqueous electrochemical characterization of p-Type CuGaO₂ nanocrystals. A.R. Combs, **B.H. Farnum**

8:50 561. Surface chemistry and intercalation as strategies to tune reactivity in colloidal transition metal dichalcogenide electrocatalysts. **B.M. Cossairt**, D. Henckel, O. Lenz

9:10 562. Copper substituted TiO₂: A novel p-type anatase metal oxide and its application in dye-sensitized solar cells. **S. McCullough**, J. Cahoon

9:30 563. Photoelectrochemical performance of BiVO₄ photoanodes

integrated with [NiFe]-layered double hydroxide water oxidation nanocatalysts. **A.M. Müller**, T.S. Sinclair, H.B. Gray
9:50 Intermission.

10:00 564. Electrochemical measurements of the redox potentials of multiply reduced colloidal semiconductor nanocrystals. C.K. Brozek, G.M. Carroll, E. Tsui, K. Hartstein, **D.R. Gamelin**

10:20 565. Nano-spectroscopy for characterization of surfaces and interfaces. **J. Atkin**

10:40 566. Fluorescence activation by visible light in conjugated polymer nanoparticles. **E.J. Harbron**, X. Zhang, H.C. Hannon

11:00 567. Design, synthesis, and passivation of metal oxide photocathodes for aqueous solution: Fixing and moving beyond NiO. **J. Cahoon**

11:20 568. Strongly coupled chromophore-base-phenol dyads: PCET oxidation on surfaces and using polymetallic chromophores. **G. Manbeck**, J.J. Concepcion, E. Fujita
11:40 569. PCET with colloidal quantum dots: Quantification of surface proton concentration and demonstrations of PCET-mediated colloidal catalysis. **E.A. Weiss**, S. Lian, D. Westmoreland, K. McClelland

Section H

Ernest N. Morial Convention Center
Room 211

Solid-State Inorganic Chemistry

C. G. Lugmair, V. Poltavets,
Organizers

B. Saparov, *Presiding*

8:30 570. The origin of unusual valence band structure in layered bismuth oxyhalides. **H. Kageyama**

8:50 571. Hybrid Organic-Inorganic Halides of Group 12 Metals (Zn, Cd, Hg): syntheses, crystal and electronic structures, and prospective optoelectronic applications. **B. Saparov**

9:10 572. Bringing node-and-linker principle out in metal-free systems: Enlarged diamond-like networks from halogen-bonded halide ions. **C.A. Gunawardana**, M. Dakovic, C.B. Aakeroy

9:30 573. Intrinsic broadband white-light emission from ultrastable, cationic lead halide materials. Z. Zhuang, C. Peng, **H. Fei**

9:50 574. Rapid microwave synthesis of organically-grafted layered perovskites and exfoliated nanosheets. S. Akbarian-Tefaghi, A. Poduval, E. Teixeira Veiga, G. Amand, **J.B. Wiley**

10:10 Intermission.
10:25 575. Chemically controlled design and discovery of new materials. **T. Tran**, M. Quintero, K. Arpino, X. Wang, T. McQueen

10:45 576. Borides and carbaborides as transition-metal-free intercalation

cathodes with redox active anions. **V. Poltavets**, M.R. Shabetai, J.Y. Do
11:05 577. Non-icosahedral high-pressure boron allotrope. **I. Chuvashova**, E. Bykova, M. Bykov, V. Prakapenka, K. Glazyrin, L. Dubrovinsky, N. Dubrovinskaia
11:25 578. Searching for new superconductors with chemistry view. **X. Gui**

11:45 579. Structurally related carbometalates grown from Pr/Ni flux. T.O. Engstrand, **S.E. Latturmer**

Section I

Ernest N. Morial Convention Center
Rooms 340/341

Bioinorganic Chemistry: DNA, RNA & Inorganic Drugs

S. A. Koch, *Organizer*

J. L. Brumaghim, R. S. Khnayer,
Presiding

8:30 580. Diiridium (III) and Ru(II) complexes as emission probes for cell imaging and cellular activities. **J. Kim**, T. Anjong

8:50 581. DNA interactions of potent thione and selone antioxidants: Control via metal coordination? S. Goodman, **J.L. Brumaghim**

9:10 582. Rational design of a cytotoxic dinuclear Cu₂ complex that binds by molecular recognition at two neighboring phosphates of the DNA backbone. **T. Glaser**

9:30 583. Withdrawn

9:50 584. Development and study of novel ruthenium complexes as potential dual-activated anticancer prodrugs: The role of pH in uptake and the use of cytotoxic ligands. **J. Gray**, F. Qu, J. Park, A. Shrestha, S. Altman, A.R. Hairston, Y. Kim, E.T. Papish
10:10 Intermission.

10:20 585. Naphthoquinone fused N-heterocyclic carbene-Gold(I) complexes as dual targeting cancer therapeutics. **K. Arumugam**, J. Arambula, M. Miles, R. McCall

10:40 586. Pyridine modified heterocycles and coordination complexes derived from first row transition metals. **K.N. Green**, S.M. Brewer, H.M. Johnston

11:00 587. Structure-activity relationships for a new class of Mn-based MRI contrast agents: Magnetic relaxation, protein binding, and pharmacokinetics. **E. Gale**
11:20 588. Syntheses, characterization, and biological activities of 2-(benzylimino)methyl)-6-methoxyphenol and its metal(II) complexes. **O. Adewusi**

11:40 589. Photodynamic therapy of cancer using a long-lived Cu(I) bis-phenanthroline sensitizer. C. Al Hageh, M. Al Assad, Z. El Masri, M. El Sibai, C. Khalil, **R.S. Khnayer**

Section J

Ernest N. Morial Convention Center
Room 212

Chemistry of Materials: Nanomaterials

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

8:00 590. Circular dichroism of CdSe nanocrystals bound by chiral carboxylic acids. **M. Puri**, V.E. Ferry

8:20 591. Halide-terminated cadmium selenide nanocrystals: From classic fundamental chemistry to devices. **N.C. Anderson**, J.S. Owen

8:40 592. Kinetically controlled heterostructure assembly of cadmium chalcogenide nanorods. **M. Enright**, B.M. Cossairt

9:00 593. Measurement and theoretical modelling of multiply charged quantum dot redox potentials. **C.K. Brozek**, H. Liu, X. Li, D.R. Gamelin

9:20 594. Insights in the nucleation and growth mechanism of colloidal stable indium phosphide nanomaterials. **M. Friedfeld**, B.M. Cossairt

9:40 595. Exfoliation and surface tunability in layered rhenium chalcogenide networks. **B. Choi**
10:00 Intermission.

10:15 596. Cation exchange induced evolution of InP magic-sized cluster physical and electronic structure. **J. Stein**, B.M. Cossairt

10:35 597. Nonclassical synthetic phase control at the nanoscale. **A. Ritchhart**, B.M. Cossairt

10:55 598. Aminophosphines as versatile precursors for the synthesis of group II metal phosphide nanocrystals. **M. Mundy**, B.M. Cossairt

11:15 599. Phase transitions in transition metal chalcogenide superatomic crystals. **E.S. O'Brien**
11:35 600. Colloidal synthesis of metal germanide nanocrystals. T. Dupper, **A. Hochbaum**

11:55 601. Frustrated quantum dots, the experimental validation of a computational model. **J.K. Bindra**, L. Gutsev, G. Strouse, N. Dalal, S. Stoian, J. van Tol

Section K

Ernest N. Morial Convention Center
Room 335

Coordination Chemistry: Synthesis & Characterization

A. Larsen, *Organizer*

M. Stollenz, E. M. Villa, *Presiding*

8:30 602. Oxygen-exchange kinetics of the Anderson-type polyoxometalate ion IM₆O₆24⁵⁻. **E.M. Villa**, M.R. Spriet

8:50 603. Reactivity of a μ₃-nitridotriiron cluster. **B.J. Cook**, D.M. Ermert, R. Garcia, L.J. Murray

9:10 604. Bioinspired monooxygenase mimics: Towards the design of functional high valent metal-oxo intermediates. **J. Bogart**, S.A. Cook, A. Weitz, N. Levi, C. Moore, A.L. Rheingold, M.P. Hendrich, A. Borovik

9:30 605. Divergent electronic structures and reactivity profiles in

bimetallic copper imide complexes.

K.M. Carsch, T. Betley

9:50 606. Trapped intermediate of Meerwein-Ponndorf-Verley reduction of hydroxy benzaldehyde using titanium alkoxides. **T.J. Boyle**, J.M. Sears, K.A. Dunnigan, D.R. Wheeler

10:10 Intermission.

10:20 607. Highly luminescent copper^I bis(amidinate) clusters and digold bis(amidine) complexes. **M. Stollenz**, O. Ugarte Trejo, A. Calderón Díaz, N. Siwabut, N. Maya, N. Bhuvanesh

10:40 608. Synthesis, characterization, and reactivity of heterobimetallic Nb/Fe complexes supported by phosphinoamide ligands. **G. Culcu**, C.M. Thomas

11:00 609. Synthesis and characterization of a Co(II)-iodosylarene adduct. **E. Hill**, A. Filatov, J. Anderson

11:20 610. Spin ground state tuning of octahedral Fe₆ clusters and their incorporation into extended magnetic structures. **K. Anderton**, B. Malbrecht, T. Betley

11:40 611. Synthesis and reactivity of bio-inspired mononuclear transition metal complexes: Hydrocarbon functionalization with reactive oxygen species. **N. Botcha**, N. Singh, A. Mukherjee

GSSPC: Finding Our Place at the Bottom

Symposium in honor of Richard Feynman

Sponsored by CHED, Cosponsored by ANYL³, COLL³, ENVR³, INOR, PMSE³ and PRES³

Actinide Complexes & Nanoclusters

Sponsored by NUCL, Cosponsored by INOR

Homogeneous Catalysis for Applied Organic Synthesis

Sponsored by CATL, Cosponsored by INOR and ORGN²

Innovative Chemistry & Materials for Electrochemical Energy Storage

Sponsored by ENFL, Cosponsored by CATL, INOR and PMSE

Catalytic Conversion of Biomass Derived Molecules to Chemicals & Fuels

Sponsored by CATL, Cosponsored by ENFL, ENVR and INOR

Activation of Light (C1-C4) Hydrocarbons: Theory & Experiments

Sponsored by CATL, Cosponsored by ENFL, INOR and PHYS

Catalytic & Photocatalytic Degradation of Pollutants & Chemical Threat Agents: New

Developments in Materials & in Situ & Operando Methods

Enabling Fundamental Advances in Catalysis & Surface Science

Sponsored by CATL, Cosponsored by ENVR, INOR and PHYS

TUESDAY AFTERNOON

Section A

Ernest N. Morial Convention Center Room 345

ACS Award for Distinguished Service in the Advancement of Inorganic Chemistry: Symposium in honor of Thomas B. Rauchfuss

Z. M. Heiden, *Organizer*

L. F. Szczepura, *Organizer, Presiding*
A. R. Fout, *Presiding*

1:30 612. Hydrogen oxidation electrocatalysis involving hydrogen atom transfer: A homolytic approach to a heterolytic reaction. **R. Bullock**, G.M. Chambers, E.S. Wiedner

1:55 613. Radical cyclizations catalyzed by [NEt₄][CpV(CO)₃H]. **J.R. Norton**, J. Kuo, J. Abuyuan, C. Lorenc

2:20 614. Supported organotungsten complexes for catalysis. **A.P. Sattelberger**, **R.R. Langeslay**, M. Delferro

2:45 615. Putting more chemistry into chemical vapor deposition, or how I learned to stop worrying and listen to Tom. **G.S. Girolami**, J.R. Abelson

3:10 Intermission.
3:25 616. Augmenting small molecule binding and activation with Lewis acids. **N.K. Szymczak**, J.B. Geri, J.J. Kiernicki, J.P. Shanahan

3:50 617. Synthesis and reactivity of BODIPY-containing metal complexes. **Z.M. Heiden**, B.L. Thompson, J.L. Fernandez, N.R. Treich

4:15 618. Redox-active and reactive ligands - new avenues for organometallic chemistry, selective bond activation and homogeneous catalysis. **J. van der Vlugt**

4:40 619. Exploring iron and cobalt-based metal-thiolate catalysts for organic synthesis. **W. Wang**
5:05 620. Iron-catalyzed oxyanion reduction. **A.R. Fout**, C. Ford, Y. Park, Z. Gordon, M. Drummond

Section B

Ernest N. Morial Convention Center Room 344

Metal-Organic Frameworks: What Are Next?

W. Lin, S. Ma, *Organizers*
H. Zhou, *Organizer, Presiding*
P. K. Thallapally, *Presiding*

1:30 621. Carbon dioxide capture in diamine-appended metal-organic frameworks. **R. Siegelman**, P.J. Milner, J. Martell, E. Kim, M.I. Gonzalez, A. Forse, T. Runcevski, J.A. Mason, T. McDonald, J.A. Reimer, **J.R. Long**

2:15 622. Metal-organic frameworks (MOFs) as a platform for energy applications. **Q. Xu**

2:45 623. Bimetallic metal-organic frameworks. **N.B. Shustova**, E. Dolgoplova, O. Ejegbavwo, A.M. Rice

3:15 624. Direct electrical readout sensors utilizing highly selective metal organic frameworks. **T.M. Nenoff**, L.J. Small
3:35 Intermission.

3:50 625. Commercialization of metal-organic frameworks and lessons learned. **O.K. Farha**, J. Arno, M. Weston, W. Morris, P. Siu

4:20 626. Strategies for the fabrication of MOF films and coatings. **B. Wang**
4:50 627. A simple strategy to immobilize enzyme in metal-organic frameworks. **W. Liu**, L. Liu, S. Lirio, C. Lin

Section C

Ernest N. Morial Convention Center Room 343

F. Albert Cotton Award in Synthetic Inorganic Chemistry: Symposium in honor of Andrew S. Borovik

D. C. Lacy, C. G. Riordan, J. Y. Yang, *Organizers*

R. Gupta, *Presiding*
1:30 628. Multiple-site concerted proton-electron transfers (MS-CPET). **J.M. Mayer**, J. Darcy, M. Ener, B. Koronkiewicz, T. Markle

1:55 629. Metal-coordinated ligand radical-driven reactivity. **R. Mukherjee**

2:20 630. Troger's base: A versatile platform for supramolecular chemistry. **D.L. Jameson**

2:45 631. Syntheses, structural and stability comparisons of [Co(DIG₃tren)X]Y, (X = halide or pseudohalide; Y = X or BPh₄). **R.C. Scarrow**, D. Suryavanshi Magar, B. Burke, G.P. Yap

3:10 632. Spectroscopy and DFT calculations of a flavo-diiron enzyme identify new structures and NO intermediates of the enzymatic cycle. **A. Weitz**, N.C. Giri, J.D. Caranto, D.M. Kurtz, E.L. Bominaar, **M.P. Hendrich**
3:35 Intermission.

3:50 633. Artificial metalloenzymes: Second coordination sphere interactions at their best. **T.R. Ward**

4:15 634. Discovery and application of 12-lipoxygenase inhibitors as anti-platelet agents. **T.R. Holman**

4:40 635. Mononuclear high-valent Fe(OH) and Mn(OH) corroles. **D.P. Goldberg**, J. Zaragoza

5:05 636. Carbon- and sulfur-bridged iron clusters of relevance to nitrogenase. **S.F. McWilliams**, A.L. Nagelski, D.E. DeRossa, N.A. Arnet, B.Q. Mercado, **P.L. Holland**

Section D

Ernest N. Morial Convention Center Room 352

Molecular Confinement Effects in Inorganic & Organic Containers

M. Fujita, B. C. Gibb, J. L. Sessler, *Organizers*

R. Custelcean, H. Li, *Presiding*
1:30 637. Crystalline sponge method for natural product chemistry. **M. Fujita**

2:00 638. Confinement of anion-water clusters in guanidine crystals. **R. Custelcean**

2:30 639. Anion protection and self-assembly inside cages formed from stacked macrocycles. **A.H. Flood**

3:00 640. Ten years of incarceration: A versatile, water-soluble cage. **D.A. Vosburg**, J. Nitschke

3:30 Intermission.
3:45 641. Molecular capsules constructed from mixed macrocycles

seamed together by metal ions. **J.L. Atwood**, C. Zhang, R. Patil, K. Sikligar, G.A. Baker, P.H. Atwood, S.G. Atwood

4:15 642. Endo-functionalized molecular tubes. **W. Jiang**

4:45 643. Unique host properties of polyaromatic coordination capsules. **M. Yoshizawa**

5:15 644. Recognition and reactions in deep cavitands. **J. Rebek**

Section E

Ernest N. Morial Convention Center Room 353

Inorganic Chemistry of Lead Halide Perovskites: Insights from Fundamentals

R. L. Brutchey, J. Vela, *Organizers*
B. C. Melot, *Organizer, Presiding*

1:30 Introductory Remarks.
1:40 645. Halide perovskites: New high performance semiconductors. **M.G. Kanatzidis**

2:20 646. Reducing the toxicity and improving the stability of two-dimensional halide perovskites. **D. Solis-Ibarra**, B. Vargas, P.I. Roman, P. Carmona-Monroy

2:40 647. Halide perovskites beyond CH₃NH₃PbI₃: Structural diversity and opportunities for semiconductor design. **D.B. Mitzi**

3:20 Intermission.
3:50 648. Looking beyond methylammonium lead iodide for next generation solar absorbers. **D. Scanlon**

4:30 649. Trends in the lone pair-induced local distortions in tin and lead halide perovskites: Are Sn and Pb in the center of the octahedron? **G. Staurita-Plankis**, D.H. Fabini, C. Stumpous, M.G. Kanatzidis, R. Seshadri

4:50 650. Capturing the properties of lead-halide perovskites with new materials. **A. Slavney**, I. Smith, L. Leppart, J. Neaton, **H. Karunadasa**

Section F

Ernest N. Morial Convention Center Room 354

Harry Gray Award for Creative Work in Inorganic Chemistry by a

Young Investigator: Symposium in honor of Dwight S. Seferos

A. M. Spokoyny, *Organizer*
M. R. Jones, *Organizer, Presiding*
T. Li, *Presiding*

1:30 Introductory Remarks.

1:35 651. Programmable metamaterials. **C.A. Mirkin**

2:00 652. Nanoparticle slurry technologies for chemical mechanical planarization. **T. Li**

2:25 653. Using nanoscale geometry to dictate molecular behavior in inorganic nanoparticle composites. **R. Macfarlane**

2:50 654. Polymers, plasmons, and patterns. **J.M. Buriak**, F. Liu, E.J. Lubber, B. Olsen

3:15 Intermission.

3:25 655. Peptide platforms for constructing plasmonic chiroptical materials. **N.L. Rosi**, A. Merg, S. Punekar

3:50 656. Spherical nucleic acids for gene regulatory and immuno therapeutic applications. **D. Giljohann**

4:15 657. Wiring-up transition metals: Translating solution chemistry to nanoscale sensors. **T.M. Swager**

4:40 658. NMR characterization of metal nanoparticle formation, structure, and performance. **J. Millstone**

5:05 659. Spatial mapping of surface-mediated nanocrystal transformations. **M.R. Jones**

5:30 Concluding Remarks.

Section G

Ernest N. Morial Convention Center
Room 210

PCET PhotoCatalysis with Inorganic Molecules & Materials

Cosponsored by PHYS

J. L. Dempsey, C. Heyer, E. Leon, G. J. Meyer, *Organizers*

T. A. White, *Presiding*

1:30 660. Proton coupled electron transfer bond cleavage of oxygen. **D.G. Nocera**, D.K. Dogutan, M. Qiu, G. Passard, C. Cosentin

1:55 661. PCET in metal organic frameworks: Toward photoinduced water oxidation. P. Celis-Salazar, S. Lin, **A.J. Morris**

2:15 662. Role of PCET in small molecule activation: Water oxidation and CO₂ reduction. Y. Xie, D.W. Shaffer, L. Wang, **J.J. Concepcion**

2:35 663. Iron polypyridyl complexes immobilized on metal oxide semiconductors for photocatalytic hydrogen generation. **W. McNamara**

2:55 664. New Ru complexes demonstrate ligand-centered reactivity for the reduction of CO₂. **M.R. Norris**, M. Gu, L. Paul

3:15 Intermission.

3:30 665. Increasing rates and lowering overpotentials in [Ni(P₂N₂)₂]²⁺ electrocatalysts for production of H₂. **R. Bullock**, C.M. Klug, A.J. Cardenas, M.J. O'Hagan, E.S. Wiedner

3:50 666. Unlocking redox reactivity through Installation of proton relays in the secondary coordination sphere. **J.Y. Yang**, J. Kotyk, R. Combs

4:10 667. Mechanistic studies on a family of carbene-supported ruthenium complexes for electrochemical CO₂ reduction. **S. Gonell**, M.D. Massey, I.P. Moseley, C.K. Schauer, J.T. Muckerman, A.J. Miller

4:30 668. Fast detection method for analyzing CO₂ electroreduction products to probe catalyst degradation mechanism. F. Zhang, **A. Co**

4:50 669. Evaluating the potential of nanocapsules to synthetically modulate the second coordination sphere of fuel forming catalysts. **N. Elgrishi**

5:10 670. Electrocatalysis and photo-electrocatalysis of the oxygen reduction reaction. **J.M. Mayer**, M.L. Pegis, C. Wise, D. Martin, O. Jung, B. Koronkiewicz, S. Raugel, N. Kumar, J. Peper

Section H

Ernest N. Morial Convention Center
Room 211

Chemistry of Materials: Synthesis & Properties

C. G. Lugmair, *Organizer*
Y. Rao, *Presiding*

1:30 671. Chemical vapor transport synthesis of Mn_xZn_(1-x)Cr₂O₄ single crystals in a closed ampoule reactor: A virtual equilibrium (steady-state) model that predicts composition (x) of the deposited crystalline solid solution. **Y. Rao**

1:50 672. Low-valent coordination networks with *m*-terphenyl isocyanides based linkers. **A. Arroyave**

2:10 673. Thermolysis of heterobimetallic single-source precursors: A springboard to the synthesis of binary intermetallic compounds. **C.L. Daniels**, S. Sahu, F.P. Gabbai, J. Vela

2:30 674. Hybrid platinum (IV) iodides: progression from perovskite to hydrogen bonded frameworks. **H. Evans**, D.H. Fabini, M. Preefer, R. Seshadri, F. Wudl

2:50 Intermission.

3:05 675. Kinetic control of one-pot core/shell nanoparticles and nanoplatelets using thio- and selenoureas. **L. Hamachi**, I. Jen-La Plante, M.P. Campos, K. Qian, G. Cleveland, I. Rreza, H. Yang, E. Chan, W. Walravens, Z. Hens, A. Kuntzmann, S. Ithurria, B. Dubertret, J.S. Owen

3:25 676. Controlled speciation of transition metal ions in cadmium thiophenolate-based molecular clusters. **K.R. Kittilstved**, F. Kato

3:45 677. Molten salt synthetic method for making complex metal oxide nanoparticles. **Y. Mao**

4:05 678. Facile and controllable synthesis of Janus two-dimensional transition metal dichalcogenide monolayers. **J. Zhang**, J. Lou

Section I

Ernest N. Morial Convention Center
Rooms 340/341

Coordination Chemistry: Characterization & Applications

A. Larsen, *Organizer*

E. V. Rybak-Akimova, K. D. Vogiatzis, *Presiding*

1:30 679. Pyridine azamacrocycles with appended functional groups: redox reactivity and catalysis. **E.V. Rybak-Akimova**, S.G. McKenzie, T. Palluccio, H. Seidel

1:50 680. Copper guanidine quinoline complexes as catalysts in ATRP: Prediction of activities via DFT and isodesmic reactions. **T. Rösener**, A. Hoffmann, S. Herres-Pawlis

2:10 681. Ruthenium(II) polypyridyl complexes with hydroxypyridine mixed ligands: Synthesis, characterization and *in vitro* cell cytotoxicity. **J.A. Obaleye**, A.O. Rajee, A.A. Ajibola, H.F. Babamale, M.O. Bamigboye, P.O. Obaleye

2:30 682. Supramolecular self-assembled metallacages as targeted drug delivery systems and for imaging. **A. Casini**, B. Woods, M. Wenzel

2:50 683. Tuning the hydricity of nickel hydrides for the electrocatalytic reduction of CO₂. **A.L. Ostericher**, C.P. Kubiak

3:10 Intermission.

3:20 684. Understanding the electronic effects that control the non-heme Fe(IV)-oxo reaction channels for C-H activation. **K.D. Vogiatzis**

3:40 685. Triiron clusters containing single atom bridging ligands for dinitrogen fixation. **R.B. Ferreira**, L.J. Murray

4:00 686. Mn(IV) complexes for biochemically activated MRI contrast. **H. Wang**, P. Caravan, T. Storr, E. Gale

4:20 687. Computational modelling of the ligand tuning effect over the transition temperature in spin-crossover systems using density functional methods. **J. Cirera Fernandez**

Section J

Ernest N. Morial Convention Center
Room 212

Organometallic Chemistry: Catalysis-Late Transition Metals

N. S. Radu, *Organizer*

T. Atesin, O. Ozerov, *Presiding*

1:30 688. Computational study of the mechanism of dehydrogenative borylation of terminal alkynes by SiNN iridium complexes. **O. Ozerov**, J. Zhou, C. Lee

1:50 689. Mechanistic observations of cross coupling reactions with PNP Cobalt. **B.J. Foley**, C. Palit, O. Ozerov

2:10 690. Preferential electrochemical reduction of CO₂ to formate by a CCC-NHC-Ni complex: A computational/mechanistic study. **R.W. Lamb**, J. Cope, N. Liyanage, P.J. Kelly,

J. Denny, J.H. Delcamp, T.K. Hollis, C.E. Webster

2:30 691. Electrocatalytic formate oxidation with an iridium hydride complex. **K.M. Waldie**, C.P. Kubiak

2:50 692. Bioorthogonal transfer hydrogenation mediated by small molecule organoiridium catalysts. **S. Bose**, L. Do

3:10 693. Understanding the thermodynamic and kinetic factors that contribute to transfer hydrogenation efficiency by organoiridium complexes. **A.H. Ngo**

3:30 694. Palladium(0)-catalyzed intramolecular allylic alkylation of diketesters. **T. Atesin**

3:50 695. Enhancing catalytic performance of phosphine-phosphinate and phosphine-phosphonate Pd alkyl polymerization catalysts by remote binding of B(C₆F₅)₃. **A. Johnson**, N.D. Contrella, J. Sampson, M. Zheng, R.F. Jordan

4:10 696. Carbon dioxide reduction by anionic chalcogenide-bridged tricopper clusters. **B.J. Cook**, L.J. Murray

4:30 697. Controlled 4e⁻ reduction of CO₂ with various hydroboranes and first row metal hydride catalysts. **S. Bontemps**

4:50 698. Substrate directed, enantioselective Heck arylation of cyclohexenols promoted by KCTf₃: Synthesis of all cis substituted, arylcyclohexenols. **R.A. Angnes**, L.M. Thompson, C.R. Correia, G.B. Hammond

5:10 699. Metal-ligand bifunctional catalysis: The "accepted" mechanism, the issue of concertedness, and the function of the ligand in catalytic cycles involving hydrogen atoms. **P.A. Dub**

5:30 700. Olefin hydroarylation catalyzed by ruthenium(II) complexes: Changes in reactivity based on auxiliary ligands. **X. Jia**, J. Gary, B.A. McKeown, T.R. Cundari, P.J. Perez, T.B. Gunnoe

Section K

Ernest N. Morial Convention Center
Room 335

Inorganic Spectroscopy

C. V. Popescu, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 701. To be or not to be: Bonding studies in heterobimetallic d¹⁰-d¹⁰ centers. **K. Melancon**, B.M. Otten, M.A. Omary

1:55 702. Multimodal micro-spectroscopies for metal complexes bio-imaging: development metal-CO as multimodal probes. **C. Policar**, F. Lambert, N. Delsuc, H.C. Bertrand

2:15 703. Near-field optical microspectroscopy and nanoscale spectroscopy (nano-FTIR) on semiconductors, plasmonic and 2D materials. **P. Schäfer**, T. Gokus

2:35 704. Time-resolved IR studies in conventional and supercritical fluids: From alkane complexes and C-H

activation to organometallic noble gas complexes. **M.W. George**
2:55 705. Effects of electron transfer on hydrogen bonds. **T.M. Porter, G.P. Heim, C.P. Kubiak**
3:15 Intermission.
3:20 706. Determination of the dramatic increase in protonation rates following one-electron reduction for a series of luminescent osmium hydride complexes. **R.E. Adams, T.A. Grusenmeyer, A.L. Griffith, R.H. Schmehl**
3:40 707. Theoretical study of substituted CCC-NHC palladium and platinum complexes for OLED applications. **V. Dixit, E.V. Dornshuld, C.E. Webster, T.K. Hollis**
4:00 708. Solid-state ^{45}Sc NMR of $\text{Cp}^*\text{Sc-R}$: Evidence for an agostic interaction in $\text{Cp}^*\text{Sc-Et}$. **M.P. Conley, D. Culver, W. Huynh, H. Tafazolian**
4:20 709. Direct identification of inner-sphere nitrogen radicals via nitrogen K-edge X-ray absorption spectroscopy. **J.T. Lukens, D. Iovan, T. Kurogi, D.J. Mindiola, T. Betley, K.M. Lancaster**
4:40 710. Magnetic resonance investigation of bonding between first row transition metals. **S.M. Greer, J. McKay, K.M. Gramigna, C.M. Thomas, S. Stoian, S. Hill**
5:00 711. Highly concentrated alkali hydroxide aqueous solutions: Classical force fields, speciation and their effects on neutron PDFs. **D. Semrouni, H. Wang, K. Page, D. Wesolowski, A.G. Stack, A.E. Clark**

GSSPC: Finding Our Place at the Bottom

Symposium in honor of Richard Feynman

Sponsored by CHED, Cosponsored by ANYL[‡], COLL[‡], INOR, PHYS[‡], PMSE[‡] and PRES[‡]

WCC Rising Star Award Symposium

Sponsored by WCC, Cosponsored by BIOT, CHED, COLL, INOR and PROF

Homogeneous Catalysis for Applied Organic Synthesis

Sponsored by CATL, Cosponsored by INOR and ORGN[‡]

Molecular Processes at Mineral-Water Interfaces: Linking Theory & Experiments

Silica/Alumina Surfaces & the Electrical Double Layer

Sponsored by GEOC, Cosponsored by ENVR and INOR

Catalytic Conversion of Biomass Derived Molecules to Chemicals & Fuels

Sponsored by CATL, Cosponsored by ENFL, ENVR and INOR

Innovative Chemistry & Materials for Electrochemical Energy Storage

Sponsored by ENFL, Cosponsored by CATL, INOR and PMSE

R&D in the Chemical Catalysis for Bioenergy Consortium

Sponsored by CATL, Cosponsored by ENFL, ENVR and INOR

Catalytic & Photocatalytic Degradation of Pollutants & Chemical Threat Agents: New Developments in Materials & in Situ & Operando Methods Enabling Fundamental Advances in Catalysis & Surface Science

Sponsored by CATL, Cosponsored by ENVR, INOR and PHYS

TUESDAY EVENING

Section A

Ernest N. Morial Convention Center Hall D

Metal-Organic Frameworks: What Are Next?

W. Lin, S. Ma, H. Zhou, *Organizers*
5:30 - 7:30

712. Hierarchical pore formation in a series of ultrastable multivariate metal-organic frameworks. **L. Feng, S. Yuan, L. Zhang, J. Li, A. Kirchner, H. Zhou**
713. Computational modeling of the degradation of MOF-2 by Brønsted acid gases. **Z. Lee, S. Zhang, L. Flores, D.A. Dixon**

714. Rational design and synthesis of heterometallic metal-organic frameworks. **P. Muldoon, C. Liu, C. Miller, N.L. Rosi**

715. Arsenic coordination materials: Design, properties, and applications. **R.E. Sikma, S.G. Dunning, P. Kunal, J. Reynolds, J. Chang, S.M. Humphrey**

716. Metal-organic framework templated formation of nanostructured conducting polymers. **T. Wang, S.K. Smoukov, A.K. Cheetham**

717. Enhancing polymer crystallinity in mixed matrix membranes using metal organic framework nanosheets for efficient CO₂ capture. **C. Youdong, D. Zhao**

718. Phosphine coordination materials as a platform for catalytic metal incorporation. **S. Dunning, G. Nandra, A.D. Conn, K.M. Walsh, W. Chai, P. Kunal, J. Reynolds, J. Chang, A. Steiner, G.A. Henkelman, S.M. Humphrey**

719. Design and synthesis of multifunctional materials comprising stratified metal-organic frameworks and plasmonic nanoparticles. **T. Luo, X. Gan, J. Millstone, N.L. Rosi**

720. Ligand removal and porosity control in gradient metal-organic frameworks. **C. Liu, Z.M. Schulte, T. Luo, N.L. Rosi**

721. Chemical modifications to tailor magneto-structural correlations in the

triangulated Kagome lattice $\text{Cu}_9\text{X}_2(\text{cpa})_6$. **S.F. Skinner, W.M. Farmer, L.W. Ter Haar**

722. Aggregation to the best: A 12-connected Zirconium MOF with a triphenylene-based hexatopic linker. **Y. Zhang, X. Yang, S. Yuan, J. Qin, H. Zhou**

723. Ultramicroporous Zr MOF for C₂ hydrocarbon separation. **Y. Wang, D. Zhao**

724. Preparation of 2D MOF materials. **Z. Li, K. He, K. Yeung**

725. Crystallization of sub-100 nanometer MOF thin film on graphene oxides. **W. Chen, K. He, K. Yeung**

726. MOF membrane microreactor for organic synthesis. **K. He, K. Yeung**

727. Rational design of a mixed-linker MOF platform based on merged net principle. **H. Jiang, J. Jia, A. Shkurenko, Z. Chen, K. Adil, Y. Belmabkhout, L. Weselinski, A. Assen, D. Xue, M. O'Keeffe, M. Eddaoudi**

728. Effects of chloride concentration on graphene analogues for thermoelectric devices. **S. Yoon, M.C. So**

729. Single-crystal electrical devices of triphenylene-based 2D MOFs. **R.W. Day, M. Dinca**

730. Fabrication and characterization of conductive metal-organic framework coatings by automated liquid phase epitaxy for electronics. **M.C. So, V. Cherrette, V. Stavila, J. Llinas, A.A. Talin, M. Allendorf**

731. Ultra-small face-centered cubic Ru nanoparticles confined with an anionic porous coordination cage for high performance catalysis. **Z. Xiao, Y. Fang, H. Zhou**

732. Towards the design and synthesis of metal-organic frameworks for targeted separation of heavy pollutants. **D. Fairchild, J. Cordova, G.S. Pour, O.A. Tarano, K. Sanchez, Z. Magnuson, F.J. Uribe-Romo**

733. Amenable and accessible functionality in covalent organic frameworks: Merits in the design of heavy metal scavenger for environmental remediation. **Q. Sun, S. Ma**

734. Installing biomimetic diiron complex in metal-organic framework for photocatalytic hydrogen evolution. **B.L. Frey, X. Zhang, J. Zhang**

735. One-pot synthesis of a series of zirconium MOFs with multifunctionalities. **Y. Sun, H. Zhou**

736. Cooperative enhanced catalysis of lipase-proline@MOF towards enantiomeric chemical transformation. **C. Lin, S. Lirio, L. Liu, W. Liu**

737. Porous layer network in indium based metal-organic frameworks with carbon dioxide adsorption and fixation. **C. Tsai, Y. Li, S. Wang, C. Lin**

738. Dual-ligand luminescent metal-organic frameworks towards environmental remediation efforts. **N.D. Rudd, H. Wang, E.M. Fuentes-**

Fernandez, S.J. Teat, F. Chen, G.S.

Hall, Y.J. Chabal, J. Li

739. Biomimetics of carbonic anhydrase via metal-organic frameworks. **Y. Chen, Z. Zhang**

740. Selective CO₂ adsorption on Cu-pyrazolato MOFs. **K. Shi, L. Mathivathanan, R.G. Raptis**

741. Fluorescent studies of metal-organic frameworks with highly conjugated linkers. **R. Ly, G.S. Pour, F.J. Uribe-Romo**

742. Titanium based metal-organic frameworks for visible light photocatalytic reduction of CO₂. **M.W. Logan, N.V. Aleger, S. Ayad, J.D. Adamson, K. Hanson, F.J. Uribe-Romo**

743. Fabricating turn on fluorescent sensors for cyanide in MOFs by sequential linker installation. **J. Li, S. Yuan, H. Zhou**

Section B

Ernest N. Morial Convention Center Hall D

Molecular Confinement Effects in Inorganic & Organic Containers

M. Fujita, B. C. Gibb, J. L. Sessler, *Organizers*

5:30 - 7:30

744. Getting specific about non-specific interactions: Functional group dependence for the inverse Hofmeister series. **J.H. Jordan, W. Yao, A. Wishard, B.C. Gibb**

745. Behavior of water under confinement in a metal-organic nanotube. **M. Payne, A.S. Jayasinghe, T. Forbes**

746. Anion specific effect on protein aggregation and precipitation. **W. Yao, B.C. Gibb**

747. Withdrawn

748. Supramolecular assemblies as a mechanistic probe: Formation and catalysis of a Si₄L₆ host. **M.**

Morimoto, C.M. Hong, E.A. Kapustin, K.N. Raymond, D. Toste, R.G. Bergman

749. Supramolecular confinement of anions, from small to large, with molecular pincers. **S. Pramanik, M. Reinmuth, H. Haque, S. Kaur, K. Motley, V. Day, K. Bowman-James**

750. Molecular face-rotating cube with emergent chiral and fluorescence properties. **H. Qu, Y. Wang, Z. Li, X. Wang, H. Fang, Z. Tian, X. Cao**

751. Larger assemblies and guest exchange in molecular containers. **A. Wishard, L. Avram, B.C. Gibb, A. Bar-Shir**

752. Does charge matter? Formation of highly reactive metal nanocluster crystal within coordination cage container. **Y. Fang, H. Zhou**

753. Designing functional supramolecules for biological applications. **I.A. Riddell**

754. Anion recognition using water-soluble hosts. **M.R. Sullivan, W. Yao, P. Sokkalingam, B.C. Gibb**

755. Electrochemical analysis of supramolecular cages as nanocapsules for catalysts. **A. Webb**, J. Bruna, S.C. Lutfallah, N. Elgrishi
756. Improving biocompatibility of nano-scale metal-organic supercontainers (MOSCs) for functional applications. **P. Jampani**, Z. Wang
757. Salt induced switching of capsular assemblies mirrors the Hofmeister effect. **M.B. Hillyer**, H. Gan, B.C. Gibb

Section C

Ernest N. Morial Convention Center Hall D

PCET PhotoCatalysis with Inorganic Molecules & Materials

Cosponsored by PHYS
J. L. Dempsey, C. Heyer, E. Leon, G. J. Meyer, *Organizers*

5:30 - 7:30

758. Homogenous hydrogen evolution system employing non-noble metal bipyridyldiamine co-catalysts. **T. Vagvala**, T. Ooyabe, V. Kalousek, K. Ikeue

759. Proton transfer and proton-coupled electron transfer reactions of heteroleptic ruthenium(II) complexes incorporating hydroxylated polypyridyl ligands. **K. Martinez**, M. Esposito, E. Milner, J.J. Paul, R.H. Schmehl

760. Use of 3D ordered macroporous cuprous oxide intercalated with MoS₂ for efficient hydrogen-evolving reaction. **D.T. Conroy**, R.A. Farrer

Section D

Ernest N. Morial Convention Center Hall D

Solid-State Inorganic Chemistry

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

5:30 - 7:30

761. Probing formation mechanisms of templated vanadium selenites using reaction informatics. **Y. Huang**, A.J. Norquist, J. Schrier

762. The role of organic structure on phase stability in templated vanadium tellurites. **X. Jia**, A.J. Norquist, J. Schrier

763. Superhard tungsten tetraboride (WB₄): Effects of variable boron concentration and the dodecaboride forming metals on its properties. **G. Akopov**, I. Roh, Z. Sobell, M.T. Yeung, L. Pangilinan, C.L. Turner, S.I. Khan, R.B. Kaner

764. Topochemical synthesis and characterization of transition metal-fluoride double-layered perovskites, (MF)LnNb₂O₇ (M = Mn, Fe, Cu; Ln = La, Pr). **P. Maji**, M. Granier, D. Montasserasadi, J.B. Wiley

765. Hydrothermal synthesis and characterization of manganese doped hematite hollow spheres. **S.A. Seraly**, A.M. Morey

766. Surface functionalization and thin film deposition of α -Fe₂O₃ hollow

spheres. **G.M. Harber**, J. Kittle, A.M. Morey

767. Synthesis of TMD's by chemical transformations of ultra-thin oxides: Effect of water (and chalcogen source) on morphology and the optical properties. **T. Kuykendall**, S. Aloni, A. Schwartzberg, C. Chen, C. Kastl

768. Promoted hydride/oxide exchange reaction in SrTiO₃ by introduction of anion vacancy. **F. Takeiri**, T. Yamamoto, Y. Kobayashi, H. Kageyama

769. Facile synthesis of metal sulfide based chevrel phases. **J. Ortiz Rodriguez**, J. Perryman, J.M. Velázquez

770. Synergy in properties and chemistry: Development of PbS QDs embedded in Pb-halide perovskite matrices. **E.A. Gauding**, J. Luther

771. New transparent conductors. **M.T. Yeung**, S.M. Flynn, A.E. Wustrow, J.C. Hancock, K.R. Poepelmeier

772. Understanding distortions in the cubic pyrochlore lattice towards the design of polar materials. **S. Husremovic**, G. Laurita-Plankis, J. Li, A. Sleight, R.T. Macaluso, M. Subramanian

773. Accelerating the discovery of inorganic phosphors with the assistance of machine learning. **Y. Zhuo**, J. Brgoch

774. Energy-efficient, microwave-assisted solid-state synthesis of phase-pure ternary Ti₂S₄ thiospinels with applications in heterogeneous catalysis. **J. Perryman**, J.M. Velázquez

775. Honeycomb network of Au-Au bonding in intermetallic, RE-Au-Sn (RE = La, Ce, Pr, Nd) ternary phase space. **S. Lotfi**, J. Brgoch, A. Oliynyk

776. (1,2,6-Trimethylpyridinium)₂Cu₂Br₆: The vicinal trimethylpyridinium cation pair as supramolecular dication. **M.R. Bond**

777. Solid state variable temperature and pressure ¹H NMR analysis of templated carbon with substitutional doping. **B. Nakamoto**, C.M. Jensen

778. Crystal packing of quasiracemic mixtures of oxidiazanones. **S. Huffman**, G. Ferrence

779. Borides and carbaborides based intercalation cathodes with redox active anions. **M.R. Shabetai**, J.Y. Do, V. Poltavets

780. Substitution effects of metal and metalloid elements at the silicon sites of TiMnSi₂ compounds. **D. Matetich**, J. Allred

781. Physical property measurements for single crystal V_{1-x}Mo_xO₂. **M.A. Davenport**, J. Jones, J. Allred

Section E

Ernest N. Morial Convention Center Hall D

Nanoscience

B. G. Trewyn, *Organizer*
5:30 - 7:30

782. Metal-enhanced fluorescence Hg²⁺ biosensor. N. Sui, L. Wang, **W. Yu**

783. Improved antimicrobial properties of copper and ascorbic acid based nanoparticle systems: Advanced drugs for a post-antibiotic era. **T.M. Dassanayake Mudiyansele**, V. Serapiglia, K.M. Greskovich, S. Huang

784. Effect of the aggregation events on the optical properties of molecular-like gold clusters. **M. Sugiuchi**, K. Konishi

785. Gram scale surface functionalization of nanodiamond. **M.E. Taylor**, J. Bandy, A. Mensch, R.J. Hamers

786. Synthesis and spectroscopic measurements of yttrium (III) oxide nanomaterials doped with europium (III) cations. W. Wang, **A. Rahman**, P. Zhu

787. Growth kinetics and cytotoxicity effects of surface modified zinc oxide quantum dots at room and cold temperatures using CsOH and NaOH. **D. Francis**, D.M. McCall-Butler, J.K. Davis-Gunn, A. Mena, B. Colon, P.P. Benz, A. Schrock, P. Cavnar, K.S. Molek

788. Probing the electronic structure of small metallic nanoparticles using conduction electron spin resonance. **S. Cruz**, A. Silakov, B.J. Lear

789. Polyarylboranates: Nanoscale materials with interesting photophysical properties. **T. Wang**, **M.W. Lee**

790. Effects of perchlorate anions on the fabrication of surface enhanced Raman spectroscopy (SERS) sensors. **W. Mihalyi-Koch**, F. Dawood

791. Ceria-Zirconia nanoparticles as an enhanced multi-antioxidant for sepsis treatment. **M. Soh**, T. Hyeon

792. Sweat-based glucose monitoring and feedback transdermal drug delivery for diabetes treatment. **C. Song**, T. Hyeon

793. Multifunctional nanoparticle as tissue adhesive for image-guided procedures. **K. Shin**, **G. Ko**, T. Hyeon

794. Nano-mechanical and physical investigations of novel oxide nanocomposites using atomic force microscopy. **T.T. Brown**, S. Akbarian-Tefaghi, A. Blanco, Z.L. Highland, N. Kuruppu Arachchige, A.M. Taylor, J.C. Garno, J.B. Wiley

795. Metal oxide support for control over electronic properties in catalytic noble metal particles. **J. Fagan**, B.J. Lear

796. Crystalline-to-amorphous phase transition of large area Mo₂O₂(μ -S)₂(Et₂dtc)₂ nanosheets. **M. Zhukovskiy**, M.K. Kuno

797. Microwave synthesis of nanocomposites via the capture of preformed nanoparticles within scrolled nanosheets. **A. Blanco**, T. Rostamzadeh, J.B. Wiley

798. Growth of gold and palladium nanoparticles inside and outside of halloysite nanotubes. **M. Islam Khan**, T. Rostamzadeh, J.B. Wiley

799. Synthesis and characterization of ZnO nanoparticles and their use as a photocatalyst. **J.D. Harris**, C.C. Pena, A.E. Harris, J. Cowan

800. Comparative toxicity of ZnO nanoparticles synthesized using different amines. **C.C. Pena**, K. Cornell, J. Cowan, J.D. Harris

801. Elucidating the mechanism of aluminum nanocrystal formation using EPR spectroscopy. **B.D. Clark**

802. Role of gold oxidation state in the synthesis of Au-CsPbX₃ heterostructured nanoparticles. **D. Dacres**, B. Roman, M.T. Sheldon

803. Nanostructured iron oxide electrodes for the water splitting reaction. **K. Koster**, L. Bradley, P. Kharel, F. Dawood

804. NiO nanoparticle synthesis, characterization, and toxicology. **P.T. Gwin**, C.C. Pena, K. Cornell, J. Cowan, J.D. Harris

805. Influence of particle size and stoichiometry on the magneto-electronic properties of La_{1-x}Sr_xCoO₃ nanoparticles. **H.A. De Santiago**, S. Mohan, M. Manno, E. McCalla, C. Leighton, Y. Mao

806. Polarization properties of semiconductor nanorods. **A. Francis**
807. Monitoring the growth of silver dendrites for large-area surface enhanced Raman spectroscopy (SERS) sensors. **A. Oh**, **N. DeBuono**, F. Dawood

808. High pressure exfoliation of layered materials. **W.H. Mak**, M.D. Kowal, E.P. Nguyen, R. Rizvi, R.B. Kaner

809. Multicolor emitting La₂Zr₂O₇ nanoparticles and its tunability on europium doping. **S. Gupta**, J. Zuniga, **Y. Mao**

810. Attachment of molecular catalysts to nanocrystal surfaces facilitated by anionic bridging ligands. **M.R. Buck**, **R.P. Murphy**

811. Development of a trimodal contrast agent for acoustic and magnetic particle imaging of stem cells. **J. Lemaster**, T. Kim, F. Chen, J.V. Jokerst

812. Characterization of electrical properties of GaAs nanowires and planar heterostructures by Kelvin probe force microscopy. **G. Matheson**, L. Geelhaar, M. Heilmann, J. Herranz

813. Translation of transition-metal based catalysis for selective sensing. **V. Schroeder**, T.M. Swager

814. Can nanotechnology help cell research for major diseases. **M. Breaux**

Section F

Ernest N. Morial Convention Center Hall D

Chemistry of Materials

C. G. Lugmair, *Organizer*
5:30 - 7:30

- 815.** Electrochemical etching of Ti_2CT_x MXene in dilute HCl solution. **W. Sun**, M.J. Green, M. Radovic
- 816.** Stabilizing CuPd nanoparticles via CuPd coupling to $WO_{2.72}$ nanorods in electrochemical oxidation of formic acid. **Z. Xi**, S. Sun
- 817.** Atomically Thin Pt Coated over Intermetallic FePt Nanoparticles for Efficient Oxygen Reduction Catalysis in Fuel Cells. **J. Li**, S. Sun
- 818.** Imaging boron nitride nanotubes (BNNTs) by single molecule fluorescence microscopy. **A. Smith**, Z. Tang, C. de los Reyes, D.M. Marincel, M. Pasquali, A.A. Martí
- 819.** In situ ligand stripping and etching of indium phosphide nanocrystals. **R. Siramdas**
- 820.** Room temperature, mild condition post-synthesis etching of InP nanocrystals. **M. Yazdanparast**, E. McLaurin
- 821.** Photophysical Studies of Isomeric *N*-Heterocyclic Carbene Ir(III) Complexes and Their Applications to Deep-Blue Phosphorescent Organic Light-Emitting Diodes (OLEDs). **B. Yun**, S. Kim, J. Kim, C. Kim, S. Kang, H. Son
- 822.** Detailed evaluation of nonradiative processes in heteroleptic cyclometalated iridium(III) complexes. **J. Kim**, S. Kim, Y. Cho, D. Cho, S. Kang, H. Son
- 823.** Optical properties of stellated metal nanocrystals grown from seeds with planar defects. **J.D. Smith**, K.M. Koczur, J.A. Burkhart, S.E. Skrabalak
- 824.** Chemical decoration of boron nitride nanotubes with aliphatic carbon chains. **C.A. de los Reyes**, K.L. Walz-Mitra, A. Smith, A. Loredó, F. Frankovsky, A.A. Martí
- 825.** Synthesis of colloidal ZnO nanoparticles and their assembly onto thin films. **R. Gaudet**, S. Ganguly
- 826.** Computational and experimental development of heterobimetallic single source precursors to Ge-Sn heterostructures. **H. Andaraarachchi**, M.A. White, J. Vela
- 827.** Preparation and characterization of a new organic-inorganic hybrid material with synergistically combined properties. **A.J. Rodriguez**, R.G. Raptis
- 828.** Studies of bulk ammonia borane – polyethylene oxide hydrogen storage materials. **K. Kharel**, R. Fu, O. Gunaydin-Sen
- 829.** New synthetic methods for generating carbon-based materials with well-controlled electronic properties: From superatomic solids to graphene nanoribbons. **I.M. Klein**, E. O'Brien, M. Paley, A. Crowther, X. Roy
- 830.** Divalent iron atom coordination in two-dimensional microporous graphitic carbon nitride. **Y. Oh**
- 831.** Large-scale synthesis of ultrathin lanthanide carbonate hydroxides nanowires for potential biomedical applications. **X. Zhang**, Y. Li, J. Ge, L. Qin, Y. Zheng, B. Lei, Y. Du, Z. Zheng
- 832.** Synthesis of magnetic $CuCr_2S_4$ chalcopinel nanoparticles using single-source precursors. **F. Akbari Afkhami**, A. Gupta
- 833.** Visible light sensitization of ferritin proteins by gold nanoparticles. **A. Bruefach**, E.B. Cerkez, K.G. Dutton, Y. Ghidry, M. Kukulka, A.M. Valentine, D.R. Strongin
- 834.** Self-assembly of PS-*b*-PEO films as a shadow mask for GaAs nanowire deposition. **L.R. Steiner**, S.C. Hall, A. Christy, J.D. Harris
- 835.** Synthesis of inorganic-organic perovskite hybrid materials via a microwave assisted method. **A. Poduval**, J.B. Wiley, S. Akbarian-Tefaghi
- 836.** Flux growth of binary and ternary metal boride single crystals as catalysts for the hydrogen evolution reaction. **L. Alameda**, R.E. Schaak
- 837.** Molten state synthesis of Pt^{3+} activated lanthanum hafnate nanoparticles as potential downconversion phosphor. **J. Zuniga**, S. Gupta, M. Pokhrel, Y. Mao
- 838.** Grafted covalent organic frameworks for fast ionic conductivity. **G. Pope**, D.A. Vazquez-Molina, A. Ezazi, F.J. Uribe-Romo
- 839.** Molecular additives for TiO_2 modification: A case study of dye-sensitized solar cells. **H. Cheema**
- 840.** Assessing effects of varying metal carboxylate coverages on lead sulfide nanocrystal properties. **I. Reza**, J.S. Owen
- 841.** Cation exchange as a synthetic entryway to complex nanomaterials. **B.C. Steimle**, J.L. Fenton, R.E. Schaak
- 842.** Ligand removal from indium phosphide nanocrystals. **S. Lee**, E.J. McLaurin
- 843.** In-situ synthesis of LaOF phases from LaF_3 and exploration for upconversion luminescence. Y. Mao, **A. Perez**, S. Gupta, M. Pokhrel
- 844.** Enhanced energy product of iron carbide nanorods induced by ruthenium. **B. Williams**, M. Tsui, E.E. Carpenter
- 845.** Rationally designed plasmonic nanostructures for biosensing. **W. Qian**, Q. Su
- 846.** Fabricating high-quality ultra-thin croconic acid film using electric field guidance. **R. Zhang**
- 847.** Surface properties of WO_3/ZnO catalysts and their catalytic performance in the direct carbonylation of glycerol with CO_2 to glycerol carbonate. **L. Jiaxiang**, D. He
- Section G
- Ernest N. Morial Convention Center Hall D
- Inorganic Chemistry of Lead Halide Perovskites: Insights from Fundamentals**
- R. L. Brutchey, B. C. Melot, J. Vela ,
Organizers
- 5:30 - 7:30**
- 848.** Persistent dopants and phase segregation in organolead mixed-halide perovskites. **B. Rosales**, L. Men, S. Cady, M.P. Hanrahan, A.J. Rossini, J. Vela
- 849.** Single crystal growth and characterization of R-M-X compounds ($R = CH_3NH_3$, $C_6H_5C_2H_4NH_3$, $C_6(CH_3)_5CH_2N(CH_3)_3$; $M = Zn, Cd, Hg$; $X = Cl, Br, I$). **R. Rocanova**, B. Saparov
- 850.** Inherent directional order of methylammonium cations in lead-iodide perovskite.. **M. Zdilla**, Y. Rao, B.B. Wayland, X. Li, A. Pender, S. Ding
- Section H
- Ernest N. Morial Convention Center Hall D
- Organometallic Chemistry: Applications to Materials & Polymer Science**
- N. S. Radu, *Organizer*
- 5:30 - 7:30**
- 851.** Methodologies of extending π -conjugation in ferrocene. **D. Daigle**, J. Bergeron, U. Pokharel
- 852.** Development of imino and amino pyridine iron(II) catalysts for atom transfer radical polymerization (ATRP). **V. Shastri**, L.M. Thierier, S.E. Jenny, M. Donley, L.M. Round, N.A. Piro, W.S. Kassel, C.L. Brown, T. Dudley, D.L. Zubris
- 853.** Design and synthesis of Ru precursors for photoassisted chemical vapor deposition. **O.M. Hawkins**, C.R. Brewer, B. Salazar, A.V. Walker, L. McElwee-White
- Section I
- Ernest N. Morial Convention Center Hall D
- Organometallic Chemistry: Applications to Organic Transformations**
- N. S. Radu, *Organizer*
- 5:30 - 7:30**
- 854.** Dearomatization and reactivity of benzene and electron-deficient arenes promoted by π -basic transition metal complexes. **J. Smith**, J.T. Myers, K. Wilson, W. Harman
- 855.** Multiple transition metal catalysts for mild hydrocarboxylation of alkenes with CO_2 . **J.A. Rogers**, B.V. Popp
- Section J
- Ernest N. Morial Convention Center Hall D
- Organometallic Chemistry: Catalysis**
- N. S. Radu, *Organizer*
- 5:30 - 7:30**
- 856.** C-H bond activation and silylation of pyridine with diruthenium complexes. **R.M. Chin**, N. Jovic, J. Prybil, N. McClendon
- 857.** *N*-Heterocyclic carbene titanium(IV) and zirconium(IV) catalysts for the copolymerization of Cyclohexene Oxide with CO_2 . **L. Ralte**, K. Törnroos, E. Le Roux
- 858.** Utilizing TiIII/IV redox catalysis for the synthesis of unsymmetrical carbodiimides. **A. Pancoast**, E. Beaumier, I. Tonks
- 859.** Influence of hydrogen bonding in photocatalytic systems. **P.L. Cheung**, C.P. Kubiak
- 860.** Withdrawn
- 861.** Nickel-mediated fluorocarbene metathesis. **J. Guan**, M.B. Hall
- 862.** Enantioenrichment of a molybdenum dearomatization agent by redox catalysis. **S. Dakermanji**, K. Welch, W. Harman
- 863.** Hydrogenation of CO_2 : A rational approach to catalyst design. **K. Grubel**, A.M. Appel, J.C. Linehan
- 864.** Ester hydrogenation catalyzed by CNN-pincer and CC-bidentate complexes of ruthenium. **L.N. Le**, J. Liu, T. He, A.R. Chianese
- 865.** A mechanistic DFT study of selective aldehyde hydrogenation by an octahedral PONOP iron catalyst. **B.S. Omar**, F. Hasanayn
- 866.** Incorporation of NADH-like hydride relays into metal-phosphine catalysts for CO_2 hydrogenation. **C. Zall**
- 867.** Base-free transfer hydrogenation of alkenones with organometallic complexes bearing a triazenide ligand functionalized with pyrazole. **L. Medrano Castillo**, M. Parra-Hake, V. Miranda-Soto, M. Collazo-Flores, D.B. Grotjahn, D. Chávez, A.L. Rheingold
- 868.** Operando infrared spectroscopic studies of iron-catalyzed hydromagnesiation of vinyl arenes. **J.A. Rogers**, B.V. Popp
- Section K
- Ernest N. Morial Convention Center Hall D
- Organometallic Chemistry: New Ligand Platforms**
- N. S. Radu, *Organizer*
- 5:30 - 7:30**
- 869.** Investigations into small molecule activation with a severely sterically crowded trigonal bipyramidal metal complex featuring a multidentate tris(phosphaalkene)phosphine ligand. **P. Miura-Akagi**, M.L. Nakashige, M. Cain, A.L. Rheingold
- 870.** Derivatized mixed-ring heterocyclic and antenna carotene ligands. **V. KomReddy**, **D. Rillema**, H. Nguyen, A.J. Cruz, C. Moore, N.K. Senaratne, L. Kadel, D.M. Eichhorn
- 871.** Acid-modulation of scorpionate ligands for modern organometallic chemistry. **P. Shivokevich**, A. Heyer, W. Harman
- 872.** Synthesis and coordination chemistry of a new PNP pincer featuring phosphaalkene and pyrrolide type-donors. **M.M. Riek**, M. Cain, A.L. Rheingold

- 873.** Efficient synthesis of imidoylamidines. **C.R. Guifarro**, E.V. Rybak-Akimova
- 874.** Synthesis and coordination of a new tris N-heterocyclic carbene. **M. Montgomery**, **S. Allison**, **A. Duenas**, **N. Harris**, **D. Tapu**
- 875.** Development of new bis N-heterocyclic carbene: Synthesis and coordination chemistry. **A. Mason**, **M.A. Baker**, **A. Carter**, **D. Tapu**
- 876.** New cerberus-type N-heterocyclic carbene: Synthesis and coordination. **R. Hooper**, **J. Malone**, **D. Tapu**
- 877.** Toward the synthesis and characterization of a new NHC-palladium complex. **N. Harris**, **G. Crimmins**, **G. Bettler**, **A. Changas**, **D. Tapu**
- 878.** Synthesis and reactivity of pincer ligands containing mixed phosphine/stibine donors. **A.J. Kosanovich**, **A.M. Jordan**, **O. Ozerov**
- 879.** Synthesis and reactivity of polydentate 1,3,5-triazine based ligands. **S. Gunther**, **O. Ozerov**

Section L

Ernest N. Morial Convention Center
Hall D

Organometallic Chemistry: Synthesis & Characterization-Early Transition Metals

N. S. Radu, *Organizer*
5:30 - 7:30

- 880.** Synthesis of Ti imidos with varying covalent donor ligands and their application in Ti redox catalysis. **T.A. Wheeler**, **I. Tonks**
- 881.** Reduction of titanium imidazolin-2-iminato complexes for the activation and cleavage of N₂. **M.A. Baeza**, **R. Aguilar**, **A. Metta-Magana**, **S. Fortier**
- 882.** Low-valent early transition metal CCC-NHC pincer complexes. **V. Adiraju**, **C.E. Webster**, **T.K. Hollis**
- 883.** Reactivity study of a masked "Ti(II)" complex. **A. Jordan**, **R. Aguilar**, **S. Fortier**
- 884.** Withdrawn

Section M

Ernest N. Morial Convention Center
Hall D

Organometallic Chemistry: Synthesis & Characterization-Late Transition Metals

N. S. Radu, *Organizer*
5:30 - 7:30

- 885.** Synthetic methodologies for organometallic polyacenes. **J.T. Bergeron**, **D. Daigle**, **U. Pokharel**
- 886.** Formic acid dehydrogenation: Ruthenium does it better. **N. Anderson**, **A.M. Tondreau**, **J.M. Boncella**
- 887.** Structure determination of PBP silver complexes. **Y. Cao**, **W. Shih**, **N. Bhuvanesh**, **O. Ozerov**
- 888.** Cyclopentadienyl pyridazines and oxazines and their applications in energy and advanced electronics. **N.C.**

- Tice**, **S. Wild**, **E. Collins**, **C. Snyder**, **D.L. Smith**
- 889.** Chameleonic nature of platinum(II) imidazopyridine complexes. **P. Pinter**, **R. Pittkowsky**, **J. Soellner**, **T. Strassner**
- 890.** Synthesis & reactivity of novel silyl/silylene pincer cobalt complexes. **J. Zhang**, **B.J. Foley**, **N. Bhuvanesh**, **M.T. Whited**, **O.V. Ozerov**
- 891.** Synthesis, characterization and reactivity of pincer-type bis(phosphine)silylene [P₂Si]Ru complexes. **S. Ma**, **J. Zhang**, **M.T. Whited**, **D.E. Janzen**
- 892.** Evidence for reversible cyclometalation in alkane dehydrogenation and C-O bond cleavage at iridium bis(phosphine) complexes. **S.M. Chapp**, **N.D. Schley**
- 893.** Reactive intermediates in silver-catalyzed nitrene transfer. **C. Mak**, **M.G. Campbell**
- 894.** Solution and solid state structures of zerovalent palladium and platinum phosphinoferrrocene complexes. **E.A. Kober**, **S.H. Schreiner**

Section N

Ernest N. Morial Convention Center
Hall D

Bioinorganic Chemistry: DNA, RNA & Inorganic Drugs

S. A. Koch, *Organizer*
5:30 - 7:30

- 895.** Mechanistic study of the reaction between KP1019 and serotonin. **L.K. Stultz**, **M. Dunbar**, **V. Krishnan**, **P. Hanson**
- 896.** Development of novel rhodium-based liver X receptor agonists. **H. Nguyen**, **M. Umetani**, **L. Do**
- 897.** Cytotoxic aldehyde detoxification by organoiridium complexes in cells and zebrafish. **A.H. Ngo**
- 898.** Design and synthesis of a carboxylate-containing ligand that increases the T1-weighted relaxivity response of a manganese complex to hydrogen peroxide. **T. Hutchinson**, **C. Goldsmith**
- 899.** Determining the mechanism by which chromium and bitter melon activates insulin signaling. **P. White**, **E. Krol**, **L.C. Scott**, **C. Nichols**, **Z. Krejpcio**, **J.B. Vincent**
- 900.** Interactions between chromium(III) and DNA. **S. Brown**, **J.B. Vincent**
- 901.** Mechanistic insights into intracellular transfer hydrogenation by unprotected organoiridium catalysts. **S. Bose**, **L. Do**
- 902.** Synthesis and evaluation of ruthenium complexes with cytotoxicity against cancer cells. **A. Shrestha**, **J. Gray**, **F. Qu**, **J. Park**, **Y. Kim**, **E.T. Papish**
- 903.** Synthesis and cytotoxic properties of organorhenium indomethacinato complexes. **T.V. Hinton**, **Y. Zhang**, **S. Pramanik**, **S. Mandal**

- 904.** Synthesis, characterization and in vitro antitumor activity of nickel (II) and platinum (II) complexes with some thiophene thiosemicarbazones.. **M.A. Al-Yafeai**, **H. Nimir**
- 905.** Synthesis, characterization & in vitro biological activity of Pt(II) and Pd(II) thiosemicarbazone. **Y. Eltayeb**
- 906.** Effects of small molecule modulators binding to Cu and remodeling the pathway of Cu-catalyzed oxidative stress and aggregation in amyloid β (1-42). **S. Mitra**, **S. Chakraborty**
- 907.** Development of iron binding assays to explore structure activity relationships of 3-AP analogs. **S. Plamthottam**, **J. Valenzuela**, **D. Sun**, **J. Van Valkenburgh**, **D. Steele**, **S. Poddar**, **C.G. Radu**, **J.I. Zink**
- 908.** NORM's and effects of exogenous agents: Copper promoted NO release from sugar appended thiol DNIC's. **C. Pectol**, **C. DeLaney**, **R.B. Chupik**, **M.Y. Darenbourg**
- 909.** Organorhenium ibuprofenato, picolinato and nicotinato complexes as anticancer agents. **S. Parnell**, **M. Stevenson**, **Y. Zhang**, **S. Pramanik**, **S. Mandal**
- 910.** Photocytotoxicity assessment of a ruthenium(II) polypyridyl complex bearing 2,9-diphenyl-1,10-phenanthroline ligand. **N. Mansour**, **S. Mehanna**, **M. El Sibai**, **R.S. Khnayzer**, **C. Daher**

Section O

Ernest N. Morial Convention Center
Hall D

Bioinorganic Chemistry: Proteins & Enzymes & Model Systems

S. A. Koch, *Organizer*
5:30 - 7:30

- 911.** Characterization of electron transfer pathways and domain binding pockets in 3-ketosteroid-9 α -hydroxylase. **S.R. Soltau**, **A. Luiz**, **P. Patel**
- 912.** Artificial bio-mineralization targeting lanthanide elements. **T. Hatanaka**, **A. Matsugami**, **F. Hayashi**, **N. Ishida**
- 913.** Formation of myoglobin-nitroso adducts from amine- and nitro-containing drugs. **S. Powell**, **B. Wang**, **X. Yang**, **V. Herrera**, **G.B. Richter-Addo**
- 914.** Studies to understand Ti(IV) speciation and transport in the human body.. **J.A. Benjamin-Rivera**, **A.D. Tinoco**, **Y. Delgado**, **M. Pandrala**, **A. Vazquez**, **A. Vazquez**
- 915.** Rate of dissociation of chromium(III) from transferrin under endosomal conditions monitored by EPR. **K.C. Edwards**, **M. Lockart**, **H.H. Kim**, **M.K. Bowman**, **J.B. Vincent**
- 916.** Mechanism of oxygen reduction in copper amine oxidases. **S.A. Mills**, **K.E. Gazica**, **M.M. Saugstad**
- 917.** Towards new titanium and vanadium enzymes. **O. Peduzzi**, **A.**

- Paredes**, **J. Pellegrino**, **A.J. Reig**, **K.M. Buettner**
- 918.** Electronic effects of a bridging Fe^I-Cyanide on {Fe(NO)₂}^{9/10} scaffolds for possible linkage isomerization. **M. Quiroz**, **P. Ghosh**, **M.Y. Darenbourg**
- 919.** Synthesis, structure and reactivity of thiolate-bridged {Fe(NO)₂}⁹ dimers with a pendant thiol. **D. Sil**, **A. Baxter**, **M.Y. Darenbourg**
- 920.** Better resolution of Co hyperfine at low frequency: CoEDTA, a model for obtaining Co hyperfine in high spin complexes of biological interest like the transmembrane metal binding site for CzcP. **W.E. Antholine**, **M. Ross**, **B.M. Hoffman**, **A.C. Rosenzweig**
- 921.** Modeling *P. aerophilium*'s nitrate reductase tungsten analogue: Understanding the connection between nitrate turnover and the proton motive force. **M.A. Cranswick**, **T. Marshall**, **B.J. Trujillo**
- 922.** Switchable stereoselectivity in monooxygenation of non-native substrates by P450BM3 using decoy molecules. **K. Suzuki**, **O. Shoji**, **J.K. Stanfield**, **H. Sugimoto**, **Y. Shiro**, **Y. Watanabe**
- 923.** Reconstitution of self-sufficient cytochrome P450 with artificial metal complexes. **K. Omura**, **Y. Aiba**, **S. Ariyasu**, **O. Shoji**, **H. Sugimoto**, **Y. Shiro**, **Y. Watanabe**
- 924.** Simple Zn-scorpionate complex to test the binding of antimicrobial drugs to Zn containing enzymes. **J. Dewar**, **A. Thakur**, **L. Peterson**, **W. Eckenhoff**
- 925.** Exploring structural and redox properties of biomimetic models of metal- β binding site in Alzheimer's disease using DFT. **S. Niu**, **S.D. Zaric**, **E.N. Brothers**, **M.B. Hall**
- 926.** "Beeting" Alzheimer's: Inhibition of Cu²⁺- β -amyloid mediated oxidation and peroxidation by betanin from sugar beets. **D.C. Cerrato**, **L. Ming**
- 927.** Assembling oxygen-evolving complex (OEC) of photosystem II: Design and synthesis of ligands. **J. Prakash**
- 928.** Synthesis of functional catalysts for CO conversion based on Mo-containing CO dehydrogenase. **M. Foster**, **E. Gladhill**, **L. Nyarko**, **D. Rokhsana**
- 929.** Models of the molybdenum cofactor: Synthesis and reactivity. **H.H. Varnum**, **V.R. Berke**, **D.R. Gisewhite**, **S.J. Nieter Burgmayer**
- 930.** Short Metallo-peptides and peptoids: A look into the oxidative reactivity. **S. Islam**, **C. Tang**, **D.C. Cerrato**, **J. Cai**, **L. Ming**
- 931.** Withdrawn
- 932.** Structural and reactivity investigation of oxomanganese(IV) and bis(μ -oxo)dimanganese(III,IV) complexes. **Y. Lee**, **A.A. Massie**, **T.A. Jackson**
- 933.** Designed metalloproteins for efficient CO₂ reduction via low valent

Fe (I/0) state in aqueous medium. **D. Selvan**, S. Chakraborty
934. Synthesis and reactivity studies of ene-dithiolate modeling molybdenum cofactor. **N. Nguyen**, D. Gisewhite, S.J. Nieter Burgmayer
935. Developing TALE proteins as a sensor for detecting pathogens. **K. Gaiko**, M. Kim

Section P

Ernest N. Morial Convention Center Hall D

Coordination Chemistry: Characterization & Applications

A. Larsen, *Organizer*

5:30 - 7:30

936. Fluorometric and colorimetric sensing of citrate with a macrocyclic-based dinuclear foldamer in water. **M. Rhaman**, M.H. Hasan, R. Tandon, **A. Hossain**
937. Discovery of the novel colorimetric chemosensor for multiple target metal ions Fe²⁺, Co²⁺, and Cu²⁺ in a near-perfect aqueous solution: experimental and theoretical studies. **H. Cho**, **M. Yang**, S. Hwang, S. Kim, C. Kim
938. Development of highly selective turn-on chemosensor for Zn²⁺ in aqueous media and living cells. **D. Yun**, **J. Chae**, J. Jung, J. Kang, C. Rha, C. Kim
939. Electrochemical investigation of [Ru(saloph)(NO)(Cl)]-type complexes (saloph = N,N'-bis-(salicylidene)-o-phenyldiamine, and derivatives). **A. Ramuglia**, A. Fadamin, M.J. Shaw
940. Ni complexes with redox-active tetradentate ligands: Structures, electrochemistry, and reactivity studies with CO₂. **K.D. Spielvogel**, **J.A. Luna**, **A. Benson**, S.K. Shaw, S.R. Daly
941. Investigated and calculated solvatochromic characteristics of MoCl₄(dimine) anions. **A. Chang**, W.T. Eckenhoff
942. Metallothiolate ligands for reversing metal ion induced aggregation of beta amyloid. **E.K. Adams**, M.R. Mackiewicz
943. Probing valence tautomerism in a cobalt verdazyl coordination compound. **C. Kung**, S. Fu, D. Chung, **D.J. Brook**
944. Novel porphyrins bearing phenothiazine pincers to encapsulate fullerenes: Synthesis and complexation study. **K. Jain**, N. Duvva, T. Roy, L. Giribabu, R. Chitta

Section Q

Ernest N. Morial Convention Center Hall D

Coordination Chemistry: Synthesis & Characterization

A. Larsen, *Organizer*

5:30 - 7:30

945. Synthesis of N-heterocyclic chalcogenone silver complexes. **F. Voges-Haupt**, A. Allen, D. Rabinovich

946. Synthesis and characterization of model copper(I) and gold(I) thiolate nanoparticle precursor complexes. **C. Tran**, R.J. Papoular, L.E. Marbella, J. Millstone, M. Gembicky, B. Chen, A.T. Royappa
947. Nitrile reactions of 1,1-bis(diphenylphosphino)ethene dirhenium compounds. **G. Crispin**, **D.J. Esjornson**
948. Coordination chemistry of *N,N'* azodioxides. **L. Balaraman**
949. A C₃ symmetric sulfate complex with an *m*-nitrophenyl-functionalized hexaurea receptor. **B. Portis**, M. Emami Khansari, C. Johnson, D.R. Powell, **A. Hossain**
950. Exploring new synthetic strategies by using novel manganese carboxylate complexes along with a well-explored ligand, 2-(Hydroxymethyl)-pyridine in the area of polynuclear coordination chemistry. **M.A. Reagan**, A. Saha
951. Extraordinarily large ferromagnetic coupling ($J \geq 150 \text{ cm}^{-1}$) via electron delocalization in a heterometallic Mo-Mo-Ni chain complex. **J.A. Chipman**, J.F. Berry
952. Multicomponent supramolecules in coordination-driven self-assembly: Preparation and photophysical studies. **H. Sepehrpour**, P.J. Stang
953. Structural and electronic properties of 1,3,6-trisubstituted fulvene chromium complexes. **A. Peloquin**, M. Smith, B. O'Connell, S.K. Adas, G.J. Balaich, S.T. Iacono
954. Novel colorimetric ligand for the detection of silver (I). **L. Patton**, E. Bosch
955. Spectroscopic and electronic properties of dissymmetric *trans* Co^{III}-cyclam acetylides and their precursors. **S.D. Banziger**, T. Ren
956. Synthesis of heteroleptic transition-metal complexes containing azodioxide ligands. **K.A. Emhoff**
957. Synthesis and coordination chemistry of new Schiff base ligands with hydrogen-bonding groups. **A. Penn**, C. Hamaker
958. Synthesis and characterization of vanadium(IV), vanadium(V) and iron(III) complexes of perfluoropinacolate ligands. **S.L. Carter**, J.K. Elinburg, J. Nelson, L.H. Doerrer
959. Structural characterization of a heterobimetallic Zn/La Schiff base complex. **J. Farnsworth**, M. Zeller, E.R. Trivedi
960. Variation of water cluster motifs in structurally similar Ni(II) complexes: Synthesis, characterization, and thermal analyses. **N. Saraci**, C.S. Mullins, M. Mashuta, R. Buchanan, C. Grapperhaus
961. Synthesis and characterization of a series of vanadium(IV) complexes with the Kläui ligand. **X. Wu**, C.C. McLauchlan
962. Molecular characterization of cationic lanthanide complexes containing phosphine oxide. **P.K.**

Yuen, C.D. Lau, E.M. Yen, A.K. Yuen, W. Chan, H. Chan
963. Multidentate aminophenols prepared from Mannich condensations. **J.R. Farrell**, M. Bender, J. Kirpas, J. Niconchuk, N. Maniatis, M. Wallace, C.J. Ziegler
964. Thiol and phenol pendant-arms for cross-bridged tetraazamacrocyclic complexes. **P.T. Nguyen**, **D. Jones**, C.C. Jacobsen, T.J. Hubin
965. Heteroatom-containing bridged azamacrocycles and C-linked bis-azamacrocycles and their coordination complexes. **D. Tresp**, T.K. Ellis, T.J. Hubin
966. 1,4,7,10,13-pentaazacyclopentadane: Streamlined synthesis and novel transition metal complexes. **F.A. Okorochoa**, **A. Shrestha**, A.G. Oliver, J.A. Krause, T.J. Hubin
967. Ethylene cross-bridged pentaazamacrocycles and their transition metal complexes. **E. Allbritton**, T.L. Fletcher, J.A. Krause, A.G. Oliver, T.J. Hubin
968. Bis-cyclometalated iridium complexes with chelating dicarbene ancillary ligands. **H. Na**, A. Maity, T.S. Teets
969. Theoretical investigations on radical bridged supramolecular metallocycles toward exploring single molecular magnets. **V. Kuduva Radhakrishnan**, D.I. Alexandropoulos, B.S. Dolinar, K.R. Dunbar
970. Halogentated formamidinate bridged dirhodium (II,II) complexes as photodynamic therapy based anti-cancer agents. **E. Song**, K.R. Dunbar
971. Synthesis, spectroscopic characterization and crystal structures of three new zinc(II) complexes of *cis*-1,2-diaminocyclohexane. **M. Monim-Ul-Mehboob**
972. Highly efficient yellow and red bis-cyclometalated iridium phosphors via ancillary ligand modification. **P. Lai**, T.S. Teets
973. New bis(amidine) ligands and digold bis(amidine) metalloligands for highly luminescent Group 11 cluster complexes. **O. Ugarte Trejo**, A. Calderón Díaz, N. Siwabut, N. Maya, N. Bhuvanesh, **M. Stollenz**
974. Role of green chemistry in the synthesis and characterization of several new copper-phenanthroline complexes. **M. Wilk**, R. Johnson, S. Scott, D. Vargas Trujillo, V. Nesterov, M. Omary
975. Reaction dynamics of the TeMo₆O₂₄⁶⁻ ion in water. **G.M. Kuhl**, E.M. Villa
976. Light assisted-oxygen atom transfer from group VI transition metals complexes. **S. Fosshat**, M.B. Chambers
977. Late transition metal complexes of selenomaltol. **M. Spiegel**, A. Hoogerbrugge, S. Truksa, A. Smith, K.L. Shuford, K. Klausmeyer, P.J. Farmer

978. Facile metal exchange reactions of ammonium and potassium magnesium dodecaborates. **D.M. Schubert**, M.B. Jacobs
979. Mononuclear and binuclear Ni complexes with pyridyltriazole ligands. **S. Gao**, T.M. Wheat, J. Theriot, F.R. Fronczek, A.W. Maverick
980. Investigating multi-electron structure and reactivity with trinuclear μ₃-nitride complexes. **A. Su**, J. Teesdale, T. Betley
981. Novel polymetallonucleosides. **C.M. Mikulski**
982. Synthesis and characterization of new copper-quinoxaline complexes via solventless and solvent synthetic routes. **K.A. Reyes**, G. Martinez, Y. Faheem, A. Henderson, V. Nesterov, M. Omary
983. Synthesis and structural characterization of mercury(II) coordination polymers based on 1,2,4,5-tetra(isopropylthio)benzene ligand. **T. Selby-Karney**, S. Kakumanu, J.T. Mague, P. Chandrasekaran
984. Synthesis, photophysical properties, and DFT studies of Cu(I,7-phen)(PPH₃)₂PF₆: An unusual three-coordinate Cu(I) compound and the concept of "inhibited" ligands. **A. Miller**, D.J. Casadonte, A.F. Cozzolino
985. Metal cluster structure types and electron counts: A survey of the Cambridge Structural Database. **D.H. Johnson**
986. Comparative studies of Co/Rh/Ni dibenzotetramethylaza[14]annulene (TMTAA) complexes with porphyrin analogs. **S. Dey**, B.B. Wayland, M. Zdzilla
987. Novel aqua and chloro Ru(II) complexes with the tripodal NNN-ligand dipyrido(2,3-a:3',2'-j)phenazine (dpop') and bidentate NN ligands 2,3-di(2-pyridyl)pyrazine(dpp) and 3,6-di(2-pyridyl)tetrazine(dpt) were prepared and characterized.. **R.R. Ruminski**, K. Engstrom, S. Hoover, M. Roe
988. Molybdenum (VI) amidate complexes: Synthesis and reactivity. **J.M. Smith**, R.K. Thomson
989. Effects of metal identity on coordination environments and electronic properties in a series of homo- and heterobimetallic complexes of iron and cobalt. **K.M. Gramigna**, R. Mathialagan, S. Kuppaswamy, C.M. Thomas
990. Designing multicobalt clusters in pursuit of dinitrogen reduction. **M. Eaton**, B.J. Knight, L.J. Murray
991. Synthesis of chiral amines via early transition metal mediated asymmetric reductive hydrogenation of prochiral imines. **B. Zhang**, R. Josef, J. Bukacek Frazier, L. Kugelmass, A. Atsango, Y. Kim, **J. Tanski**
992. Metal-Metal bonded complexes supported by artificial sweeteners: Synthesis and characterization of tetra saccharinate and acesulfamate

complexes of dirhodium(II,II). **S.C. Haefner**

993. Synthesis and characterization of novel dinitrosyl iron complexes with chelating ligands. **J.M. Grant, M.W. Jones**

994. Microwave assisted synthesis and characterization of Cr(III) pyrazolate-formate mixed ligand complexes. **J.M. Lopez, R.G. Raptis**

995. Synthesis and characterization of a novel non-innocent NNP-type pincer ligand and its first-row transition metal complexes. **K. Talukdar, A. Issa, J.W. Jurss**

996. Computation investigation of carbonyl and ammine gases for the production of solid urea *Via* 5d metal complex. **A. Taylor, B. Prince**

997. The use of bovine milk for the generation of LacDiNac (LDN) bearing N-glycans for the chemenzymatic synthesis of Schistosoma-type antigenic N-glycans. **K.K. Robinson**

Section R

Ernest N. Morial Convention Center Hall D

Lanthanide & Actinide Chemistry

A. De Bettencourt Dias, *Organizer*
5:30 - 7:30

998. EPR of lanthanide complexes: exploring the consequences of ligand induced anisotropy. **K. Fisher, G. Moise, A. Bowen, C. Timmel, S. Faulkner, A. Kenwright**

999. New family of *d/f*-heterobimetallic cationic materials with anion exchange capabilities. **T. Poe, M. Polinski**

1000. Variable coordination motifs of (silyl)anilide ligands on uranium. **A.M. Tondreau, J.M. Boncella**

1001. Separation of americium from europium using soft donor ligands in ionic liquids. **J. Dehaut, N.J. Williams, H. Luo, S. Dai**

1002. Anionic lanthanide complexes containing tetradentate halogen-substituted Schiff base ligands. **P.K. Yuen, C.D. Lau, E.M. Yen, A.K. Yuen, W. Chan, H. Chan**

1003. X-ray diffraction of 1D polymeric lanthanide-transition metal compounds. **P.K. Yuen, C.D. Lau, E.M. Yen, A.K. Yuen, W. Chan, H. Chan**

1004. Novel ionic f-f bimetallic complexes containing salen. **P.K. Yuen, C.D. Lau, E.M. Yen, A.K. Yuen, W. Chan, H. Chan**

1005. Recent advances in lanthanide chemistry. **R. Beattie, J.K. Pagano, K. Erickson, S.K. Cope, B. Scott, D.E. Morris, J.L. Kiplinger**

1006. Synthesis, characterization, and photophysical properties of two new organic ligands for the sensitization of lanthanide ions. **D. Tapia, J.H. Monteiro, A. De Bettencourt Dias**

1007. Development of Gd(III)-based magnetic resonance agents for molecular imaging of hydrogen peroxide and hypoxic tumor conditions.

C. Lynch, J.O. Massing, E.A. Bajema, K. MacRenaris, T.J. Meade

1008. Syntheses and crystal structures of lanthanide dithiooxamide complexes. **B.M. Amanda, E.M. Villa**

1009. Syntheses and crystal structures of lanthanide periodate compounds. **R.N. Colin, E.M. Villa**

1010. Homoleptic uranium and lanthanide phosphinodiboranate complexes. **T.V. Fetrow, A.V. Blake, Z. Theiler, S.R. Daly**

1011. CMPO groups and their derivatives to separate rare earth elements. **H.A. Pearson, B.G. Wackerle, M.L. Hudson, S.M. Biros**

1012. Solution and solid state structural chemistry of Th(IV) and U(IV)-monocarbonylates. **N.A. Vanagas, K.E. Knope**

1013. Identifying actinyl intermolecular interactions of the U(VI)O₂²⁺ cation in coordination compounds. **M. Pynch, T. Forbes**

1014. Coordination chemistry and redox-activity of uranium complexes of tetradentate BIAN-type ligands. **J. Niklas, B.H. Farnum, J.D. Gorden, A.E. Gorden**

1015. Synthesis, structural characterization, and magnetic properties of hexanuclear lanthanide(III) complexes of an extended tritopic picolinic dihydrazide ligand with terminal oxime groups. **S.S. Tandon, S.D. Bunge, V. Hogan, M. Murugesu**

Radiopharmaceutical Chemistry

Sponsored by FLUO, Cosponsored by INOR[‡], MED[‡] and NUCL[‡]

WEDNESDAY MORNING

Section A

Ernest N. Morial Convention Center Room 345

Bioinorganic Chemistry: Proteins & Enzymes & Model Systems

S. A. Koch, *Organizer*

S. A. Toledo, *Presiding*

8:30 1016. Selective light-driven chemoenzymatic oxytrifluoromethylation. **L.E. Cheruzel**

8:50 1017. Incorporation of phosphoryl amide moieties to support high valent metal oxido/hydroxido complexes. **V. Oswald, A. Weitz, E. Hill, N. Sickerman, M.P. Hendrich, A. Borovik**

9:10 1018. Biomimetic reactivity of a family of structural analogues of the resting state of the enzyme nickel-acireductone dioxygenase (Ni-ARD). **S.A. Toledo, A. Gremillion, J. Jaimes, A.D. Ivan, D. Saldana, A. Sanchez, V. Lynch**

9:30 1019. Design of artificial metalloproteins using Biotin-Streptavidin Technology. **K.R. Miller, A. Borovik**

9:50 1020. Immobilization of synthetic Cu complexes within a protein host. **D. Brazzolotto, A. Borovik**

10:10 Intermission.

10:20 1021. Hydroxylation of gaseous alkanes and benzene catalyzed by cytochrome P450BM3 using decoy molecules as a substrate analogue. **O. Shoji, Y. Watanabe**

10:40 1022. Cellular mapping of carbonic anhydrase and zinc: Towards understanding the bound and labile zinc pool. **R. Mehta, E.L. Que**

11:00 1023. Modulating intramolecular hydrogen bonding networks in metal complexes to mimic enzyme active sites. **J. Lee, A. Borovik**

11:20 1024. Three-coordinate iron in an unusual planar iron-sulfur cluster. **D.E. DeRoshia, E. Bill, S. DeBeer, P.L. Holland**

11:40 1025. Insights into the design of synthetic analogues of metalloenzymes. **T.J. Paul, G. Sharma, J. Mahesha, Q. Hu, R. Prabhakar**

12:00 1026. Advances in modeling the photosynthetic oxygen evolving complex with geometrically flexible manganese clusters. **M. Zdilla, S. Vaddypally, S.K. Kondaveeti, I.G. McKendry, D.J. Jovinelli, M.R. Gau, A. Polyak, C. Koellner**

Section B

Ernest N. Morial Convention Center Room 344

Metal-Organic Frameworks: What Are Next?

W. Lin, H. Zhou, *Organizers*

S. Ma, *Organizer, Presiding*

P. McGrier, *Presiding*

8:30 1027. Porous materials from new framework-forming chemistries. **M.J. Rosseinsky**

9:15 1028. Expanding the MOF toolkit: Phosphines, arsines and chalcogenides. **S.M. Humphrey, S. Dunning, R.E. Sikma, R. Riparetti, J. Reynolds, I. Malaestean, J. He**

9:45 1029. Extraction of rare earth elements from geothermal brine solution using magnetic core shell nanoparticles. **P.K. Thallapally, P. McGrail, J. Liu**

10:15 1030. General and direct method for preparing oligonucleotide-functionalized metal-organic framework nanoparticles. **S. Wang, C.A. Mirkin**

10:35 Intermission.

10:50 1031. Design and functions of sp² carbon covalent organic frameworks. **D. Jiang**

11:20 1032. Benzobisoxazole-linked covalent organic frameworks. **P. McGrier**

11:50 1033. Homochiral porous framework as a platform for durability enhancement of molecular catalysts. **F. Xiao, Q. Sun**

12:10 Concluding Remarks.

Section C

Ernest N. Morial Convention Center Room 343

F. Albert Cotton Award in Synthetic Inorganic Chemistry: Symposium in honor of Andrew S. Borovik

D. C. Lacy, C. G. Riordan, J. Y. Yang, *Organizers*

A. Borovik, *Presiding*

8:30 1034. Chiral recognition of amino alcohols using binuclear Ni(II) complex anion as host. **M. Ray**

8:55 1035. Cobalt-mediated reactions for sustainable C-H activation processes. **C.E. MacBeth**

9:20 1036. Coordination polymers and molecular assemblies decorated with hydrogen bonds. **R. Gupta**

9:45 1037. Developing Single-site organometallic complexes for photochemical water splitting. **D.C. Lacy**

10:10 Intermission.

10:25 1038. Materials for display applications. **N.S. Radu, G. Rossi, C.K. Ngai, A. Fennimore**

10:50 1039. Experiments in support of safeguards for aqueous spent nuclear fuel reprocessing. **J.F. Krebs, C. Pereira**

11:15 1040. Mechanistically driven catalyst design for oxidative coupling reactions. **D. Pappo**

11:40 1041. Shuttling protons and electrons via the secondary coordination sphere for anion reduction. **J.D. Gilbertson**

Section D

Ernest N. Morial Convention Center Room 352

Molecular Confinement Effects in Inorganic & Organic Containers

M. Fujita, B. C. Gibb, J. L. Sessler, *Organizers*

M. Hardie, W. Jiang, *Presiding*

8:00 1042. The inner space environment in coordination chemistry supramolecular clusters. **K.N. Raymond, C.M. Hong, M. Morimoto**

8:30 1043. Reversible photoswitching in the confinement of coordination cages. **R. Klajn, D. Samanta**

9:00 1044. Metallo-cages from cyclotrimeratylene-type ligands – chiral self-sorting and speciation control, luminescence and photoswitching behavior. **M. Hardie, J. Henkelis, V. Pritchard, S. Oldknow, F. Colin, D. Rota Martir, E. Zysman-Colman**

9:30 1045. Guest packing and reactivity within containers assembled via the hydrophobic effect. **B.C. Gibb**

10:00 Intermission.

10:15 1046. Molecular discrimination and quantitative detection by luminescent lanthanide-based microporous sensors. **S.M. Humphrey, S.G. Dunning, A.J. Nunez, R.E. Sikma, M. Moore, A. Steiner, J.L. Sessler**

10:45 1047. Characterization of double and triple decker naphthylsalophen

complexes with *f*-elements: tunable emission from stacking and extended interactions. **A.E. Gorden**
11:15 1048. Molecular face-rotating polyhedra. **X. Cao**
11:45 1049. Let's get them talking: Systems of container molecules that work together. **J. Nitschke**
12:15 Concluding Remarks.

Section E

Ernest N. Morial Convention Center Room 333

Inorganic Chemistry of Lead Halide Perovskites: Insights from Fundamentals

B. C. Melot, J. Vela, *Organizers*
R. L. Brutchey, *Organizer, Presiding*
8:30 1050. Synthesis and spectroscopy of nanocrystals of compositionally complex haloperovskite semiconductors. S.E. Creutz, M.C. De Siena, E.N. Crites, T.J. Milstein, X. Yuan, J. Zhao, **D.R. Gamelin**
9:10 1051. Highly dynamic ligand binding and light absorption coefficient of cesium lead bromide perovskite nanocrystals. **J. De Roo**, M. Ibáñez, P. Geiregat, G. Nedelcu, W. Walravens, J. Maes, J.C. Martins, I. Van Driessche, M. Kovalenko, Z. Hens

9:30 1052. Quantum dot perovskite solar cells: Realizing the best of both worlds for revolutionary optoelectronic applications. **J. Luther**

10:10 Intermission.

10:40 1053. Colloidal nanocrystals of APbX₃ [A=Cs⁺, CH₃NH₃⁺, CH(NH₂)₂⁺, X=Cl, Br, I] perovskites with bright photoluminescence spanning the entire visible spectral range. **M. Kovalenko**
11:20 1054. Computational chemistry to design colloidally stable and trap-free perovskite nanocrystals. S. Boehme, **I. Infante**

11:40 1055. Single particle luminescence and Raman spectroscopy analyses of lead halide perovskite nanocrystals. **E.A. Smith**, B. Boote, L. Men, D. Freppon, H. Andaraarachchi, J.W. Petrich, J. Vela

Section F

Ernest N. Morial Convention Center Room 354

Chemistry of Materials: Materials for Energy & Catalytic Applications

C. G. Lugmair, *Organizer*
I. McKendry, C. G. Read, *Presiding*
8:30 1056. Understanding the role of graphene as an overlayer on nanostructured hematite photoanodes for improved solar water oxidation. **M.P. Cardona**, C. Yang
8:50 1057. Doping-treated BiVO₄ for photocatalytic H₂ fuel production from water. **W. Jo**, K. Gleason, J. Lee
9:10 1058. High throughput, multi-pH evaluation of earth-abundant pseudo-quaternary metal oxide catalysts for the oxygen evolution reaction. **J. Haber**,

D. Guevarra, R. Jones, K. Kan, J. Gregoire
9:30 1059. Understanding of metal (Ni, Co, Fe) (oxy)hydroxides on graphene as efficient electrocatalysts for water oxidation. **J. He**, R. Miao, W. Zhong, S.L. Suib
9:50 1060. Cu₂S conformal layer on cubic Cu₂O photocatalytic nanoparticles to increase stability in water splitting reaction. **N.P. Drago**, S. do Amaral Carminati, R.M. Welch, M. Alves de Melo Junior
10:10 Intermission.

10:25 1061. Growth and characterization of single-crystalline oxynitride materials for solar fuels production. **C.G. Read**, P.P. Buabthong, N.S. Lewis
10:45 1062. The role of inter- and intralayer dopants in 2D layered manganese complexes for cheap and efficient water oxidation catalysis. **I. McKendry**, L. Mohamad, A. Thenuwara, H. Peng, R. Remsing, D.R. Strongin, M. Zdilla

11:05 1063. Modifying layered manganese oxides for enhanced water oxidation: Turning a cheap, poor catalyst into a cheap, excellent catalyst. **M. Zdilla**, D.R. Strongin, E. Borguet, M.L. Klein, J.P. Perdew, I.G. McKendry, R. Ding, R. Remsing, H. Peng, R.K. Bhullar, L. Mohamad, A. Thenuwara, S.L. Shumlas, Y. Aulin, Q. Kang

11:25 1064. Operando Raman interrogation of the synthesis and activation of a CoSe HER catalyst. **K.Z. Rinaldi**, A. Carim, N.S. Lewis
11:45 1065. α -Zirconium phosphate frameworks as supports for active oxygen evolution reaction electrocatalysts. **M. Ramos-Garces**, J. Sanchez, T.F. Jaramillo, J.L. Colon

Section G

Ernest N. Morial Convention Center Room 210

PCET PhotoCatalysis with Inorganic Molecules & Materials

Cosponsored by PHYS
J. L. Dempsey, C. Heyer, E. Leon, G. J. Meyer, *Organizers*
B. H. Farnum, *Presiding*
8:00 1066. Making solar fuels. **T.J. Meyer**, L. Alibabei, D. Wang, B. Shan, B.J. Sherman, M.V. Sheridan, M.K. Brennaman, A. Nayak, M. Eberhart, Y. Wang, R. Sampaio, L. Troian-Gautier, M.K. Gish, G.J. Meyer, J.M. Papanikolas, K. Wee

8:25 1067. Moving electrons and protons with visible light-absorbing heteroleptic Cu(I) photosensitizers. B.J. McCullough, B.J. Neyhouse, S.E. Roe, **T.A. White**

8:45 1068. Modulating electron transfer dynamics at dye-semiconductor interfaces via self-assembled bilayers. **K. Hanson**, J.C. Wang, O. Ogunsolu
9:05 1069. Chromophore-catalyst assemblies for solar fuels. **K.S. Schanze**, G. Leem, J. Jiang, B.

Sherman, Y. Eom, T. Pho, L. Nhon, Z. Morseth, J.R. Reynolds, J.M. Papanikolas, T.J. Meyer
9:25 1070. Pyridyl-NHC ligated Re and W complexes for the photocatalytic reduction of CO₂ to CO and H⁺ to H₂ without photosensitizers. **J.H. Delcamp**, A. Huckaba, H. Shirley, H. Cheema, N. Liyanage, C. Carpenter, R.H. Schmehl, J.W. Jurss, C.E. Webster, N. Hammer
9:45 Intermission.

10:00 1071. New robust photo- and electrocatalysts for H₂ evolution and CO₂ reduction. **C. Turro**, H.J. Sayre, S. Witt

10:20 1072. In search for metal-free catalytic motifs for solar fuels. **K. Glusac**

10:40 1073. Excited state ion-pairs that undergo diffusional excited-state electron transfer. **L. Troian-Gautier**, W. Swords, S.A. Wehlin, M.D. Turlington, E.E. Beauvilliers, G.J. Meyer

11:00 1074. Light absorption and bond formation from the excited states of metal hydrides. **A.J. Miller**, M.B. Chambers, J.A. Rose, A. Bonn, C.L. Pitman, T. Wong

11:20 1075. Photocatalytic CO₂ reduction with nickel complexes supported by tunable bipyridyl-*N*-heterocyclic carbenes. X. Su, H. Shirley, J.H. Delcamp, **J.W. Jurss**

11:40 1076. Homogeneous hydrogen evolving photocatalysis using charge transfer and ligand localized triplet excited states. K. El Roz, M.M. McGoorty, J.E. Yarnell, M. Yang, C.M. Taliaferro, P.M. De La Torre, **F.N. Castellano**

Section H

Ernest N. Morial Convention Center Room 337

Organometallic Chemistry: New Ligand Platforms

N. S. Radu, *Organizer*
C. H. Larsen, M. Nippe, *Presiding*
8:30 1077. On-surface synthesis of low coordinate highly reducing metal complexes. **K.G. Caulton**, I.J. Huerfano, A.V. Polezhaev, C. Tempas, T. Morris, D. Wisman, T.S. Rahman, D. Le, S.L. Tait, N. Din

8:50 1078. Catalyst design for Ti-catalysed [2+2+1] pyrrole formation. **X. See**, I. Tonks

9:10 1079. Metallocenophane chemistry of the lanthanides: Structure and Magnetism. T. Latendresse, G. Risica, **M. Nippe**
9:30 1080. Metal-ligand cooperativity with redox-active tetradentate ligands. G. Durgaprasad, J.A. Luna, K.D. Spielvogel, C. Haas, S.K. Shaw, **S.R. Daly**

9:50 1081. Synthetic strategies to nitrilotriacetamide and tren ligand systems. **D.R. Manke**

10:10 1082. Impacts of hemilabile moieties in C-H and C-X activation at

late transition metals. **E.B. Hulley**, T. Morrow, W. Christman, L. Pap, N. Arulsamy
10:30 1083. Synthesis of electronically diverse triazole-pyridine ligands: Structure and catalytic activity of corresponding palladium(II) and gold(III) complexes. **C.H. Larsen**, Z.L. Palchak, M.D. Sterling, W.J. Richards, H.M. Ruvalcaba

10:50 1084. SNAP(O) ligands and their Ru complexes for the practical chemoselective hydrogenation of bio- and oil-derived functionalized esters. **P.A. Dub**, J.G. Schmidt, R.F. Williams, J.C. Gordon

11:10 1085. Efficient synthesis of imidoamidines: Liberation of imidoamidine ligands from heteroleptic nickel (II) complexes. **C.R. Guifarro**, E.V. Rybak-Akimova

Section I

Ernest N. Morial Convention Center Rooms 340/341

Chemistry of Materials: Metal Organic Frameworks

C. G. Lugmair, *Organizer*
E. D. Bloch, W. Huang, *Presiding*
8:30 1086. Selective catalytic olefin epoxidation with Mn^{II}-exchanged MOF-5. **A.W. Stubbs**, M. Dinca
8:50 1087. Design of porous metal organic frameworks (MOFs) for heterogeneous catalysis. **N.C. Mallaiha**

9:10 1088. Tandem nitrene synthesis using cooperative multifunctional metal-organic framework catalysts. X. Li, B. Zhang, T. Goh, V. Alexander, C. Tsung, L.M. Stanley, **W. Huang**
9:30 1089. Polyvinylidene fluoride (PVDF)/UiO-66 polymer composite fibers with enhanced catalytic activity towards chemical agents. **D. Dwyer**, D. Cooke, W.E. Bernier, M. Hall, T. Tovar, J. DeCoste, N. Hoffman, N. Dugan, N. Pomerantz, W. Jones

9:50 1090. MOF catalysis for ethanol to butanol upgrading. **C.N. Neumann**, M. Dinca
10:10 Intermission.

10:25 1091. Catalytic carbonylation of heterocycles by Co(CO)₄⁻-incorporated Cr-MIL-101. **H.D. Park**, M. Dinca, Y. Roman-Leshkov

10:45 1092. Ultramicroporous metal-organic materials with benchmarkselectivities of acetylene/ethylene. Y. Chen, **Z. Zhang**

11:05 1093. Ethylene dimerization in metal-organic frameworks. **E. Metzger**
11:25 1094. *Cis*-decalin oxidation as a stereochemical probe of *in-MOF* versus *on-MOF* catalysis. **A.D. Cardenal**, H. Park, D. Powers, C. Chalker
11:45 1095. Small molecule storage and activation with novel metal-organic materials. **E.D. Bloch**

Section J

Ernest N. Morial Convention Center Room 212

Organometallic Chemistry: Applications to Organic Transformations

N. S. Radu, *Organizer*

C. Hahn, J. T. York, *Presiding*

8:30 1096. Hydroarylation of alkenes catalyzed by late transition metal complexes. **C. Hahn**, B.J. Garcia, C.J. Adams, J. Medina

8:50 1097. Study of LiX (X=Cl, I, R) in THF: Aggregation states and reactivity, a theoretical study at the QM and QM/MM levels. **A. Milet**, R. David, P. Girard, M. Khazri

9:10 1098. Studies toward enantioenriched molybdenum dearomatization. **J.T. Myers**, P. Shivokevich, S. Dakermanji, J. Smith, C. Trindle, W. Harman

9:30 1099. Base metal catalyzed, and regioselective hydroboration of pyridines. **S.R. Tamang**, M. Findlater

9:50 1100. Terminal Rh^{III} methylidene from formal trinuclear oxidative addition of CH₂Cl₂. **T. Morrow**, E.B. Hulley, N. Arulsamy

10:10 1101. Tethered axial coordination in dirhodium paddlewheel complexes. **A. Darko**, D. Cressy, W. Sheffield, B. Anderson

10:30 1102. Investigating the binding and electrophilic activation of ethylene by group 12 metal ions. **J.T. York**

10:50 1103. Kinetics and mechanism of iron-catalyzed transfer hydrometallation. **B.V. Popp**

11:10 1104. Catalytic photoredox arene and heteroarene C-C bond-forming reactions driven without sacrificial reagents by tungsten-alkylidene chromophores. **H.B. Vibbert**, M.D. Hopkins

Section K

Ernest N. Morial Convention Center Room 335

Organometallic Chemistry: Applications to Materials & Polymer Science

N. S. Radu, *Organizer*

T. W. Hudnall, *Presiding*

8:30 1105. Synthesis of diverse C-H bond activated nonmetallocene lanthanides as a versatile tool for functionalized homo- and blockcopolymers *via* group-transfer polymerization. **F. Adams**, B. Rieger

8:50 1106. Substitution effects in highly syndioselective styrene polymerization catalysts based on single-component allyl *ansa*-lanthanidocenes: A theoretical study. **E. Louyriac**, L. Maron

9:10 1107. Electrophilic carbenes: Tales of main group chemistry, radicals, and photochemistry. **T.W. Hudnall**, T.A. Perera, R.N. Arias, M.B. Gildner

9:30 1108. Synthesis, characterization and applications of highly modular polyphosphonates. **T.R. Totsch**, G. Gray

9:50 1109. New complexes for nickel-catalyzed olefin polymerization. **A. Kocen**, M. Brookhart, O. Daugulis

10:10 1110. Synthesis of hyperbranched polyethylene with triazolocarboxamidate supported nickel complexes. **D. Xiao**, L. Do

10:30 1111. *In situ* Lewis acid recruitment effects on (b)py-appended late transition metal catalyzed ethylene polymerization. **A. Smith**, I. Tonks

10:50 1112. Rhodium-catalyzed dehydropolymerization of arsine boranes. **B. Ackley**, R. Waterman

11:10 1113. Photochemical reactions of Ru precursors for photoassisted chemical vapor deposition. **C.R. Brewer**, O.M. Hawkins, B. Salazar, A.V. Walker, L. McElwee-White

Radiopharmaceutical Chemistry Fluorine

Sponsored by FLUO, Cosponsored by INOR[‡], MEDI[‡] and NUCL[‡]

Molecular Processes at Mineral-Water Interfaces: Linking Theory & Experiments

Confinement: Clay Mineral Geochemistry

Sponsored by GEOC, Cosponsored by ENVR and INOR

Innovative Chemistry & Materials for Electrochemical Energy Storage

Sponsored by ENFL, Cosponsored by CATL, INOR and PMSE

Catalytic Conversion of Biomass Derived Molecules to Chemicals & Fuels

Sponsored by CATL, Cosponsored by ENFL, ENVR and INOR

R&D in the Chemical Catalysis for Bioenergy Consortium

Sponsored by CATL, Cosponsored by ENFL, ENVR and INOR

Catalytic & Photocatalytic Degradation of Pollutants & Chemical Threat Agents: New Developments in Materials & in Situ & Operando Methods Catalysis & Surface Science Applied to the Destruction of Threat Agents

Sponsored by CATL, Cosponsored by ENVR, INOR and PHYS

WEDNESDAY AFTERNOON

Section A

Ernest N. Morial Convention Center Room 345

Coordination Chemistry: Synthesis & Characterization

22 | Page

A. Larsen, *Organizer*

J. L. Brumaghim, J. R. Jeitler, *Presiding*

1:30 1114. Complexes of 2,6-pyridinedicarboxylate: Understanding the complex chemistry of a simple ligand. **J.R. Jeitler**, M. Jeitler, S. Patberg, E. Schafhausen

1:50 1115. Coordination sphere effects on unusually large zero field splitting and slow magnetic relaxation in trigonally symmetric 3d molecules. **K. Schulte**, V. Kuduva Radhakrishnan, K.R. Dunbar

2:10 1116. Effects of second coordination sphere on the properties and reactivity of Mn(III)-oxido complexes. **S. Barman**, J.R. Jones, C. Sun, A. Borovik

2:30 1117. Anisotropic exchange in polynuclear complexes containing Mo^{III}. **D.K. Kempe**, T.J. Woods, K. Schulte, H. Zhao, M.R. Saber, K.R. Dunbar

2:50 1118. Homo- and heterobimetallic complexes supported by an unsymmetric redox-active ligand. **C. Hess**

3:10 Intermission.

3:20 1119. Copper-thione complexes are truly complex: Redox and sulfur extrusion reactions. **J.M. Murphy**, C.D. McMillen, **J.L. Brumaghim**

3:40 1120. Rhenium metal-metal bonded fluoro complexes. **S. Mariappan Balasekaran**, A.P. Sattelberger, A. Hagenbach, F. Poineau

4:00 1121. Preparation and structure of lanthanide complexes coordinated to FeCOO and DTBpy ligands. **N. Johns**, S. Mariappan Balasekaran, A. Chang, P.K. Bhowmik, F. Poineau

4:20 1122. Employment of non-innocent ligands in transition metal coordination chemistry. **D.I. Alexandropoulos**, B.S. Dolinar, V. Kuduva Radhakrishnan, K.R. Dunbar

Section B

Ernest N. Morial Convention Center Room 344

Electrochemistry

Ernest N. Morial Convention Center Room 344

B. L. Lucht, *Organizer*

M. Zdilla, *Presiding*

1:30 1123. Highly conductive molecular electrolytes for safer lithium batteries designed through use of the Pearson hard-soft acid-base concept. **M. Zdilla**, S.L. Wunder, P.R. Chinnam, B. Fall, M. Van Vliet, A. Jalil, R.N. Clymer, A. Venkatnathan, P. Prakash, J. Aguirre

1:50 1124. Crystalline-amorphous Co@CoO core-shell heterostructures for efficient electro-oxidation of hydrazine. **X. Yan**, Y. Liu, J. Lan, Y. Yu, J. Murowchick, X. Yang, Z. Peng

2:10 1125. Benchmarking the effects of surface ligands on CoP for the hydrogen evolution reaction. **D. Ung**, B.M. Cossairt

2:30 1126. Pollutant detection with electrochemical biosensors. **A.L. Furst**, M.B. Francis

2:50 Intermission.

2:55 1127. Reduction potential and stability trends in heterobimetallic complexes containing trivalent redox-inactive cations. **A. Kumar**, V. Day, J.D. Blakemore

3:15 1128. Single-electron redox chemistry of [Cp*Rh] enabled by a nitrated bipyridine ligand. **W. Moore**, W.C. Henke, D. Lionetti, V. Day, J.D. Blakemore

3:35 1129. The electrochemical quartz crystal microbalance as a probe of molecular catalyst homogeneity. **D.J. Sconyers**, J.D. Blakemore

3:55 1130. Catalysis of the oxygen evolution reaction in strongly acidic electrolytes with earth-abundant crystalline nickel-manganese antimonate. **I.A. Moreno-Hernandez**, C.A. MacFarland, C.G. Read, K. Papadantonakis, B.S. Brunshwig, N.S. Lewis

4:15 1131. Scalable redox-active coordination network films toward molecular devices. **M. Haga**, K. Yoshikawa, D. Motoyama, H. Ozawa

Section C

Ernest N. Morial Convention Center Room 343

F. Albert Cotton Award in Synthetic Inorganic Chemistry: Symposium in honor of Andrew S. Borovik

Ernest N. Morial Convention Center Room 343

C. G. Riordan, J. Y. Yang, *Organizers*

D. C. Lacy, *Organizer, Presiding*

1:30 1132. Recent advances in the +2 oxidation state chemistry of the rare-earth and actinide metals. **W.J. Evans**

1:55 1133. Cytochrome P450 compound I: A direct link between electron donation and reactivity. **M. Green**

2:20 1134. Further studies in ligand non-innocence: Managing electrons and protons. **A.F. Heyduk**, K. Rosenkoetter, B. Charette, C. Ramirez

2:45 1135. Electrifying the secondary coordination sphere: Proximal cations and their effect on redox reactivity. **J.Y. Yang**, A. Reath, T. Chantarojsiri

3:10 Intermission.

3:25 1136. Structural biology of redox partner binding: Simple and complicated. **T.L. Poulos**

3:50 1137. The 6,6'-biazulenyl motif: From unusual polyelectrochromism to molecular nanostructures with remarkably high redox capacity. **M.V. Barybin**

4:15 1138. What do molecules want?

C.B. Aakeroy

4:40 1139. Nickel-dioxygen complexes: Synthesis, structure and reactivity.

C.G. Riordan

5:05 Concluding Remarks.

Section D

Ernest N. Morial Convention Center Room 352

Lanthanide & Actinide Chemistry

A. De Bettencourt Dias, *Organizer*

I. Hartenbach, E. M. Villa, *Presiding*

1:30 1140. Isolation of lanthanide cryptate complexes by ligand rearrangement and encapsulation. **D.N. Huh, J.W. Ziller, W.J. Evans**

1:50 1141. Facile linking of lanthanide cations with soft metals *via* thiosulfate. **E.M. Villa, E.Z. Dalton**

2:10 1142. Weak field ligands in *f*-element chemistry. **H.S. La Pierre, N.T. Rice, T.P. Gomba, B.J. Yik, L.M. Aquirre-Quintana**

2:30 Intermission.

2:40 1143. Molecular approaches to rare earth separations: Tuning ligand electronics for a greener system. **B.E. Cole, I.B. Falcones, T. Cheisson, B.C. Manor, P.J. Carroll, E.J. Schelter**

3:00 1144. Prism inside: Lanthanide chloride oxidotungstates and -molybdates of the formula $Ln_3Cl_3[MO_6]$ ($Ln = La - Nd, Sm - Er; M = Mo, W$). **K.V. Dorn, I. Hartenbach**

3:20 1145. Structural chemistry of Ce(IV), Th(IV), and U(IV) complexes isolated from acidic aqueous media. **J.N. Wacker, O.C. Stewart, Jr., K.E. Knope**

3:40 Intermission.

3:50 1146. An exploration of the lanthanide fluorite structure, MO₂ (Ce, Pr, and Tb) by microRaman. **J.T. Stritzinger, G. Goff, K. Boland**

4:10 1147. Reactivity of the isolated divalent lanthanide complexes $\{Ln[N(SiMe_3)_2]_3\}^{1-}$ with small molecules: CO, CO₂, N₂. **A. Ryan, J.W. Ziller, W.J. Evans**

4:30 1148. Ferrocene-based redox switches for reversible single-molecule magnet behaviour in dysprosium(III) and erbium(III) bis-diamidoferrocene complexes. **C.M. Dickie, A.L. Laughlin, J.D. Wofford, N. Bhuvanesh, M. Nippe**

4:50 1149. Formation of thorium and uranium – phosphorano - stabilized carbene. **P. Rungthanaphatsophon, L. Maron, J.R. Walensky**

Section E

Ernest N. Morial Convention Center Room 353

Inorganic Chemistry of Lead Halide Perovskites: Insights from Fundamentals

R. L. Brutchey, B. C. Melot, *Organizers*
J. Vela, *Organizer, Presiding*

1:30 1150. Interfaces, cations, and carrier dynamics in halide perovskites. **D.S. Ginger**

2:10 1151. Rationalizing the size-dependent Stokes shift in CsPbBr₃ nanocrystals. **M.C. Brennan, J.E. Herr, T.S. Nguyen-Beck, J. Parkhill, M.K. Kuno**

2:30 1152. Enhancing the sensitivity of ²⁰⁷Pb solid-state NMR spectroscopy for characterization of organolead halide perovskites. **M.P. Hanrahan, B. Rosales, L. Men, J. Vela, A.J. Rossini**

3:10 Intermission.

3:40 1153. Is mesoscopic TiO₂ in perovskite solar cells an innocent

bystander or a direct participant. **R.A. Scheidt, E. Kerns, P.V. Kamat**

4:20 1154. Transition path of organic cation induced anomalous photoluminescence in hybrid lead perovskites from real-time single crystal neutron diffraction. **X. Wang, B. Yang, K. Xiao**

4:40 1155. Synthesis and optical properties of 2D halide perovskites. **W.A. Tisdale**

Section F

Ernest N. Morial Convention Center Room 354

Chemistry of Materials: Materials for Energy & Catalytic Applications

C. G. Lugmair, *Organizer*
R. Coridan, O. Gunaydin-Sen, *Presiding*

1:30 1156. Search, discovery, and properties of ternary nitrides. **S. Lany, A. Holder, W. Sun, E. Arca, S. Bauers, G. Ceder, A. Zakutayev**

1:50 1157. Selective metal oxide atomic layer deposition: Toward precision few-atom clusters synthesis. **D. Cao, J. Emery, M. Pellin, A.B. Martinson**

2:10 1158. Physical and chemical applications of photodoping in electrodeposited cuprous oxide thin films. **J. Lowe, R. Coridan**

2:30 1159. Synthesis of fluorinated tungsten (VI) oxo-alkoxide complexes as precursors for the chemical vapor deposition of WO_x. **N. Ou, D.C. Bock, L. McElwee-White**

2:50 Intermission.

3:05 1160. The effect of different molecular weight and catalyst on ammonia borane: Polvinylpyrrolidone hydrogen storage composites. **O. Gunaydin-Sen, R. Seemaladinne, S. Pati, K. Kharel, A. Bafana, A. al-Wahish, E. Wujcik**

3:25 1161. Manganese(I) and rhenium(I) molecular CO₂ reduction catalysts heterogenized on gold electrodes at bipyridine sites in Rh(I) 5,5'-diisocyanide-2,2'-bipyridine coordination polymers. **G. Lee, C.P. Kubiak**

3:45 1162. Microwave-assisted hydrothermal carbonization of waste plant materials: An approach for improving their energy properties. **S. Elaigwu**

Section G

Ernest N. Morial Convention Center Room 210

PCET PhotoCatalysis with Inorganic Molecules & Materials

Cosponsored by PHYSS
C. Heyer, E. Leon, G. J. Meyer, *Organizers*

J. L. Dempsey, *Organizer, Presiding*

1:30 1163. Multiple proton transfers coupled to a single electron transfer in benzimidazole-phenol derivatives. **S. Mora, E. Odella, B. Wadsworth, M.T. Huynh, G.F. Moore, S. Hammes-Schiffer, D. Gust, T.A. Moore, A.L. Moore**

1:55 1164. Switching the mechanism: Proton-coupled electron transfer reactivity of a tungsten hydride complex. **J.L. Dempsey, T. Huang**

2:15 1165. Mechanistic roles of hydrogen bonding interactions in photoinduced PCET. **D.E. Polyansky, S. Lyamar, M. Ertem**

2:35 1166. Innovating bimetallic active sites for small-molecule catalysis. **C. Lu, R. Cammarota, M.V. Vollmer, S.P. Desai, J. Vitillo, J. Xie, J. Ye, L. Gagliardi**

2:55 1167. Excited State PT, ET and PCET in Hydroxybipyridine Ru(II) Complexes in Nonaqueous solution. **K. Martinez, M. Esposito, J.J. Paul, R.H. Schmehl**

3:15 Intermission.

3:30 1168. Toward light-driven multiple-electron-coupled proton-transfer (ECPT) reactions. **S. Luo, C. Sanborn, W. White, L. Renna, S. Ardo**

3:50 1169. Excited-state proton transfer in transition metal compounds. **R. Sampaio, R.M. O'Donnell, G. Li, G.J. Meyer**

4:10 1170. Free energy relationships in the formation of cobalt hydrides through PCET. **D. Kurtz, N. Elgrishi, B. Kandemir, W. Howland, J.L. Dempsey**

4:30 1171. PCET branch-points in CO₂-to-fuels catalysis. **Y. Surendranath, A. Wuttig, Y. Yoon, S. Khan, M. Schreier**

4:50 1172. Charge transfer through metal oxides on semiconductors for hydrogen evolution. **M.J. Rose, J. Seo, H. Kim, R. Pekarek**

5:10 1173. Probing the elementary steps of PCET catalysis. **R. Lomoth, T. Liu, S. Wang, S. Ott, L. Hammarstrom**

Section H

Ernest N. Morial Convention Center Room 211

Chemistry of Materials: Metal Organic Frameworks

C. G. Lugmair, *Organizer*
C. Mulzer, I. Stassen, *Presiding*

1:30 1174. O₂ electroreduction catalyzed by conductive metal-organic frameworks. **E. Miner, M. Dinca**

1:50 1175. Signature of metallic behavior in the metal-organic frameworks M₃(hexaiminobenzene)₂ (M = Ni, Cu). **J. Dou, M. Dinca**

2:10 1176. Vertical and lateral charge transport in ultrathin films of metal organic frameworks. **C. Marti-Gastaldo**

2:30 1177. Tunable, high single crystal conductivity in a permanently porous metal-organic framework. **L. Xie, L. Sun, R. Wan, S. Park, J. DeGayner, C.H. Hendon, D. Harris, M. Dinca**

2:50 1178. Synthesis and electromagnetic properties of square-symmetry π -conjugated metal-organic frameworks. **I. Stassen, M. Dinca**

3:10 Intermission.

3:25 1179. Charge transfer within MOF: The role of polar node. **P. Deria**

3:45 1180. Systematic study of conductive metal-organic frameworks as electrocatalysts for oxygen reduction reaction. **L. Wang, E. Miner, M. Dinca**

4:05 1181. Synthesis and characterization of novel palladium- and platinum-based metal-organic frameworks for thermoelectrics. **M.C. So, N.D. Mackie, S. Yoon, V. Cherrette, Y. He, V. Stavila, A.A. Talin, J. Llinas, M. Allendorf, K.L. Mulfort**

4:25 1182. Design and synthesis of highly stable metal organic frameworks with pre-designed interactions with light. **W. Newsome, G.S. Pour, R. Ly, J. Cordova, F.J. Uribe-Romo**

Section I

Ernest N. Morial Convention Center Rooms 340/341

Organometallic Chemistry: Applications to Organic Transformations

N. S. Radu, *Organizer*
J. M. Camara, *Presiding*

1:30 1183. New fluoro-organometallic chemistry of nickel and copper. **D.A. Vivic, M. Kosobokov, S. Yu**

1:50 1184. Carbon-fluorine bond formation from copper(I) vinyls: Synthesis of fluoroalkenes from alkynes. **A. Jordan, P.K. Thompson, J.P. Sadighi**

2:10 1185. Copper-catalyzed P-C cross-coupling for the synthesis of secondary phosphines and related ligands. **M. Frik, A.L. Haber, E.B. Schiff, J.M. Camara**

2:30 1186. Cobalt complexes of tripodal ligands with mixed P, N donors: Applications for catalytic dehydrogenative coupling reactions. **K. Ding, S. Xu, K. Paudel, B. Pandey, D.L. Tyler**

2:50 1187. Immobilization of molecular nickel cross-coupling catalyst on oxide supports via atomic layer deposition. **R. Key, A.K. Vannucci**

3:10 1188. How to predict reactivity on organometallic reactions from user-friendly computational tools. **A. Poater**

3:30 1189. Multiple aromatic C-H bond activations by a dirhenium carbonyl complex. **P. Dhull, R.D. Adams**

3:50 1190. Toward absolute measurements of Pd(π -arene) C-H acidity. **W. Christman, T. Morrow, N. Arulsamy, E.B. Hullay**

4:10 1191. Homogeneous (transfer) hydrogenation for the selective conversion of α,β -unsaturated aldehydes. **J.G. De Vries, R. Farrar-Tobar, P. Puylaert, B. Stadler, S. Hinze**

Section J

Ernest N. Morial Convention Center Room 212

Organometallic Chemistry: Synthesis & Characterization-Late Transition Metals

N. S. Radu, *Organizer*
 A. M. Tondreau, *Presiding*
1:30 1192. 1st row transition metals supported by dianionic PNP-chelate ligands; Reactivity and electronic structure. **A.M. Tondreau, N.H. Anderson, J.M. Boncella**
1:50 1193. Nickel complexes bearing the ¹⁸Pn^HP and ¹⁸Pn^HNOP ligands: Synthesis, characterization, and substrate reactivity. **N. Anderson, A.M. Tondreau, J.M. Boncella**
2:10 1194. Photoinduced electron transfer reaction of bis-cyclometalated iridium complexes with β -diketiminato ancillary ligands. **J. Shon, T.S. Teets**
2:30 1195. Monometallic and bimetallic platinum complexes with fluorinated β -diketiminato ligands. **K. Choung, T.S. Teets**
2:50 1196. Phosphorescent platinum(II) complexes with mesoionic NHC ligands – tuning the excited state. **J. Soellner, T. Strassner**
3:10 1197. Synthesis and reactivity of reduced CCC-NHC rhodium pincer complexes. **J. Denny, R.W. Lamb, C.E. Webster, T.K. Hollis**
3:30 1198. CCC-NHC pincer iron complexes: Synthesis of bis CCC-NHC complexes and ligand functionalization after complexation. **J. Cope, R.W. Lamb, J. Denny, C.E. Webster, T.K. Hollis, B. Donnadieu**
3:50 1199. Synthesis, characterization, and photophysics of CCC-NHC pincer Platinum complexes. **M. Zhang, S. Autry, V. Dixit, E.V. Dornshuld, J. Denny, N. Hammer, C.E. Webster, T.K. Hollis**
4:10 1200. Accessing reactive oxo intermediates: Oxidation of a CCC-NHC-Pt complex. **G.M. Lang, J. Denny, V. Dixit, C.E. Webster, T.K. Hollis**
4:30 1201. Boryl participation in H-X cleavage facilitated by (PBP)Ir and (PBP)Rh complexes. **Y. Cao, W. Shih, N. Bhuvanesh, O. Ozerov**

Section K

Ernest N. Morial Convention Center
 Room 335

Main Group Chemistry

T. W. Hudnall, *Organizer*
 A. F. Cozzolino, *Presiding*
1:30 1202. Novel Cu(I)- and Co(II)-Sb complexes: Magnetic properties, luminescence, and catalysis. **L. Taylor**
1:50 1203. Advances in the synthesis of Te, N-containing heterocycles: Potential building blocks for supramolecular frameworks. **N.L. Silar, B.A. Larson, F.R. Fronczek, T. Junk**
2:10 1204. Metalated ylides: Unique donor ligands for main group chemistry. **V.H. Gessner**
2:30 1205. Flexible nature of the carbodiphosphorane, C(PPh₃)₂, and its reactivity towards main group alkyl complexes. **P. Quinlivan, G. Parkin**

2:50 1206. Development of hypervalent 10–P–3 compounds for use as transition metal surrogates: The journey continues.... **M. Cain**
3:10 1207. Controlling molecular recognition and self-assembly with pnictogen(III) secondary bonding interactions in the solid and solution states. **S. Moaven, J. Qiu, A.F. Cozzolino**
3:30 1208. Cationic antimony containing compounds as Lewis acid catalysts for transfer hydrogenation reactions. **M. Yang, M. Hirai, F.P. Gabbaï**
3:50 1209. Platinum→trifluorostiborane complexes as carbophilic catalysts: Activation by fluoride anion abstraction from the trifluorostiborane Z-type ligand. **D. You, H. Yang, S. Sen, F.P. Gabbaï**
4:10 1210. Understanding Te and Sb separations in support of targeted Auger therapy using X-ray absorption spectroscopy. **S. Bone, K.T. Bennett, M.G. Ferrier, B.W. Stein, J. Engle, S.A. Kozimor**
4:30 1211. 2,2'-Bipyridine synthesis via phosphorus extrusion. **B.F. Wicker, K.M. Gass, Z. Araki**
4:50 1212. Synthesis, spectroscopic properties and biological activities of spiro-4-bromobenzylaminophosphazenes. **N. Guven Kuzey, N. Asmafiliz, L. Acik, T. Hokelek**
5:10 1213. Phonon-induced superstructures in layered titanium-oxypnictides superconductors. **R. Maazono, K. Nakano, K. Hongo**

Celebrating Over Four Decades of Research in Nanomaterials & Commercialization: Symposium in honor of Kenneth Klabunde
 Sponsored by I&EC, Cosponsored by INOR[‡]

Radiopharmaceutical Chemistry Carbon-11 & Radionuclide Production

Sponsored by FLUO, Cosponsored by INOR[‡], MED[‡] and NUCL[‡]

Unconventional Catalysis Targeting Stable Molecules

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

Molecular Processes at Mineral-Water Interfaces: Linking Theory & Experiments

Carbonates, Phosphates & Rare Earth Elements
 Sponsored by GEOC, Cosponsored by ENVR and INOR

Catalytic Conversion of Biomass Derived Molecules to Chemicals & Fuels

Sponsored by CATL, Cosponsored by ENFL, ENVR and INOR

Innovative Chemistry & Materials for Electrochemical Energy Storage

Sponsored by ENFL, Cosponsored by CATL, INOR and PMSE

R&D in the Chemical Catalysis for Bioenergy Consortium

Sponsored by CATL, Cosponsored by ENFL, ENVR and INOR

Catalytic & Photocatalytic Degradation of Pollutants & Chemical Threat Agents: New Developments in Materials & in Situ & Operando Methods Photocatalytic Approaches

Sponsored by CATL, Cosponsored by ENVR, INOR and PHYS

WEDNESDAY EVENING

Fluid-Solid Interfacial Phenomena at the Nexus of Energy & Geochemistry Research: A Symposium in Honor of David J. Wesolowski

Sponsored by GEOC, Cosponsored by COLL, ENFL, ENVR and INOR

Molecular Processes at Mineral-Water Interfaces: Linking Theory & Experiments

Sponsored by GEOC, Cosponsored by ENVR and INOR

Theoretical & Experimental Studies of Supercritical Fluids in the Subsurface

Sponsored by GEOC, Cosponsored by ENVR and INOR

THURSDAY MORNING

Section A

Ernest N. Morial Convention Center
 Room 345

Chemistry of Materials: Metal Organic Frameworks

C. G. Lugmair, *Organizer*
 P. J. Milner, J. P. Vizuet, *Presiding*

8:30 1214. Record-setting sorbents for water and ammonia: Engineering capacity, kinetics, and stability. **A.J. Rieth, M. Dinca**

8:50 1215. Cracking down on vapo-chromic materials: Vapor induced stress in gas sensing platinum salts. **A.E. Norton, S. Taylor, J.A. Krause, W.B. Connick**

9:10 1216. Holmium-based metal-organic framework for gas separations and cancer therapy. **J.P. Vizuet, K.J. Balkus**

9:30 1217. Understanding the mechanism of carbon dioxide uptake by a photoresponsive MOF. **R. Poloni, C. Yang, A. Charaf Eddin, L. Lin**

9:50 1218. Diamine-appended metal-organic frameworks for carbon dioxide capture from fossil fuel-fired power

plants. **P.J. Milner, R. Siegelman, J. Martell, A. Forse, M.I. Gonzalez, T. Runcevski, D. Gygi, J.A. Reimer, J.R. Long**

10:10 Intermission.

10:25 1219. Adsorption and sensing properties of metal-organic frameworks with mixed organic ligands. **W. Sun**

10:45 1220. Exploring the effect of ligand design on porphyrin metal-organic framework separation performance. **H. Rubin, M.M. Reynolds**

11:05 1221. Withdrawn

11:25 1222. Gas separations in a metal-organic framework featuring exposed vanadium(II) sites. **D. Reed, D. Jaramillo, J.R. Long**

11:45 1223. In-situ characterization of adsorbates in nanoporous materials with infrared spectroscopy. **H. Jiang, J. Long**

Section B

Ernest N. Morial Convention Center
 Room 344

Solid-State Inorganic Chemistry

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

8:30 1224. Structural and optical properties of two new non-centrosymmetric compounds: MgSiAs₂ and Mg₃Si₆As₈. **K. Woo, J. Wang, K. Lee, J. Dolyniuk, K. Kovnir**

8:50 1225. Withdrawn

9:10 1226. Polyamorphism induced multi-level electronic states in phase change K₂Sb₈Se₁₃. **M.S. Islam, L. Peng, L. Zeng, C. Malliakas, D. Chung, B. Buchholz, T. Chasapis, R. Li, K. Chrissafis, J. Medvedeva, G. Trimarchi, M. Grayson, T.J. Marks, M.J. Bedzyk, R. Chang, V. Dravid, M. Kanatzidis**

9:30 1227. Utilizing heterostructural alloying to design improved piezoelectrically active nitrides. **S. Millican, K. Talley, C. Musgrave, G. Brennecke, A. Holder**

9:50 Intermission.

10:05 1228. Magnetic properties of Ln₂CoGe₄O₁₂ and related compositions. **P.D. Battle, D. Xu, M. Avdeev, D. Ryan**

10:25 1229. Cu₂IrO₃: Toward the quantum spin liquid phase in honeycomb iridates. **M. Abramchuk, C. Ozsoy-Keskinbora, J.W. Krizan, K.R. Metz, D.C. Bell, F. Fallah Tafti**

10:45 1230. Synthesis of α -Fe₂O₃ hollow spheres: photonic crystal mimics. **A.M. Morey, S.T. Iacono**

11:05 1231. Real-time observation of nanoscale manipulation of metal oxide phase transformations using *in situ* transmission electron microscopy. **L. Yu, B.M. Hudak, R. Han, G. Waetzig, S. Depner, X. Sang, J. Liu, A. Talapatra, R. Arroyave, K. Page, S. Banerjee, B. Guiton**

11:25 1232. Investigation of the effect of rare-earth substitution on the Debye temperature of YAG:Ce³⁺ and

BAM:Eu²⁺. **A.C. Duke**, W. Zeier, J. Brgoch

Section C

Ernest N. Morial Convention Center Room 343

Nanoscience

B. G. Trewyn, *Organizer*
A. A. Marti, *Presiding*

8:30 1233. Flow synthesis of MOF nanoparticles in microfabricated reactors. **K. He**, K. Yeung

8:50 1234. High efficiency and long-term intracellular activity of an enzymatic nanofactory based on metal-organic frameworks. **X. Lian**, H. Zhou
9:10 1235. Grafting organic functionalities to boron-nitride nanotubes using Billups-Birch reaction. **A.A. Marti**, C. de los Reyes, A. Smith, K. Walz, M. Pasquali

9:30 1236. Polyarylboranes: Unexpected reactivity from some of the most stable ions. **M.W. Lee**, T. Wang
9:50 1237. Phase directing ability of an ionic liquid solvent for the synthesis of colloidal Ni₂P nanocrystals. **E.J. Roberts**, C.G. Read, N.S. Lewis, R.L. Brutchey

10:10 1238. Synthetic phase control over colloidal nickel sulfide nanocrystals. **G. Barim**, R.L. Brutchey
10:30 Intermission.

10:30 1239. Dynamic nature of thiolate monolayer in Au₂₅(SR)₁₈ nanoclusters. **G. Salassa**, A. Seles, F. Mancin, T. Bürgi

10:50 1240. Exploiting surface plasmon resonance in Au/ZnO photocatalysts for the selective oxidation of phenols. F. Lin, B.E. Cojocaru, **L.W. Colaciello**, C.A. Cadigan, C. Tian, M.N. Grecu, H. Xin, S. Vyas, V.I. Parvulescu, R.M. Richards

11:10 1241. Colloidal synthesis, energy gap tuning, and carrier dynamics of Ge_{1-x-y}Si_xSn_y alloy quantum dots. E. Eladgham, V. Tallapally, T.A. Nakagawara, D.O. Demchenko, U. Ozgur, **I.U. Arachchige**

11:30 1242. Cyclohexane oxidation over rock-salt structured metal oxides as catalysts. **Q. Yao**, C.A. Cadigan, A.R. Corpuz, G. Jeong, R. Bhattacharjee, R.M. Richards

11:50 1243. Microwave synthesis of Ir-based binary alloy nanoparticles and catalytic properties for hydrogenation. **H. Guo**, H. Li, K. Javis, H. Wan, P. Kunal, S. Dunning, D.S. Fernandez, S.M. Humphrey, G.A. Henkelman

Section D

Ernest N. Morial Convention Center Room 352

Main Group Chemistry

T. W. Hudnall, *Organizer*
C. Chiu, *Presiding*

8:00 1244. Reduction of aryl(hydro)boranes: Versatile bond-formation reactions. **T. Kaese**, M. Wagner

8:20 1245. Carbon-fluorine bond activation by low valent aluminum(I) complexes. **X. Wang**

8:40 1246. Boraflorenes with ultra-large Stokes shifts. **J. Cassidy**, P.A. Rupar, I. Adams, M. Smith

9:00 1247. Utilization of BODIPY dyes to introduce redox chemistry into main group complexes. **Z.M. Heiden**, I.A. Kieffer, R.J. Allen, J. Deobald

9:20 1248. One step conversion of potassium organotrifluoroborates to metal organoborohydrides. **E.R. Abbey**

9:40 1249. Boron containing radicals. M. Chung, H. Tsai, W. Liu, **C. Chiu**

10:00 1250. Microwave-promoted reactions of the CB₁₁⁻ carborane anion. **M.A. Juhász**

10:20 1251. Lewis superacidic ionic liquids with borenium cations. **M. Swadzba-Kwasny**, S. Coffie, J.M. Hogg, F. Coleman, A. Ferrer-Ugalde, J.D. Holbrey

10:40 1252. Alkyl groups as electron density donors in π -hole bonding. **J. Echeverria**

11:00 1253. Lanthanum catalyzed heterodehydrocoupling of silanes with amines. **M. Cibuzar**, R. Waterman

11:20 1254. Facile access to organometallic heavy alkaline earth metal species using environmentally friendly redox transmetalation protolysis (RTP). Y. Takahashi, A.Y. O'Brien, G.B. Deacon, P.C. Andrews, M. Wolf, A. Torvisco, **M.M. Gillett-Kunnath**, K. Ruhlandt-Senge

11:40 1255. Reductive CO₂ homologation: C-C homocoupling and asymmetric carbon generation. **S. Bontemps**

Section E

Ernest N. Morial Convention Center Room 353

Coordination Chemistry: Synthesis & Characterization

A. Larsen, *Organizer*

M. P. Marshak, F. Poineau, *Presiding*

8:30 1256. Speciation and reactivity of heptavalent technetium in strong acids. **F. Poineau**

8:50 1257. Molecular magnets utilizing anisotropic coupling with 4d and 5d cyanometallate compounds. **F.J. Birk**, D. Pinkowicz, K.R. Dunbar

9:10 1258. An investigation into the reactivity profile of high-spin iron hydride clusters. **B.J. Knight**, K. Anderton, M. Eaton, L.J. Murray

9:30 1259. Diosmium carbonyl complexes containing multiple ligands derived from ferrocene. **G.L. Powell**

9:50 1260. Structural elucidation of chemical compounds in reaction conditions that preclude standard characterization techniques. **J. Fehrs**, C.H. Hendon

10:10 Intermission.

10:20 1261. Bulky β -diketonate ligands and implications for catalysis. **M.P. Marshak**

10:40 1262. Steps towards the elucidation of the electronic structure of a family of open-shell trinuclear iron clusters. **J. Teesdale**, T. Betley

11:00 1263. Exploring cooperative redox chemistry using dipyrin pacman complexes. **E.J. Johnson**, C. Kleinlein, T. Betley

11:20 1264. Copper(I) and silver(I) complexes with unsaturated N-heterocyclic chalcogenones. **A. Allen**, D. Rabinovich

Section F

Ernest N. Morial Convention Center Room 354

Environmental & Energy-Related Inorganic Chemistry

S. A. Koch, *Organizer*

J. D. Blakemore, M. Nippe, *Presiding*

8:00 1265. Modulating electrocatalytic CO₂ reduction via secondary coordination sphere functional groups. S. Sung, J. Meeder, **M. Nippe**

8:20 1266. Controlled synthesis of earth-abundant tin sulfides Sn₂S₃ thin films for photoelectrochemical water splitting. **Y. Liu**, L. Zhang, H. Zhu

8:40 1267. Bipolar phthalocyanine-based electrolyte for symmetric redox flow batteries. **C. Hunt**, G. Menard

9:00 1268. Photolytic conversion of light alkanes to alkyl esters by iodine oxides and chloride salts in non-superacidic media. **N. Schwartz**, S.E. Kalman, N. Boaz, J.M. Goldberg, R. Fu, R.J. Nielsen, W.A. Goddard, J.T. Groves, T.B. Gunnoe

9:20 1269. Carbon dioxide-expanded liquids as media for electrochemistry and catalysis. **J.D. Blakemore**, T. Kerr, C. Shaughnessy, D.J. Sconyers, B. Subramaniam, K.C. Leonard

9:40 1270. Electrocatalytic reduction of nitrate in water by a highly-fluorinated Cu(II) precatalyst. **J.K. Elinburg**, S. Hannigan, L.H. Doerrer

10:00 1271. Identification of high ZT thermoelectrics from complex oxide screening. **A. Ganose**, W. Leung, A. Jackson, R. Palgrave, D. Scanlon

10:20 Intermission.

10:40 1272. Withdrawn

11:00 1273. Coordination sphere effects on the activity and selectivity of electrochemical CO₂ reduction by a polymer-encapsulated cobalt complex. **Y. Liu**, C.C. McCrory

11:20 1274. Causes and cures of the photodecomposition of manganese tricarbonyl complexes. **W.C. Henke**, C.J. Otolski, W.N. Moore, K.V. Prather, C.G. Elles, J.D. Blakemore

11:40 1275. Total utilization of biomass, lignin and carbohydrate: Using earth abundant nickel catalyst. **H. Luo**

12:00 1276. Palladium N-heterocyclic carbene based CCC-NHC pincer complexes: Air and water stable organometallic emitters. **G.M. Lang**, J. Denny, S. Atry, V. Dixit, N. Hammer, C.E. Webster, T.K. Hollis

Section G

Ernest N. Morial Convention Center Room 210

Inorganic Catalysts

S. A. Koch, *Organizer*

T. Hamann, D. Powers, *Presiding*

8:30 1277. Mechanistic insights into the aerobic copper catalyzed decarboxylative thiolation of benzoic acids. **K. Green**, J.M. Hoover

8:50 1278. Copper cryptand complexes as catalysts for CuAAC click reactions and their prospects for in vivo applications. **T. Tran**

9:10 1279. Iodine redox catalysts for selective O₂ utilization. **D. Powers**

9:30 1280. Electrocatalytic reduction of carbon dioxide by finely tuned molecular catalysts. **S. Sung**, D. Kumar, M. Gil-Sepulcre, M. Nippe

9:50 1281. The influence of ligand environment on the deoxydehydration of polyols by early-metal oxo-complexes. **S.M. Kilyanek**, R. Tran

10:10 Intermission.

10:25 1282. Understanding the fast rates of open butterfly [2Fe-2S] cluster-based catalysts for the hydrogen-evolving reaction (HER). **K. Clary**, H. Petersen, D.H. Evans, R.S. Glass, D.L. Lichtenberger

10:45 1283. Formic acid oxidation by surface attached Ni(P₂N₂)₂ complexes. **F.M. Brunner**, C.P. Kubiak

11:05 1284. A molecular palladium catalyst immobilized on heterogeneous metal oxide supports for the hydrodeoxygenation of model lignin monomers. **N.A. DeLucia**, A.K. Vannucci

11:25 1285. Electro-catalytic ammonia splitting. F. Habib-Zadeh, **T. Hamann**, M.R. Smith

11:45 1286. Fabrication of magnetically retrievable metal nanocatalysts for organic transformations. **R.K. Sharma**

12:05 1287. Withdrawn

Section H

Ernest N. Morial Convention Center Room 211

Lanthanide & Actinide Chemistry

A. De Bettencourt Dias, *Organizer*
M. Mazzanti, J. D. Rinehart, *Presiding*

8:30 1288. Generating robust erbium(III) anisotropy without full coordinative saturation for scalable molecule-based magnetic materials. **J.D. Rinehart**, J. Hilgar, M.G. Bernbeck, B. Flores

8:50 1289. Stabilization of neptunyl crown ether complexes: Characterization by spectroscopic and diffraction approaches. **T. Forbes**

9:10 Intermission.

9:20 1290. New carbocyclic uranium compounds and their unusual reactivity. **K. Erickson**, J.L. Kiplinger

9:40 1291. Synthesis and reactivity of complexes of f elements supported by siloxide ligands. **M. Mazzanti**

10:00 1292. Synthesis, characterization and reactivity of U(IV) and U(III) imido and amido complexes with bulky terphenyl substituents. **J.M. Boncella**, B. Billow, A.L. Odom, C. Mokhtarzadeh

10:20 Intermission.

10:30 1293. Heterometallic single-molecule magnets: Synthetic challenges and solutions. C. Burns, B. Wilkins, C.M. Dickie, T. Latendresse, **M. Nippe**

10:50 1294. Synthesis of mixed tris(imido) uranium complexes. **K.E. Gettys**, N. Anderson, M. Zeller, S.C. Bart

11:10 1295. New bond forming events using organometallic actinide chemistry. **J.K. Pagano**, J. Xie, K. Erickson, D.E. Morris, B. Scott, R. Wu, M. Sykora, P. Yang, R. Waterman, L. Gagliardi, J.L. Kiplinger

Section I

Ernest N. Morial Convention Center
Rooms 340/341

Organometallic Chemistry: New Ligand Platforms

N. S. Radu, *Organizer*

E. T. Papish, *Presiding*

8:30 1296. Development of new phosphalkene-pyridine ligands, their coordination chemistry, and use as a noninnocent platform for “waste-free” catalytic processes. **M.L. Nakashige**, M. Cain, A.L. Rheingold

8:50 1297. Carbon dioxide reduction with transition metals and proton responsive pyridinol based pincer ligands. **E.T. Papish**, S. Das, D.B. Burks, C. Boudreaux, N. Liyanage, S.B. Davis, R.W. Lamb, V. Dixit, F. Qu, C.E. Webster, J.H. Delcamp

9:10 1298. Synthesis and characterization of “nucleo-pincers” and their transition metal complexes. **S. Gunther**, A.J. Kosanovich, Y. Cao, N. Bhuvanesh, O. Ozerov

9:30 1299. Robust ruthenium(II) CNC-pincer catalysts selectively reduce carbon dioxide. **C. Boudreaux**, N. Liyanage, S. Das, H. Shirley, S. Siek, D. Gerlach, F. Qu, J.H. Delcamp, E.T. Papish

9:50 1300. New synthetic route to acridone, and acridine-based PNP ligands for low-coordinate late first- and second-row transition metal complexes. **K. Omolo**, J.P. Sadighi

10:10 1301. Facile dearomatization and metal-ligand cooperation in an unfunctionalized PCP-pincer. **A.J. Kosanovich**, C.H. Komatsu, O. Ozerov

10:30 1302. Use of a protic bis-(N-heterocyclic carbene)phosphine ligand to explore metal-ligand cooperativity for CO₂ reduction and as a scaffold for bimetallic complexes. **M. Johnson**, S.E. Flowers, B.M. Cossairt

10:50 1303. Tridentate phosphine ligands bearing aza-crown ether lariats: Applications to Pd and Mo coordination chemistry. **L. Pap**, N. Arulsamy, E.B. Hulley

11:10 1304. Efficient synthesis of imidoamidines: The trapping and confirmation of an imidoamide intermediate. **C.R. Guifarro**, E.V. Rybak-Akimova

Section J

Ernest N. Morial Convention Center
Room 212

Organometallic Chemistry: Synthesis & Characterization-Late Transition Metals

N. S. Radu, *Organizer*

B. Captain, U. R. Pokharel, *Presiding*

8:30 1305. Synthetic methodologies for ferrocene-fused acenes. **U.R. Pokharel**, J. Bergeron, D. Daigle, J.P. Selegue

8:50 1306. Development of electronic unsaturation in transition metal cluster complexes: Addition of Pt(IPr) groupings as sterically demanding ligands. **V. Zollo**

9:10 1307. Influence of the isocyanide and Tm ligands on the reductive coupling of [Tm^RFe(CNR)₃]OTf. **O. Mitevski**, A.S. Gowda, A. Baur, J.M. Hoover

9:30 1308. N₂O binding on RCo(CNR)₃ and O-atom transfer reactions. **C. Chan**, J.S. Figueroa

9:50 Intermission.

10:15 1309. Synthesis of formazanate complexes with third row transition metals and analysis of their spectroscopic and electrochemical properties. **E. Kabir**, T. Teets

10:15 1310. Further developments in synthesis from [M(S₂C₂Ph₂)₂] (M = Ni, Pd, Pt) by direct ligand substitution. **A. Obanda**, K. Martinez, R.H. Schmehl, I.V. Rubtsov, J.T. Mague, J.P. Donahue

10:35 1311. Small molecule activation by platinum complexes containing bulky tin groups. **B. Captain**, A. Koppaka, M. Gamage

10:55 1312. Synthesis, structures and properties of copper complexes with diamino bis(thiolato) ligands. **B. Wang**, S.J. Ferrara, S. Sproules, R. Pascal, J.T. Mague, J.P. Donahue

11:15 1313. Group 10 dithiolene compounds with an open-ended 1,2,4,5-Tetrakis(diphenylphosphino)benzene ligand: Synthesis, structure, properties. **M. Pratheepkumar**, K. Arumugam, J.T. Mague, **J.P. Donahue**

Section K

Ernest N. Morial Convention Center
Room 335

Chemistry of Materials: Nanomaterials

C. G. Lugmair, *Organizer*

M. Devadas, *Presiding*

8:00 1314. Combinatorial synthesis of multimetallic nanoparticles. **P. Chen**, J. Hedrick, C.A. Mirkin

8:20 1315. Host-guest design to access the lead halide perovskites nanocrystals under strong confinement using metal organic frameworks as a matrix. **L. Protesescu**, M. Dinca

8:40 1316. Photo-inks based on porphyrins and diarylethenes (DAEs). A. Galanti, T. Biellmann, J. Wytko, J. Boixel, V. Guerschais, P. Samori, **J. Weiss**

9:00 1317. Introducing room temperature liquid metals as a reaction solvent for the synthesis of atomically thin 2D metal oxides. **T. Daeneke**, A. Zavabeti, R.B. Kaner, K. Kalantar-zadeh

9:20 1318. Investigating inter-particle exchanges and crystallographic changes in gold nanoclusters. **C. Hosier**, C. Ackerson

9:40 Intermission.

9:55 1319. Synthesis of first row transition metals nanoparticles for aerosol deposition. **L.J. Treadwell**, T.J. Boyle, A.W. Cook, D. Perales, D. Woodard, N.S. Bell

10:15 1320. Controlled growth of Mn₁₂ single-molecule magnet polymers and oligomers. M. Shmunis, E.R. Williams, S.M. Stone, A.M. Mowson, G. Christou, T.M. Pekarek, **C. Lampropoulos**

10:35 1321. Au(I) precursors for electron beam induced deposition. **W.G. Carden**, J. Pedziwiatr, K.A. Abboud, L. McElwee-White

10:55 1322. Magic numbered gold clusters - optical and electrochemical properties. **M. Devadas**, A. Meola, B. Hutson, N. Hondrogiannis, K. Reber

11:15 1323. Pulsed microwave energy: A kinetic control approach to highly branched nickel multipod nanostructures. **P. Vakil**, B. Ashley, D. Hardy, G.F. Strouse

11:35 1324. Surfactant-free shape control of gold nanoparticles enabled by unified theoretical framework of nanocrystal synthesis. **C.M. Drain**, M. Wall, M. Kircher

Celebrating Over Four Decades of Research in Nanomaterials & Commercialization: Symposium in honor of Kenneth Klabunde

Sponsored by I&EC, Cosponsored by INOR[‡]

Radiopharmaceutical Chemistry

Sponsored by FLUO, Cosponsored by INOR[‡], MEDI[‡] and NUCL[‡]

Molecular Processes at Mineral-Water Interfaces: Linking Theory & Experiments

Iron Oxyhydr-Oxides: Redox Processes

Sponsored by GEOC, Cosponsored by ENVR and INOR

Unconventional Catalysis Targeting Stable Molecules

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

Theoretical & Experimental Studies of Supercritical Fluids in the Surface

Sponsored by GEOC, Cosponsored by ENVR and INOR

Catalytic Conversion of Biomass Derived Molecules to Chemicals & Fuels

Sponsored by CATL, Cosponsored by ENFL, ENVR and INOR

Control of Zeolite Structure, Composition & Sites for Catalysis

Sponsored by CATL, Cosponsored by INOR

THURSDAY AFTERNOON

Section A

Ernest N. Morial Convention Center
Room 345

Chemistry of Materials: Metal Organic Frameworks

C. G. Lugmair, *Organizer*

C. H. Hendon, *Presiding*

1:30 1325. Development of a computational method for simple DFT calculation of pore volume and surface area of porous materials. **C.H. Hendon**, K. Butler, T.Z. Crawford

1:50 1326. Screening of ZIF topologies using mechanochemistry: Fast, simple, and effective route to the discovery of new ZIFs. **I. Brekalo**, K. Holman, T. Friscic

2:10 1327. Tubes vs sheets: A mechanistic investigation of MOF dimensionality. **K.M. Vailonis**, U. Shrestha, M.D. Dadmun, D.M. Jenkins

2:30 1328. Biocompatible near-infrared MOF fluorophores for bio-imaging applications. **D.F. Sava Gallis**, L.S. Rohwer, K.S. Butler, T.S. Luk

2:50 1329. Fluorescent porous materials for chemical sensing. **D. Zhao**

3:10 Intermission.

3:25 1330. Mesoporous MOFs for DNA and protein Inclusion. **H. Deng**

3:45 1331. Lanthanide metal-organic frameworks for proton conduction. **M. Fairley**, L. Qin, Z. Zheng

4:05 1332. Luminescent conductive metal-organic frameworks. **G. Skorupskii**, K. Williams, R.W. Day, C. Perkinson, M. Cotlet, M. Baldo, W.A. Tisdale, M. Dinca

4:25 1333. Electronic structure of electrically conductive metal organic frameworks. **J. Fehrs**, C.H. Hendon

4:45 1334. Boosting transport distances for molecular excitons within photo-excited metal-organic framework films. **S. Goswami**, M. Chen, M.R. Wasielewski, O.K. Farha, J.T. Hupp

Section B

Ernest N. Morial Convention Center
Room 344

Coordination Chemistry: Synthesis & Characterization

A. Larsen, *Organizer*

C. Martin, N. C. Tomson, Presiding
1:30 1335. Exploiting the Lewis acidity of boroles to access boron-containing heterocycles. S. Yruegas, V. Adiraju, **C. Martin**

1:50 1336. Structural and spectroscopic characterization of five-coordinate iron and cobalt bis(dithiolene)-phosphine complexes. **P. Chandrasekaran, L. Mootha, D. Williams**

2:10 1337. Coordination chemistry of extended pyridyl-acetylacetonate ligands. **C.A. Gunawardana, A. Sinha, V. Day, C.B. Aakeroy**

2:30 1338. Oxidative reactivity of a rhenium nitride complex. **G.P. Connor, P.L. Holland, J.M. Mayer**
2:50 Intermission.

3:00 1339. Synthesis and structure of octahedral cobalt clusters. **R.A.**

Musgrave, A.R. Fout, R. Hernandez Sanchez, T. Betley

3:20 1340. Synthesis, characterization, and reactivity of thermally stable cupric superoxides. S. McCollom, A.B. Weberg, P.J. Carroll, **N.C. Tomson**

3:40 1341. Experimental and computational studies of trans-Rh₂ compounds: Improving the photochemistry by manipulating the configurational isomerism. **A. Millet, C. Xue, C. Turro, K.R. Dunbar**

4:00 1342. Synthesis, characterization, and reactivity of luminescent CuCl complexes with triaminoborane-bridged diphosphines. **C.M. Donahue, K. Lee, B.A. Massman, S.R. Daly**

4:20 1343. Cyclic double-butterfly iron carbonyl clusters. **C.A. Mebi, S. Johnson**

Section C

Ernest N. Morial Convention Center
Room 343

Organometallic Chemistry: Synthesis & Characterization-Late Transition Metals

N. S. Radu, *Organizer*

J. P. Donahue, *Presiding*

1:30 1344. Homoleptic platinum azoiminato complexes via hydrogenative cleavage of formazans. **G. Mu, T.S. Teets**

1:50 1345. The 4-electron reduction of benzo[c]cinnoline by a trimetallic Ni₂Ti complex. **P. Dunn, I. Tonks**

2:10 1346. Revisiting the cluster-surface analogy: Surface-like behavior in strong field iron clusters. **M.J. Drance, J.S. Figueroa**

2:30 1347. Structure and reactivity of mono-anionic rhodium and iridium tris-isocyanides. **M.L. Neville, J.S. Figueroa**

2:50 1348. Investigations of a reactive open shell trigold(I) carbide and its adducts. **N.T. Daugherty, J.P. Sadighi, J. Bacsa**

3:10 1349. Thermodynamics of ligand-metal complex binding: An isothermal titration calorimetry study. **W. Li, S.**

Ivanov, S. Mozaffari, N. Shanaiah, A.M. Karim

3:30 1350. Isolation and characterization of in-situ species formed in iron-catalyzed cross-coupling reactions with aryl nucleophiles. **S. Carpenter, M.L. Neidig**
3:50 1351. Synthesis and characterization of high-spin iron carbene complexes. **A. Wrobel, T. Betley**

Section D

Ernest N. Morial Convention Center
Room 352

Bioinorganic Chemistry: Proteins & Enzymes & Model Systems

S. A. Koch, *Organizer*

W. M. Ames, H. R. Lucas, *Presiding*

1:30 1352. New chemical tools for studying cellular iron homeostasis. **A. Fikes, E.L. Que**

1:50 1353. Biological on/off switch for bacterial biofilm formation in *Agrobacterium vitis*. **D. Williams, N.M. Nesbitt, E.M. Boon**

2:10 1354. Formation of benzothiazoles from 2-mercaptoaniline and O₂-dependent oxidation of primary alcohols by thiol dioxygenase enzymes. **S. Sardar, W.P. Morrow, F.W. Foss, B.S. Pierce**

2:30 1355. Mutations on the superoxide reductase: A theoretical study of the 2nd coordination sphere and formation of an oxo-iron intermediate. **R. David, H. Jamet, V. Nivière, Y. Moreau, A. Millet**

2:50 1356. Reactivity of diiron clusters containing sulfide and hydride bridges. **D. Singh, B. Knight, L.J. Murray**

3:10 1357. Investigating unique *J*-values for Mn^{III}Mn^{III} and Mn^{III}Mn^{IV} dimers containing a single unsupported μ -oxo bridge with BS-DFT. **W.M. Ames**

3:30 Intermission.

3:45 1358. Triplet, high-spin, linear {Fe(NO)}⁸: Redox feature of a stable diiron trinitrosyl complex. **P. Ghosh, S. Ding, M. Quiroz, C. Hsieh, M.B. Hall, M.Y. Darensbourg**

4:05 1359. Nickel and cobalt macrocycles for oxidative transformations. **H.R. Lucas**

4:25 1360. Molecular modelling on the driving force the acylation of β -lactam antibiotics. **C.U. Ibeji**

Section E

Ernest N. Morial Convention Center
Room 353

Chemistry of Materials: Nanomaterials

C. G. Lugmair, *Organizer*

A. L. Eckermann, *Presiding*

1:30 1361. Europium-doped cerium oxide nanomaterials: Synthesis and exposure to l-dopa and eumelanin. **A. D'Achille, J.L. Coffey**

1:50 1362. Gold nanoparticles stabilized by organic-inorganic hybrid polyoxometalates: Synthesis, surface

studies and catalytic applications. **M. Martin Gandul, G. Newton**

2:10 1363. Thermal decomposition of Prussian blue analogue as precursors for magnetic nanoparticles. **D.A. Hardy, G.F. Strouse**

2:30 1364. Synthesis of 2D metal borides derived from ternary MAB phases. **L. Alameda, R.E. Schaak**

2:50 1365. Synthesis and leaching of strontium-doped hydroxyapatite. **A.L. Eckermann, A. Washburn, K. Libson**
3:10 1366. Minerals to materials: Bulk synthesis of aqueous aluminum clusters and their use as precursors for metal oxide thin films. **B. Fulton**
3:30 Intermission.

3:45 1367. Carbon nanorods for water expulsion at high humidity. **J.**

Kothandaraman, S.K. Nune, D.J. Heldebrant, M.J. Olszta, D. Lao, K. Stoerzinger, Y. Shin, X. Yu

4:05 1368. Molybdenum promoted mesoporous Co₃O₄: Study of acid-base switchable surface chemistry. **C. Weerakkody, S.L. Suib**

4:25 1369. Temperature dependant stabilities of various isomers of C32 endohedral metallofullerenes. **T.J.**

Fuhrer, S. Church, J. Coello

4:45 1370. Purification of metallic nanowires and their uses in low density aerogels. **Y. Han, F. Qian**

5:05 1371. Van der Waals assembly of two-dimensional fullerene thin films. **K. Lee, B. Choi, I. Jen-La Plante, C. Goulbourne, X. Zhu, X. Roy**

5:25 1372. Exploring synthetic pathways to pluronics-derived mesoporous nitrides with *in situ* SAXS/WAXS. **P. Beaucage, S.M. Gruner, U.B. Wiesner**

Section F

Ernest N. Morial Convention Center
Room 354

Chemistry of Materials: Synthesis & Properties

C. G. Lugmair, *Organizer*

F. Fallah Tafti, T. E. Stevens, *Presiding*

1:30 1373. Tuning superconductivity and magnetism in [Li_{1-x}Fe_xOH]FeS by controlling the hydrothermal synthesis conditions. **F. Fallah Tafti, E. McDonnell**

1:50 1374. Plasmonic excitations in strained Sr_{1-x}Nb_{1-y}O_{3+ δ} nanoparticles. **T. Ofoegbuna, W. Shelton, J.A. Dorman**

2:10 1375. Near-infrared aza-BODIPY fluorescence probes for selective Cu²⁺ detection and their potential in living cell imaging. **N. Wanichacheva, Y. Tachapermpoon, P. Praikaew, S. Thavornpradit, A. Charoenpanich, J. Sirirak, K. Burgess**

2:30 1376. Chemically tunable photoluminescence in Si₂Te₃ nanoplates through doping and intercalation. **M. Wang, B. Wang, K.J. Koski**

2:50 Intermission.

3:05 1377. Synthesis of a magnetically frustrated organometallic ferrous oxide

cluster from partial oxidation. **Z.H. Hecht, J. Kephart, N. Arulsamy, B. Livesay, M.P. Shores, C.V. Popescu, E.B. Hulley**

3:25 1378. Synthesis of γ' -Fe₄N, a new soft magnetic material for inductors and transformers. **T.E. Stevens, C.J. Pearce, S. Atcity, T.C. Monson**

3:45 1379. Using different synthetic conditions to achieve maximum dye loading of Brooker's merocyanine within zeolite L channels. **J.S. Holt, L. Engerer, T. Dabertin, B. Henning, S. Mattis, K. Weber**

4:05 1380. Kinetic control of ZnS and ZnSe nanocrystal syntheses. **E. Bennett, L. Hamachi, H. Yang, B. Abecassis, J. De Roo, M. Greenberg, J.S. Owen**

Section G

Ernest N. Morial Convention Center
Room 210

Coordination Chemistry: Characterization & Applications

A. Larsen, *Organizer*

K. L. Mulfort, M. Zdilla, *Presiding*

1:30 1381. Vectorial charge transfer from heteroleptic Cu(I)diimine complexes. **K.L. Mulfort, L. Kohler, D. Hayes, R.G. Hadt, L.X. Chen**

1:50 1382. Pyrazole-based ligands for complexation, extraction and recovery of Hg(II) from nuclear waste. **S. Kandel, K. Chambers, L. Mathivathanan, R.G. Raptis**

2:10 1383. Aminotriphenolate complexes for catalysis and enantioselective molecular recognition. **C. Zonta, A.W. Kleij, G. Licini**

2:30 1384. Synthesis and elucidation of novel phosphonate-based biocompatible coordination polymers with enhanced dissolution properties. **G. Quinones Velez, V. López-Mejías**

2:50 1385. Breaching the "CHNO ceiling" in energetic materials by the inclusion of redox-frustrated inorganic elements. **M. Zdilla, O. O'Sullivan**

3:10 1386. Tunable dimetal tetraguanidinate paddlewheel complexes with unprecedented electron donor abilities. **M. Humphries, B.R. Smith, E. Wusterbarth, J.T. Njardarson, D.L. Lichtenberger**

3:30 1387. Inorganic-organic hybrid material for the cyanide sensing using Co(II)-bis-terpyridine type coordination complexes. **I. Bhowmick, C. Collins, D.J. Boston**

3:50 Intermission.

4:00 1388. Synthesis, characterization, and reactivity studies of a zirconium-cobalt bis(phosphinoamide) complex. **K.M. Gramigna, C.M. Thomas**

Section H

Ernest N. Morial Convention Center
Room 337

Nanoscience

B. G. Trewyn, *Organizer*

J. E. Johns, *Presiding*

1:30 1389. Cancer nanotherapy promoted by a nuclear targeting molecular capsule. **Y. Fang**, H. Zhou
1:50 1390. Ultrastable metal nanoparticles studied for the development of biomedical applications, nanomedicine and water purification. **E. Rauwel**, P. Rauwel, S. K  nial, O. Volobujeva, A. Ivask, D. Wragg

2:10 1391. Controlling DNA delivery from gold nanoparticles in human cells, studied via live-cell fluorescence microscopy. **K.J. Carnevale**, G.F. Strouse

2:30 1392. Nanobioplar electrodeposition in nanoparticle arrays for tunable optical materials. **G. Crouch**, D. Han, S. Fullerton, D. Go, P.W. Bohm

2:50 Intermission.

3:00 1393. Impact of natural organic ligands structure on the colloidal stability of silver nanoparticles. **K. Afshinnia**, M. Baalousha

3:20 1394. Oil separation from water under environmentally relevant conditions using polymer-coated iron oxide nanoparticles. **S. Mirshahghassemi**, J. Lead

3:40 1395. Ultrathin nanowires of Mo₆Te₆ grown by chemical vapor deposition. **J.E. Johns**, Y. Yoo, J. Jeong

4:00 1396. Structural characterization and sulfide oxidation of V-DTPA immobilized on mesoporous silica. **J.R. Taft**, C.C. Landry

Section I

Ernest N. Morial Convention Center
Rooms 340/341

Chemistry of Materials: Materials for Energy & Catalytic Applications

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

1:30 1397. Synthetic manipulation of hybrid thermoelectric materials. **K.A. Mazzi**, M. Raja Thulasimani, B. Ryll, D. Kojda, K. Habicht, S. Raoux

1:50 1398. Bismuth chalcogenides as earth-abundant and non-toxic photovoltaics. **A. Ganose**, K. Butler, A. Walsh, D. Scanlon

2:10 1399. Structured Si/Co-P photocathodes: Designs for efficient light absorption in earth abundant solar fuels devices. **P. Kempler**, M. Gonzalez, K. Papadantonakis, N.S. Lewis

2:30 1400. Quantum dot nucleation and the future of LED lighting. **M.P. Campos**, L. Hamachi, M.P. Hendricks, I. Rreza, J. De Roo, J.S. Owen

2:50 Intermission.

3:05 1401. Sequential series multijunction dye-sensitized solar cells (SSM-DSCs): Concept, optimizations and novel applications. **H. Cheema**, J.H. Delcamp

3:20 1402. (Photo)electrocatalytic properties of copper gallium delafossite nanoflakes. **Y. Mao**, S. Mohan

3:40 1403. Ultrathin metal/semiconductor nanosheets for photocatalytic oxidation of alcohols and H₂ evolution. **G. Han**, Y. Sun
4:00 1404. Photocatalytic degradation of low concentration toluene by atomically platinum dispersed nanoporous TiO₂ film with exposed {001} facets. **H. Zheng**, T. Xu, P. Zhang

Section J

Ernest N. Morial Convention Center
Room 212

Organometallic Chemistry: Catalysis-Late Transition Metals

N. S. Radu, *Organizer*

B. P. Carrow, E. A. Ison, *Presiding*

1:30 1405. Synthesis and reactivity studies of a [Cp*Rh] monohydride. **E. Boyd**, K.V. Prather, D. Lionetti, J.D. Blakemore

1:50 1406. Mechanism of the Tishchenko reaction catalyzed by an octahedral d⁶-rhodium dihydride catalyst. **J. Mallah**, **F. Hasanayn**

2:10 1407. Azaphosphatriptycene in rhodium-catalyzed hydroformylation.

Y. Cao, J. Napoline, J. Bacsaj, J.P. Sadighi

2:30 1408. Pentamethylcyclopentadiene as a ligand in rhodium-catalyzed hydrogen evolution. **Y. Peng**, D. Lionetti, J.D. Blakemore

2:50 1409. Insights into catalytically active rhodium complexes. **D. Selent**, C. Kubis, A. Boerner, W. Baumann, K. Neymeyr, M. Sawall, H. Schroeder

3:10 1410. Rhodium complexes ligated by an unconjugated bipyridine analogue: Electronic properties and effects on H₂ evolution reactivity. **D. Lionetti**, V. Day, J.D. Blakemore

3:30 1411. Nickel dipyrin imides capable of C–H bond amination. **Y. Dong**, T. Betley

3:50 1412. Through-space ligand effects on reaction rate and selectivity in gold(acyclic diaminecarbene)-catalyzed organic transformations. **A.A. Ruch**, J.K. Nguyen, M.C. Ellison, **L.M. Slaughter**

4:10 1413. Non-covalent interactions in rhenium oxo/nitrido frustrated Lewis pairs. **E.A. Ison**, N.S. Lambic

4:30 1414. Selective reduction of CO₂: A rational thermodynamic approach to disfavor proton reduction pathways. **D.W. Cunningham**, J.Y. Yang

4:50 1415. Unstable boronic acid and pinacol ester cross-coupling enabled by an “on-cycle” precatalyst. **B.P. Carrow**

5:10 1416. Catalytic N-formylation of amines using CO₂ and H₂. **U. Jayarathne**, N. Hazari, W.H. Bernskoetter

Section K

Ernest N. Morial Convention Center
Room 335

Chemistry of Materials: Metal Organic Frameworks

C. G. Lugmair, *Organizer*

T. Gadzikwa, Q. Zhang, *Presiding*

1:30 1417. Synthesis and characterization of high valence metal phosphonate metal-organic frameworks. **D.B. Barbee**, A.R. Barron

1:50 1418. Bio-template synthesis of zeolitic imidazolate framework-8 (ZIF-8). **Q. Wang**, H. Qin, H. Zhou

2:10 1419. Phase-purity and size control of NU-1000. **T. Webber**, S. Bingham, R. Combs, W. Liu, S.P. Desai, C. Lu, D.G. Truhlar, R. Penn

2:30 1420. Precise control of the pore hydrophilicity enabled by post-synthetic cation exchange in a metal-organic framework. **A.M. Wright**, A.J. Rieth, M. Dinca

2:50 1421. Synthesis and applications of hierarchically structured metal-organic frameworks. **Y. Yue**, S. Armentrout

3:10 Intermission.

3:25 1422. Some general considerations made for controlled guest materials formation in the confined environments of metal-organic frameworks. **T. Wang**, S.K. Smoukov, A.K. Cheetham

3:45 1423. Topological transformation of luminescent metal-organic frameworks. **Q. Zhang**

4:05 1424. Synthetic strategies for constructing enzyme-inspired metal-organic framework materials. **T. Gadzikwa**, C.S. Satterfield, K.P. Samarakoon, M.C. McCoy

4:25 1425. *Quo vadis niobium?* Multifaceted coordination behavior of MOF-5. **M.D. Korzynski**, L. Braglia, E. Borfecchia, A. Baldansuren, C.H. Hendon, C. Lamberti, M. Dinca

4:45 1426. Cross-linking Zr-based metal-organic polyhedra via postsynthetic polymerization. **D. Nam**, J. Huh, J. Lee, J. Kwak, H. Jeong, K. Choi, W. Choe

Celebrating Over Four Decades of Research in Nanomaterials & Commercialization: Symposium in honor of Kenneth Klabunde

Sponsored by I&EC, Cosponsored by INOR[‡]

Radiopharmaceutical Chemistry

Sponsored by FLUO, Cosponsored by INOR[‡], MEDI[‡] and NUCL[‡]

Molecular Processes at Mineral-Water Interfaces: Linking Theory & Experiments

Uranium Incorporation: Sulfate Mineral Geochemistry

Sponsored by GEOC, Cosponsored by ENVR and INOR

Catalytic Conversion of Biomass Derived Molecules to Chemicals & Fuels

Sponsored by CATL, Cosponsored by ENFL, ENVR and INOR

Theoretical & Experimental Studies of Supercritical Fluids in the Subsurface

Sponsored by GEOC, Cosponsored by ENVR and INOR

Control of Zeolite Structure, Composition & Sites for Catalysis

Sponsored by CATL, Cosponsored by INOR