

INOR
DIVISION OF INORGANIC
CHEMISTRY

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

SUNDAY MORNING

Section A

Venue

Placeholder

Harry Gray Award for Creative Work in Inorganic Chemistry by a Young Investigator: Symposium in honor of Nilay Hazari W. H. Bernskoetter, A. Valentine, Organizers J. E. Bercaw, Presiding

9:00 . Towards a thermochemical hydrogen-affinity scale for oxide materials, and its implications in reactivity and catalysis. **J.M. Mayer, J. Peper, J. Lora, S. Laga, D. Damatov, C. Valdez, J. Peng, B. Broudy**

9:25 . Bonding in pentalene complexes and their recent applications. **J.C. Green**

9:50 . Small molecule activation with molybdenum complexes supported by diphosphine-arene ligands. **T. Agapie**

10:15 intermission.

10:25 . Reversible C-H bond cleavage in the formation of cationic iridium alkoxycarbenes from ethers. **N.D. Schley**

10:50 . Siderophore-Promoted release of titanium(IV) from metal oxide materials. **A. Valentine**

11:15 . Electronic structures of diplatinum complexes. **H.B. Gray**

11:40 . Near-miss synthesis of a noble gas compound in 1933: Could it have been Harry Gray award-worthy?. **J.A. Labinger**

Section B

Venue

Placeholder

Celebrating 60 Years of the Division of Inorganic Chemistry

The early days of the Division of Inorganic Chemistry (DIC)

M. J. Clarke, *Organizer* D. C. Crans, *Organizer, Presiding* T. J. Marks, A. P. Sattelberger, *Presiding*

8:30 Introductory Remarks.

8:40 . Sixty years of inorganic chemistry. **H.B. Gray**

9:10 . Synthesis and properties of selected transition metal complexes over half a century - a retrospective. **S.J. Lippard**

9:40 . My experiences inside the Division of Inorganic Chemistry.

D.J. Nelson 10:10

Intermission.

10:25 . Inorganic and supramolecular pincer chemistry. **K. Bowman-James**

10:55 . Whither goest inorganic chemistry: What goes around, comes around. **R. Eisenberg**

11:25 . How the Division of Inorganic Chemistry brought the ACS into the 21st Century: E-

Lectons and the DIC's first ChemLuminary Award. **M.J. Clarke**

Section C

Venue

Placeholder

Undergraduate Research at the Frontiers of Inorganic Chemistry Coordination Chemistry A. K. Bentley, C. Nataro, S. R. Smith, Organizers B. B. Sears, Presiding

9:00 Introductory Remarks.

9:05 . Selective f-element extraction utilizing tripodal CMPO ligands. **E.J. Werner, S.M. Biros,**

M. Patterson, A.K. Mulville, E.K. Connor

9:25 . N-heterocyclic thione and selones: New tricks for old dogs. **D. Rabinovich**

9:45 . Exploring the reactivity of hexaphenylcarbodiphosphorane with electron-deficient metallic species. **G. Risica, C.D. Abernethy, M. Findlater**

10:05 . Structure and properties of coordination polymers containing conformationally flexible dipyritylamide ligands: An introductory undergraduate research program at Lyman Briggs College at Michigan State University. **R.L. Laduca, T.A. Beard, J.Z. Travis**

10:25 Intermission.

10:40 . Ligand replacement on 1D and 2D coordination polymers. **B.J. Johnson, M. Johnson, N.**

Beattie

11:00 . Synthesis, electronic structure, and reactivity of iron complexes bearing donor-modified BIAN ligands. **H.M. Hoyt, G.N. Tran, C.C. Cody, M. Takemura, L. Darko, A. Volkov, E.Y. Martinez, W.R. Fuller, J.M. Darmon, C.E. Schulz, K.A. Wheeler**

11:20 . Synthesis and characterization of cobalt(II) SNS pincer model complexes for liver alcohol dehydrogenase. **J.R. Miecznikowski, S. Bonitatibus, J. Jasinski, L. Li**

11:40 . Peptoid ligands: Bioinspired chelators for lanthanide and actinide complexation. **A.**

Ricano, I. Captain, G. Deblonde, R.J. Abergel

Section D

Venue

Placeholder

ACS Award in Inorganic Chemistry: Symposium in honor of Lawrence Que, Jr.

M. J. Maroney, E. L. Que, *Organizers*

T. A. Jackson, J. Kovacs, *Presiding*

8:30 Introductory Remarks.

8:35 . Diiron enzymes in antibiotic biosynthesis: Similar metal centers - different chemistry. **A.J.**

Komor, C.J. Knot, A. Jasniewski, B.S. Rivard, L. Que, **J.D. Lipscomb**

9:00 . Mössbauer, EPR and DFT studies of Fe(V)=O, Fe(IV)Fe(IV) and Fe(III)Fe(IV) complexes of biological relevance. **E. Munck**

9:25 . Metal selectivity in nickel trafficking proteins. **M.J. Maroney, C.E. Carr, H.Q. Hu, H. Huang, R.C. Johnson, S.L. Ciurli, D.S. Merrell**

9:50 . DNA repair glycosylase MUTYH: From Fe-S clusters to MAP. **S.S. David**

10:15 Intermission.

10:30 . Mechanistic enzymology of tryptophan oxidizing enzymes. **A. Liu**

10:55 . Gallium complexes targeting FepA: An inorganic approach to fighting antimicrobial resistance. **V.C. Pierre**

11:20 . Metal scaffolds for biological sensing using ¹⁹F magnetic resonance imaging. **E.L. Que**

11:40 . Spectroscopic and kinetic studies of a bifunctional α -ketoglutarate dependent non-heme iron enzyme, AsqJ. **Y. Guo, J. Li, J. Lee, J. Dicks, R. Fan, W. Chang**

12:00 . Developing x-ray spectroscopic toolkits for mechanistic studies of cobalt and nickel catalysts. **F. Li**

Section E

Venue

Placeholder

Inorganic Nanomaterials: Structure & Function in 0, 1 & 2 Dimensions

Financially supported by Chemistry of Materials

E. J. McLaurin, *Organizer*

K. R. Kittilstved, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 . Mechanistic investigations of colloidal metal chalcogenide nucleation and growth. **J.S. Owen, M.P. Campos, I. Rreza**

9:05 . Germanium alloy nanocrystals and hollow spheres prepared via colloidal synthesis. **S.**

Kauzlarich, K. Tabatabaei, K.A. Newton, X. Qi

9:35 . Inorganic-Capped luminescent InP nanocrystals. **E.J. McLaurin**

10:05 Intermission.

10:20 . High throughput nanomaterial synthesis and its application to technology. **G.F. Strouse 10:50** .

Design of multi-functional nanocrystal membranes and the fabrication of thin film nanocrystal devices. **C.B.**

Murray, Y. wu, N. Gogotsi, T. Zhao, N.J. Greybush, D. Straus, D. Jishkariani, K.C. Elbert, C.R. Kagan

11:20 . Dislocation-Driven growth of 1D, 2D and 3D nanomaterials and the applications in lead halide perovskite nanostructures. **S. Jin, Y. Fu**

11:50 . Synthesis of magnetic semiconductor nanostructures. **S.L. Stoll**

Section F

Venue

Placeholder

Sustainability in Electrocatalytic Fuel & Chemical Production

Cosponsored by CATL

L. A. Berben, J. L. Dempsey, *Organizers*

V. Thoi, *Presiding*

8:30 Introductory Remarks.

8:35 . Why is Ni(cyclam)²⁺ a better CO₂ reduction catalyst when supported on a mercury surface? B. Rudshteyn, Y. Wu, J. Froehlich, A. Zhanaidarova, W. Ding, V.S. Batista, **C.P.**

Kubiak

9:00 . Engineered biomolecular electrocatalysts for hydrogen evolution from water. **K. Bren, Y. Guo, B. Kandemir, V. Fourmond**

9:25 . Paired electrochemical reactions: A lesson learned from microelectrode arrays and the onsite generation of chemical reagents. **K.D. Moeller**

9:50 . Promoting selective electrocatalytic carbon dioxide reduction through modification of a metal's secondary and outer coordination spheres. **C.C. McCrory**

10:15 . Towards electrocatalytic reduction of carbon dioxide to methanol: Adventures in hydricity. **E.S. Wiedner, S.A. Burgess, M.J. Wilding, D.L. Miller, M. Helm, J.C. Linehan, A.M.**

Appel

10:40 Intermission.

10:55 . Mechanistic details of CO₂ reduction processes revealed by pulse radiolysis with timeresolved infrared detection. **D.C. Grills, K.T. Ngo, J.J. Rochford**

11:20 . Rational design of catalysts for fuel generation: Controlling the secondary coordination sphere. **D.J.**

Harrison, E. Jarvis, Z.R. Relethford,
C.A. Caputo

11:40 . Mechanistic insight into the cleavage and coupling of CO with molybdenum complexes:

Toward upgrading oxygenated C₁ precursors. **T. Agapie**

12:05 . H₂ Evolution by Metal Chalcogenide Coordination Polymers, Highly Active Molecular Models of [NiFe] Hydrogenases. **S.C. Marinescu**

Section G

Venue

Placeholder

F. Albert Cotton Award in Synthetic Inorganic Chemistry: Symposium in honor of Pingyun Feng

X. Bu, q. Zhang, D. Zhao, *Organizers*
P. Yang, N. Zheng, *Organizers*,
Presiding

8:30 . Pingyun Feng – the quintessence of synthetic materials chemistry. **G.D. Stucky**

9:00 . Nanostructured and single phase thermoelectrics. **M.G. Kanatzidis**

9:20 . Interfacial assembly and engineering of ordered functional mesoporous materials. **D. Zhao**

9:40 . Sol-gel assembly of metal chalcogenide nanoparticles into multicomponent architectures. J. Davis, **S. Brock**

10:00 Intermission.

10:30 . Oxygen evolution reaction electrocatalysis: Redefining intrinsic activity trends and illustrating design principles. **S.W. Boettcher**

10:50 . Synthesis and applications of conducting polymer nanofibers. **R.B. Kaner**, W.H. Mak,

C. Lin, R. Li, D. Maung, X.W. Huang, K. Wang, Y. Wang, T. Farrell

11:10 . Design and synthesis of novel porous materials for energy and environmental applications. **T.M. Nenoff**

11:30 . Synthesis and substitution chemistry of complex bismuth sulfide iodides in sulfur/iodine melts. R.A. Groom, **S.E. Latturmer**

11:50 . Spark plasma sintering of Zintl phases. **S. Kauzlarich**, E.L. Kunz Wille, J. Cooley, D. Barrett, N. Grewal

Section H **Bioinorganic Chemistry**

Proteins & Enzymes & Model Systems

S. A. Koch, *Organizer*

M. Knapp, F. Li, *Presiding*

8:00 . Theoretical studies of the mechanism of the second half-reaction step of nitric oxide synthase:

Nondynamical electron correlation drives the reaction to the intended products. **I. Shamovsky**, G. Belfield,

R. Lewis, F. Narjes, L. Ripa, C. Tyrchan, L. Öberg, P. Sjö

8:20 . Proton-facilitated transformations of molybdenum-oxo compounds as synthetic models for molybdoenzymes. **F. Li**

8:40 . Metal capture and sensing in porous polymers for disease and environmental diagnostics.

S. Lee, G. Barin, J.R. Long, C.J. Chang

9:00 . Mechanistic investigations of guest binding in a self-assembled Ga₄L₄ host reveals the first example of a conformational selection mechanism in a synthetic host. **C.M. Hong**, D.M. Kaphan, D. Toste, K.N. Raymond, R.G. Bergman

9:20 . Engineering the alpha-ketoglutarate oxygenase FIH for alternate rebound chemistry. **M. Knapp**

9:40 . Urease inhibitors: In search for a key to control a nickel-enzyme. **S.L. Ciarli**

10:00 Intermission.

10:10 . Iron-assisted CO₂ activation at a nickel center. **C. Yoo**, Y. Lee

10:30 . Mechanistic, structural and computational studies of the catalytic multifunctional hemoglobin dehaloperoxidase from *Amphitrite ornata*. **R.A. Ghiladi**, L.M. Carey, N.L. McCombs

10:50 . Mechanistic nuances of hydrogen atom abstraction by the copper(III)-hydroxide unit. **D. Dhar**, G.M. Yee, J.M. Mayer, C.J. Cramer, W.B. Tolman

11:10 . Structure-function studies of tetranuclear iron clusters with a variable interstitial μ_4 -atom as models of biological active sites. **C. Reed**, T. Agapie

11:30 . Bio-inspired nonheme iron catalyst: Electrophilic versus nucleophilic iron-based active oxidant – effect on alkane hydroxylation. **S. Kal**, L. Que

11:50 . Over and under: Fe-HNO vs. H-Fe-NO formation from hydride attack at ferric nitrosyl porphyrins. **E.G. Abucayon**, R.L. Khade, D.R. Powell, M.J. Shaw, Y. Zhang, G.B. RichterAddo

Section I

Venue

Placeholder

Chemistry of Materials: Materials for Energy & Catalytic Applications

C. G. Lugmair, *Organizer*

X. Chen, M. V. Sheridan, *Presiding*

8:30 . Polydiacetylene-(phen)Ru(bpy)₂ for cofactor regeneration and CO₂ reduction as an artificial photocatalytic system. **J. Kim**, S. Kim, T. Anjong, H. Lee

8:50 . Bismuth-based double perovskites for non-toxic photovoltaics. **A. Slavney**, T. Hu, A. Lindenberg, H. Karunadasa

9:10 . Three-dimensional graphene nanoribbon-based materials and its applications. **T. Yi**

9:30 . Pulsed-laser synthesis of advanced nanomaterials for water-oxidation catalysis and sunlight capture. **A.M. Mueller**, J.R. Winkler, H.B. Gray

9:50 . Metal chalcogenide coordination polymers as catalysts for the hydrogen evolution reaction. **C.A. Downes**, S. Marinescu

10:10 Intermission.

10:25 . All-in-one, derivatized tandem p⁺n-Si/SnO₂@TiO₂ water splitting device. **M.V. Sheridan**, T.J. Meyer

10:45 . General strategy for electrocatalytic hydrogen production integrated with oxidative organic upgrading. **Y. Sun**

11:05 . Chemically tailoring two-dimensional transition metal dichalcogenides. **X. Chen**, A.R. McDonald

11:25 . Polydopamine coatings for stabilizing the interface between cobalt-based water oxidation catalysts and electrode. **I. Kim**, Y. Nam

Section J

Coordination Chemistry: Synthesis & Characterization

S. A. Koch, *Organizer*

P. Yin, *Presiding*

8:30 . Electron hopping through double-exchange coupling in a mixed-valence diiminobenzoquinone-bridged Fe₂ complex. **A. Gaudette**, I. Jeon, J.S. Anderson, G.J. Long, F.

Grandjean, D. Harris

8:50 . Enhancement of magnetic anisotropy in a heterobimetallic Mn-Bi complex. **T. Pearson**,

M. Fataftah, D.E. Freedman

9:10 . Redox series of gallium complexes: Characterization of four oxidation states and electrocatalytic hydrogen production by a Ga(III) complex in water. **A. Arnold**, L.A. Berben

9:30 . Self-assembly processes: Connected spherical nano-sized supramolecules. **B. Krämer**, M. Scheer

9:50 . Host-guest systems: Encapsulation of various templates by self-assembled supramolecules. **H. Brake**, M. Scheer

10:10 Intermission.

10:20 . X-ray and neutron scattering study of the formation of giant molecular metal oxide clusters. **P. Yin**

10:40 . Cobalt supramolecular triple-stranded helicate-based discrete molecular cage. **H. Yoo**

11:00 . Synthesis, structure, and substitution reactivity of trinuclear molybdenum cluster compounds. **J.R. Houston**

11:20 . Accessing a copper(III)-alkylperoxo complex. **B.D. Neisen**, D. Dhar, N.L. Gagnon, W.B. Tolman

11:40 . Enhanced magnetic anisotropy and single-molecule magnet behavior in tetranuclear clusters featuring low-coordinate cobalt centers. **K. Chakarawet**, P. Bunting, J.R. Long

Section K

Venue

Placeholder

Lanthanide & Actinide Chemistry
Cosponsored by WCC

A. De Bettencourt Dias, *Organizer*

B. E. Cohen, L. Doerr, J. Monteiro, *Presiding*

8:30 . Comparing molecular and band-based approaches to the antenna effect in lanthanide coordination polymers. **J. Einkauff**, D.T. de Lill

8:50 . Thiophene-based lanthanide complexes as photosensitizers for singlet oxygen generation.

M.A. Gracia-Nava, A. De Bettencourt Dias

9:10 . Broadband porphyrin dyes for near-infrared emission of lanthanide ions. R.W. Arachchi, A. Kukoyi, **H. He**

9:30 . Lanthanide complexes of fluorinated alkoxy ligands. J. Weber, C. Kotyk, A.T. Royappa, A.L. Rheingold, **L. Doerr**

9:50 Intermission.

10:00 . Lanthanide-doped nanocrystals engineered for low fluence multiphoton imaging. **B.E. Cohen**, B. Tan, A. Fernandez-Bravo, E. Chan, P. Schuck

10:20 . Template-directed synthesis of actinide nanoparticles. **A. Herve**, A. Braun, S. Alayoglu,

C. Booth, D. Olive, M. Straub, S.G. Minasian

10:40 . Challenges in the design of luminescent markers and cation sensors based on lanthanide complexes. **J. Monteiro**, D. Tapia, A. De Bettencourt Dias

11:00 . Comparison of Li with K and Na in rare-earth metal reduction chemistry: Isolation of [Li(2.2.2-cryptand)]⁺ in unique coordination environments. **D.N. Huh**, J.W. Ziller, W.J. Evans **11:20** Intermission.

11:30 . New vistas in organometallic actinide chemistry. **J.K. Pagano**, K. Erickson, J. Xie, D.E. Morris, B. Scott,

R. Wu, L. Gagliardi, R. Waterman, J.L. Kiplinger

11:50 . Investigations of the electronic structure of actinide-aluminum bimetallics: Synthesis, reactivity and XAS characterization of actinide-alanate molecules and other actinide-aluminum materials. **A.B. Altman**, A. Brown, J. Arnold, S.G. Minasian, S. Pemmaraju, D. Prendergast,

D.K. Shuh, T. Tylliszczak, D. Vine

12:10 . Synthesis and reactivity of a homoleptic uranium(III) tris(aryl) complex. **M. Boreen**, B. Parker, T.D. Lohrey, J. Arnold

Section L

Organometallic Chemistry:

Catalysis N. S. Radu, Organizer A. Poater, Presiding

8:30 . Evolution of reactivity of olefin metathesis of Ru, and a step forward to other metals. **A. Poater**

Poater

8:50 . Ruthenium-based olefin metathesis: Insight into catalyst decomposition. **G.G. Lavoie**, T.G. Larocque, A.C. Badaj

9:10 . Synthesis, structure and characterization of new ruthenium(II) complexes and their catalytic activities towards selective C-O bond formation via activation of terminal alkynes. **R.K. Jena**, M. Bhattacharjee

Jena, M. Bhattacharjee

9:30 . Catalytic upgrading of ethanol to butanol: Mechanistic insights. **H. Aitchison**, D. Wass, R. Wingad

Wingad

9:50 . CO₂ and formic acid, a winning couple in reduction chemistry. **T. Cantat**

10:10 . Mechanistic studies of oxidative arene vinylation catalyzed by late transition metals.

B.A. Vaughan, S.K. Khani, J.B. Gary, J.D. Kammert, J. Chen, M.S. Webster-Gardiner, B.A. McKeown, R.J. Davis, T.R. Cundari, T.B. Gunnoe

10:30 . Mechanistic study of thermal oxidative addition of si-h bond to mixed n-heterocyclic carbene oxazolonylborato rhodium bis(carbonyl) complex. **A. Biswas**

10:50 . Cationic rhenium(III) complexes: Synthesis, characterization, and reactivity for catalytic hydrosilylation of aldehydes. **D.E. Perez**, E.A. Ison

11:10 . Rh-catalyzed C-H cyanation of imidazopyridine using N-cyano-N-phenyl-pmethylbenzenesulfonamide as the cyano source. X. Shen, J. Qu, C. Liu, Y. Guo, **X. Zhu**, X. Hao, M. Song

11:30 . Mechanistic studies of Rh(diphosphine)-catalyzed methanol reductive carbonylation. **S. Chotchatchawankul**, C.R. Landis

Section M

Venue

Placeholder

Organometallic Chemistry: New Ligand Platforms

N. S. Radu, *Organizer*

R. Blanski, D. Mendoza-Espinosa, *Presiding*

8:30 . Bicyclic (alkyl)(amino)carbenes (BicAACs): Introducing the first of a new family of stable carbenes. **E. Tomas Gonzalez de Mendivil**, M.M. Hansmann, r. jazzar, M. Melaimi, G. Bertrand

8:50 . Imidazolin-2-ylidenaminophosphines: A highly electron-rich phosphorus(III) superbase that splits CO₂. **P. Mehlmann**, F. Dielmann

9:10 . Coordination chemistry of a hybrid NHC-MIC biscarbene proligand. **D. MendozaEspinosa**

9:30 . New class of N-heterocyclic carbenes featuring closo-carborane anions. **S. Lee**, V. Lavallo

9:50 . Highly functionalized N-heterocyclic carbenes bearing icosahedral carborane anions. **S.G. McArthur**

10:10 . Chiral acyclic diaminocarbene gold complexes as catalysts for enantioselective intramolecular hydroamination of allenes: Systematic study of ligand substituent effects on enantioselectivities. **A. Ruch**, V. Nesterov, L.M. Slaughter

10:30 Intermission.

10:40 . Synthesis of backfunctionalized imidazolinium salts and NHC carbene complexes. **R. Blanski**, H. Phan, R.H. Grubbs

11:00 . Novel phosphine ligand with NH linker for ligand cooperative catalysis. **K. Ding**, L. Alhthol, D. Tyer, S. Xu

11:20 . Mono/di/tri-phosphine complexes of transition metals based on tris(3-methyl-1H-indol-2yl)methane as a model system for the study of apical metal-H-C_{sp3} interactions. **E. Smirnova**, J. Lloret-Fillol

11:40 . Synthesis of Co and Mo hydroxycyclopentadienyl complexes and their catalytic activities in transfer hydrogenation. **W. Wu**, R.M. Waymouth, T. Seki, D. Solis, K. Nozaki, H. Ando, S. Kusumoto

12:00 . P-P bond formation via unique metal-ligand cooperation. **Y. Kim**, Y. Lee **Multicenter Molecules & Coupled Molecular Assemblies: Synthesis, Characterization & Theory**

Experimental Characterization

Sponsored by PHYS, Cosponsored by INOR

LGBT Graduate & Postdoctoral Student Chemistry Research Symposium

Emerging Applications in Inorganic Chemistry: Energy, Materials, Catalysis, & Spectroscopy

Sponsored by PROF, Cosponsored by ANYL[‡], BIOL[‡], CHED, CMA, COLL, COMP, CWD,

ENVR, INOR[‡], MEDI, MPPG, ORGN, PHYS, PMSE[‡], POLY, PRES[‡] and WCC

Synthesis of Catalysts by Non-Traditional Methods

Nanoparticle Catalysts

Sponsored by CATL, Cosponsored by COLL and INOR

Deposition & Etching of Nanostructures

Sponsored by COLL, Cosponsored by INOR

SUNDAY AFTERNOON

Section A

Venue

Placeholder

Harry Gray Award for Creative Work in Inorganic Chemistry by a Young Investigator: Symposium in honor of Nilay Hazari W. H. Bernskoetter, A. Valentine, Organizers A. Hazari, Presiding

1:30 . Operando NMR studies of hydroformylation. **C.R. Landis**, A. Brezny

1:55 . Lewis acid additives in organotransition metal chemistry. **G. Dobereiner**

2:20 . Gold(III) catalyst design for alkene and alkyne functionalization reactions. **A. Nova**

2:45 intermission.

2:55 . Lewis acid-transition metal promoted carbon dioxide functionalization. **W.H. Bernskoetter**, D. Jin

3:20 . Proton-Assisted Reduction of CO₂ by Cobalt Aminopyridine Complexes. **S.C. Marinescu**, A. Chapovetsky

3:45 . Catalytic hydrogenolysis of carbon oxygen bonds. **D.M. Heinekey**,

K.I. Goldberg, J.M. Goldberg, L.M. Guard, T. Lekich

4:10 . Molecular catalysts for water oxidation. **G.W. Brudvig**, R.H. Crabtree, S.B. Sinha, D.Y.

Shopov, L.S. Sharninghausen, T. Michaelos, H. Lant, K. Fisher

Section B

Venue

Placeholder

Celebrating 60 Years of the Division of Inorganic Chemistry

The Next Decades: 1990'es & 2000'es M. J. Clarke, D. C. Crans, Organizers B. E. Bursten, S. Ronco, M. Scott, Presiding

1:30 Introductory Remarks.

1:35 . From siderophores to supermolecules, fifty years of coordination chemistry. **K.N. Raymond**

2:05 . Electrochemically-promoted catalytic asymmetric hydrogenation using chiral organorhodium complexes. **B.T. Donovan-Merkert**

2:35 . Solid state chemistry, Zintl phases, and the Division of Inorganic Chemistry. **S. Kauzlarich**

3:05 . Surface chemistry of II-VI nanoplatelets and nanoribbons. Y. Zhou, Y. Yao, C. Morrison, **W.E. Buhro**

3:35 intermission.

3:50 . Antimony(V) Lewis acids: Applications in anion sensing and small molecule activation. **F.P. Gabbai**

4:20 . Metalloprotein design: Examination of mononuclear redox centers. **V.L. Pecoraro**, A. Tebo, K. Koebke

4:50 . Synthesis of new bismuth based materials. J. Walsh, S.M. Clarke, **D.E. Freedman**

5:20 . Celebrating 60 Years - Inorganic chemistry at the National Science Foundation. **C.A.**

Bessel

Section C

Venue

Placeholder

Undergraduate Research at the Frontiers of Inorganic Chemistry Organometallic Chemistry

A. K. Bentley, C. Nataro, S. R. Smith, *Organizers*

A. Johnson, *Presiding*

1:30 . Synthesis and reactivity of compounds containing a κ^3 -1,1'-bis(diphenylphosphino)ferrocene ligand. **K. Cabrera**, C. Nataro

1:50 . Synthesis and characterization of antimony(V) Lewis Acids. **N. Capra**, A.M. Christianson, F.P. Gabbai

2:10 . Heterogeneous and homogeneous phosphonothioate alcoholysis by supported molybdenum-peroxo complexes. **L.Y. Kuo**, A. Bennett

2:30 . Evaluating the role of linker flexibility in base-free transfer hydrogenation of aldehydes and ketones catalyzed by Cp*Ir(pyridinesulfonamide)Cl complexes. **T.M. Townsend**, A.R. O'Connor

2:50 . Alkane functionalization with (dm^{pe}box)Ir(OAc)₂(OH)₂. **Z.H. Syed**, A.M. Wright, S.B. Rubashkin, K.I. Goldberg

3:10 Intermission.

3:25 . Group VI metal complexes of tris(diisopropylphosphinomethyl)phenylborate. **P.J.**

Fischer, S. Senthil, J.T. Stephan, M.D. Storlie, M.L. Swift, V.G. Young, Jr.

3:45 Reactivity of titanium-aluminum heterobimetallics. **A. Brown**, A.B. Altman, S. Hohloch,

T.D. Lohrey, S.G. Minasian, J. Arnold

4:05 . Palladium complexes of amine bis(phenolate) ligands: Complex isolation and catalytic evaluation. E. Collins, B.J. Graziano, A.K. Bowser, **B. Wile**

4:25 . Synthesis, reactivity, and catalytic applications of isolable NHC-CuCF₂H complexes. **S.**

Kariofillis, J.R. Bour, M.S. Sanford
Section D

Venue

Placeholder

ACS Award in Inorganic Chemistry: Symposium in honor of Lawrence Que, Jr.

M. J. Maroney, *Organizer*

E. L. Que, *Organizer, Presiding*

F. Li, *Presiding*

1:30 Introductory Remarks.

1:35 . Rational design of biologically inspired catalysts for selective oxidation reactions. **M. Costas**, J. Serrano Plana, O. Cussó, a. company, M. Milan

2:00 . Biomimetic metal-oxygen intermediates in dioxygen activation chemistry. **W. Nam**

2:25 . Spectroscopic, and/or crystallographic characterization of metastable intermediates involved in cysteine-ligated non-heme iron-promoted reaction mechanisms. M.N. Blakely, M.A. Dedushko, A.S. Ganas, G. Villar-Acevedo, P. Lugo-Mas, **J. Kovacs** **2:50** . High valent metal oxo

and nitrene cores in chemistry and biology. **K. Ray**

3:15 Intermission.

3:30 . Catching transient intermediates in non-heme iron oxidation chemistry with high speed Raman spectroscopy. D. Unjaroen, S. Padamati, j. chen, A. Draksharapu, M. Swart, **W.R. Browne**

3:55 . Insights into metalloenzyme function from bio-inspired manganese complexes. **T.A. Jackson**, D. Rice, A.A. Massie, M. Denler

4:20 . Tuning the reactivity of high-valent nickel-oxygen adducts for hydrocarbon oxidation.

A.R. McDonald

4:40 Relationship between electronic structure and reactivity in nonheme dioxygenase models. **A.T. Fiedler**, A.A. Fischer, S.V. Lindeman

5:00 . Spectroscopic studies and oxidizing reactivity of two high-valent nickel-oxygen species. T. Corona, A. Draksharapu, S. Padamati, F.F. Pfaff, F. Acuña-Parés, V. Martin-Diaconescu, J. Lloret Fillol, K. Ray, **A. Company**

Section E

Venue

Placeholder

Inorganic Nanomaterials: Structure & Function in 0, 1 & 2 Dimensions

Financially supported by Chemistry of Materials

K. R. Kittilstved, E. J. McLaurin, *Organizers*

R. Beaulac, *Presiding*

1:30 . Correlating structure and function in symmetric and asymmetric core/shell optical nanomaterials. **J.A. Hollingsworth**

2:00 . Understanding localized surface plasmon resonance in doped metal oxide nanocrystals.

D.J. Milliron

2:30 . Controlling dopant-defect interactions in doped SrTiO₃ colloidal nanocrystals. **K.R. Kittilstved**

3:00 Intermission.

3:15 . Enhanced Multiple Exciton Generation in PbS/CdS Janus-like Heterostructure Nanocrystals. D. Kroupa, G. Pach, B. Chernomordik, **M.C. Beard**

3:45 . Sample-Transmitted Excitation Photoluminescence (STEP) technique for quantifying the energy flow in nanocrystals and their solids. **M. Zankov**

4:15 . Optical Stark metrology of CdSe nanocrystal quantum dots: On the size-dependence of the oscillator strength. Y. Tang, M. Saniepay, C. Mi, R. Beaulac, **J. McGuire**

Section F

Venue

Placeholder

Sustainability in Electrocatalytic Fuel & Chemical

Production Cosponsored by CATL L. A. Berben, J. L. Dempsey, Organizers E. S. Wiedner, Presiding

1:30 . Use of polyoxometalates as redox-active reservoirs: Towards small molecule activation.

E.M. Matson

1:55 . Iron-thiolate catalysts for photo-electrochemical hydrogen production in organic solvents and water. **F. Gloaguen**

2:20 . Studies of electrocatalytic dioxygen reduction. **J.M. Mayer**, M.L. Pegis, C. Wise, D.J. Martin, S. Rauegi, N. Kumar

2:45 . Observing molecular vibrations of catalytic intermediates at electrode surfaces. **T. Cuk**, S. Pemmaraju, D. Prendergast, X. Chen, M. Waegle, D. Herlihy

3:10 Intermission.

3:25 . Hydricity as an activity descriptor for molecular hydrogen evolution electrocatalysts. **C.**

Tsay, B. Ceballos, D. Cunningham, S. Ruelas, **J.Y. Yang**

3:50 . Solar fuel devices with molecular catalysts – mechanistic insights. **L. Hammarstrom**

4:15 . Designing small molecule electrocatalysts for selective C-H bond formation with CO₂: [Fe₄N(CO)₁₂]⁻, [Fe₄N(CO)₁₂]²⁻, and the role of the hydride intermediate, [H-Fe₄N(CO)₁₂]⁻ in catalysis. N.D. Loewen, A. Taheri, **L.A. Berben**

4:40 . CO₂ splitting into CO and O₂ : From mechanistic studies to efficient electrolyzer. **c.**

cyrille

Section G

Venue

Placeholder

F. Albert Cotton Award in Synthetic Inorganic Chemistry: Symposium in honor of Pingyun Feng

X. Bu, P. Yang, D. Zhao, N. Zheng, *Organizers*

q. Zhang, *Organizer, Presiding*

1:30 . Hybrid nanomaterials for treating resistant cancers. **W. Lin**

1:50 . Dynamic metal-organic frameworks: Design and properties. **X. Bu**

2:10 . Nanostructured and nanoporous materials for energy application. **S.H. Tolbert**

2:30 . Towards robust hierarchical porous metal-organic frameworks. S. Yuan, **H. Zhou** **2:50** . Porous ionic

liquids: Challenges and

opportunities. **S. Dai** **3:10** Intermission.

3:40 . Organometallic chemistry of macrocycles, cages. **G. Jin**

4:00 . Metal-Organic Frameworks (MOFs): Platforms for multifunctional materials. **B. Chen**

4:20 . Luminescent coordination networks: Structure, functionality and applications. W. Liu,

W.P. Lustig, Y. Fang, K. Zhu, **J. Li**

4:40 . Development of metal-organic frameworks as a versatile platform for heterogeneous catalysis. **S. Ma**

Section H

Venue

Placeholder

Spectroscopic Elucidation of Metalloenzyme Mechanism: Current Successes & Future Challenges

Cosponsored by BIOL

Financially supported by Northwestern U, U of California-Davis

V. DeRose, *Organizer*

J. A. Telsler, *Organizer, Presiding*

1:30 . High resolution x-ray spectroscopic studies of soluble methane monooxygenase. **S. DeBeer**

2:00 . Mechanism and control in radical SAM enzymes. **J.B. Broderick**, M. Horitani, A.S. Byer, K.A. Shisler, T. Chandra, R.U. Hutchison, K.S. Duschene, A.R. Marts, W.E. Broderick, B.M. Hoffman

2:30 . Structure of a heme peroxidase compound II. H. Kwon, J. Basran, A.J. Fielding, T.E. Schrader, A. Ostermann, M.P. Blakeley, P.C. Moody, **E. Raven**

3:00 . Vibrational studies of the single turnover reaction cycle and substrate inhibition reaction in denitrifying NO reductases. **P. Moënn-Loccoz**

3:20 Intermission.

3:30 Effects of heme conformation on spin state, spin distribution, and electron transfer in cytochromes. **K. Bren**, J. Kleingardner, B. Kandemir

4:00 . Using biosynthetic models of heteronuclear metalloenzymes for spectroscopic elucidation of their mechanisms in multi-electron processes. **Y. Lu**, A. Bhagi-Damodaran, C. Cui, Y. Yu, J. Reed

4:20 . Developing protein-based model systems to mimic hydrogenase, carbon monoxide dehydrogenase, and acetyl coenzyme A synthase. **H.S. Shafaat**, J.W. Slater, C.R. Schneider, A. Manesis, S.C. Marguet, M.J. Stevenson

4:40 . Biosynthesis of the [FeFe]-hydrogenase active site. **D. Suess**

5:00 . Nitrogen fixation by nitrogenase: The heart of the mechanism. **B.M. Hoffman**

Section I

Venue
Placeholder

2017 Priestley Medalist: Symposium in honor of Tobin J. Marks

Homogeneous Catalysis

Cosponsored by PMSE

Financially supported by Dow-Dow Corning, ExxonMobil, STRENGTH, Argonne National Lab, Northwestern University. **A. Facchetti, Organizer** **T. Lohr, Organizer, Presiding**

1:30 Introductory Remarks.

1:35 . Design and synthesis of phosphine-olefin ligands with planar-chiral metal complex scaffold and application in asymmetric catalysis. **M. Ogasawara**

2:05 . Late stage functionalization of bioactive natural products under catalytic control. **M.R. Gagne** **2:35** . Development of cooperative asymmetric catalysts. **S. Hong** **3:05** Intermission.

3:15 . Catalytic challenges in organoactinide chemistry. **M.S. Eisen**

3:45 . Chemical transformation of dinitrogen mediated by pincer complexes. **S. Schneider**

4:15 . Transition-metal-catalyzed functionalization using carbon dioxide. **Y. Tsuji**

Section J

Venue
Placeholder

ACS Award in Organometallic Chemistry: Symposium in honor of Marcetta Y. Darensbourg C. G. Riordan, Organizer **D. Mason, Organizer, Presiding**

1:30 Introductory Remarks.

1:35 . Insights into the catalytic mechanisms of [FeFe] hydrogenase: Inspiration for the design of molecular catalysts. **W. Lubitz**, A. Adamska-Venkatesh, J.A. Birrell, C. Sommer, S. Rumpel, O.

Rudiger, E. Reijerse

2:00 . Control of the activity of [FeFe]-subsite analogues by interactions of their ligated cyanides. **C. Pickett**, J. Woods

2:25 . Effect of the dithiolate cofactor on the reactivity, spectroscopy, and electrochemistry of models for the [FeFe]-hydrogenases. **T.B. Rauchfuss**, N. Lalaoui, C.P. Richers, M.R. Carlson,

W. Wang

2:50 . Computational modeling of hydrogenases and biomimetic complexes. **M.B. Hall**

3:15 . Effect of the outer coordination sphere on molecular catalysts: A tribute to Marcetta, the hydrogenase whisperer. **W.J. Shaw**, N. Boralugodage, A. Dutta, B. Ginovska, S. Rauegi

3:40 Intermission.

3:55 . Solar fuels science. **H.B. Gray**

4:20 . Hydrogen evolution without metal-hydrides: Ligand-centered HER catalysts with transition metals and non-transition metals. **C.A. Grapperhaus**, A.Z. Haddad, B. Garabato,

R.M. Buchanan, P.M. Kozlowski

4:45 . Pyridine and pyrazine pincer coordination chemistry. **K. Bowman-James**

5:10 . Redox-active ligand complexes in artificial photosynthesis and the reductive side of water splitting. **R. Eisenberg**, G. Li

Section K Venue

Placeholder

Chemistry of Materials: Metal Organic Frameworks

C. G. Lugmair, *Organizer*

I. Kim, T. Runcevski, *Presiding*

1:30 . Effect of different synthesis methods and strategies on the properties of copper based and iron based metal organic frameworks. **A. Yurdusen**, Y. Yurum

1:50 . Redox active metal-organic frameworks with multi-components in order. B. Tu, **Q. Li**

2:10 . Site specific post-modification of Metal-Organic Frameworks (MOFs) via Atomic Layer

Deposition (ALD). **I. Kim**, Z. Li, L.C. Gallington, K.W. Chapman, L. Gagliardi, O.K. Farha,

J.T. Hupp, A.B. Martinson

2:30 . *In Situ* diffraction and spectroscopic studies of metal-organic frameworks under variable temperature and gas pressure. **T. Runcevski**, J.R. Long

2:50 . Coordination polymers featuring coordinatively unsaturated, low-valent metal centers.

D.W. Agnew, J.S. Figueroa

3:10 . General interfacial synthesis route to free-standing metal-organic framework membrane. **Z. Li**, W. Han, K. Yeung

3:30 Intermission.

3:45 . Self-assembled coordination polymer as intermediate in synthesis of porous oxide from bulk metal. **B.**

Chang, J. Chen, I. Tevis, S. Cinar, S. Oyola-Reynoso, G. Rodriguez, A.J. Rossini, M. Thuo

4:05 . Phosphine and arsine coordination materials with well-defined open metal sites: New examples with Pd(II) and Au(I). **S.M. Humphrey**, S.G. Dunning, E. Sikma, J. He

4:25 . POMOFs and POMzites: A family of zeolitic polyoxometalate frameworks from a minimal building block library. **L. Cronin**

4:45 . Coordinative alignment of molecules in chiral metal organic frameworks structure determination of molecules coordinated and aligned in MOFs by single crystal x-ray diffraction.

S. Lee, E.A. Kapustin, O.M. Yaghi

5:05 . Nanocasting in metal-organic framework materials. **A. Stein**, C. Malonzo, Z. Wang, W.

Zhao, T.E. Webber, R. Penn

5:25 . Nomenclature, terminology guidelines, and database issues for topology representations in metal-organic frameworks. **L.R. Ohrstrom**

Section L

Venue

Placeholder

Inorganic Catalysts

S. A. Koch, *Organizer*

J. Blumel, E. V. Rybak-Akimova, *Presiding*

1:30 . Mechanistic investigations of oxygen evolution at a manganese-doped cobalt cubane catalyst. **E.**

Darby, A. Nguyen, S. Gul, J. Yano, T. Tilley

1:50 . Pt NPs ligated by zwitterionic imidazolium-amidates: A notable ligand effect in hydrogenation of carbonyl groups. **L.M. Martínez-Prieto**, B. Chaudret, J. Campora, P.W. van Leeuwen

2:10 . Synthesis and characterization of tin (II) complexes supported by N₂O₂ bis(phenoxy)amine ligands for the ring-opening polymerization of lactide. **S. Praban**, K. Phomphrai

2:30 . Computational study of the vanadium-catalyzed decomposition of alkyl hydroperoxides to ketones. **M. Hermsen**, A. Schmidt, A. Schäfer, T. Schaub

2:50 . Dizinc lactide polymerization catalysts: Hyperactivity by control of ligand conformation and metallic cooperativity. **A.A. Thevenon**, C. Romain, M. Bennington, h. davidson, A. White, S. Brooker, C.K. Williams

3:10 Intermission.

3:20 . One-pot synthesis of double-capped oligoesters using simple metal amides. **P.**

Piromjitpong, K. Phomphrai

3:40 . Mechanism for the oxidation of alcohols by a μ -oxido-diiron(III)bis-phenolato polypyridyl complex. **D. Unjaroen**, a. draksharapu, M. Swart, W.R. Browne

4:00 . Towards inert C–H bond functionalization using main group multiple bonds. **J. Chu**, G.

Menard

4:20 . Immobilized Sonogashira catalyst systems. **J. Blumel**, J.C. Pope

4:40 . Kinetics and mechanisms of hydrocarbon oxidations with H₂O₂/HOAc catalyzed by iron and manganese complexes with rigid aminopyridine ligands. **E.V. Rybak-Akimova**, G. Yang, M. Piquette

Glenn T. Seaborg Award for Nuclear Chemistry: Symposium in honor of David L. Clark

Sponsored by NUCL, Cosponsored by INOR

LGBT Graduate & Postdoctoral Student Chemistry Research Symposium

Novel Reactions, Methodologies & Syntheses in Organic Chemistry

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

Multicenter Molecules & Coupled Molecular Assemblies: Synthesis, Characterization & Theory

Theory & Modeling

Sponsored by PHYS, Cosponsored by INOR

Synthesis of Catalysts by Non-Traditional Methods

Model Catalysts, Microporous Materials & Oxides

Sponsored by CATL, Cosponsored by COLL and INOR

Deposition & Etching of Nanostructures

Sponsored by COLL, Cosponsored by INOR

SUNDAY EVENING

Section A

Venue

Placeholder

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

L. M. Berreau, P. L. Holland, *Organizers*

5:30 - 7:30

- Characterization of a copper(III)-phenoxide complex. **N.L. Gagnon, D. Dhar, W.B. Tolman**
- Probing the effect of ligand electronics on the C-H reactivity of copper-oxygen cores. **C. Elwell, W.B. Tolman**
- Analysis of novel tetradentate zinc catalysts used for the polymerization of rac-lactide. **A.M. Luke, D.E. Stasiw, T. Rosen, M. Kol, W.B. Tolman**
- New strategy for the hydroxylation of strong C-H bonds. **H. Sajjad, W.B. Tolman**
- Mechanistic analysis of the alternating copolymerization of epoxides with cyclic anhydrides utilizing a cocatalyst system. **L.A. Mitchell, M. Fieser, D. Urness, M.J. Sanford, C.R. Dunbar, M. Mandal, C.J. Cramer, G.W. Coates, W.B. Tolman**
- Resonance Raman spectroscopy of copper(III)-hydroxide core and structural implications based on a unified Badger's rule. **A.D. Spaeth, N.L. Gagnon, W.B. Tolman**
- Mechanistic studies of ϵ -caprolactone polymerization by (salen)AlOR complexes and a predictive model for cyclic ester polymerizations. **J.A. Macaranas, A.M. Luke, E.E. Marlier, M. Mandal, D. Marell, C.R. Dunbar, M. Johnson, Y.C. DePorre, M.O. Miranda, B.D. Neisen, C.J. Cramer, M.A. Hillmyer, W.B. Tolman**
- Cu(I) complexes of TBDPhos: Synthesis, structures, and reactivity. **B. Massman, S.R. Daly**

Section A

Venue

Placeholder

ACS Award in Inorganic Chemistry: Symposium in honor of Lawrence Que, Jr.

M. J. Maroney, E. L. Que, *Organizers*

5:30 - 7:30

- Green synthesis of Nd-La doped $\text{Sr}_2\text{Cu}_2\text{Fe}_{28}\text{O}_{46}$ and Nd-La doped $\text{Sr}_2\text{Mg}_2\text{Fe}_{28}\text{O}_{46}$ nanoparticles and comparison their magnetic and microwave absorbing properties with Nd-La doped $\text{Sr}_2\text{CuMgFe}_{28}\text{O}_{46}$ nanoparticles. **p. alimard**
- Characterization of (μ -oxo)heterobimetallic complexes derived from $[\text{Fe}^{\text{IV}}(\text{O})\text{TMC}]$ with Fe

- coordination numbers that depend on ligand topology. **A. Zhou, J. Prakash, G. Rohde, J. Klein, S.T. Kleespies, a. draksharapu, R. Fan, Y. Guo, C.J. Cramer, L. Que**
- Tuning the C—H bond cleavage ability of an oxoiron(IV) complex structural properties of an oxoiron(IV) complex supported by a pentadentate ligand. **W. Rasheed, M. Puri, a. draksharapu, L. Que**
- Inner side of high-valent metal-oxo reactivity. **M. Swart, K. Ray**
- Exploring the H_2O_2 interaction and catalytic activity of mononuclear Cu (II) coordination complexes containing N-rich ligand architecture. **N. SINGH, J. Niklas, O. Poluektov, K.M. Van Heuvelen, A. Mukherjee**
- Two isomers of oxoiron(IV) complex supported by tetramethylcyclam ligand: Interconversion and reactivity. **J. Prakash, J. Klein, a. draksharapu, C.J. Cramer, L. Que**
- Reversible formation of $\text{Fe}^{\text{III}}\text{—O—Ce}^{\text{IV}}$ intermediate from the reaction of $\text{Fe}^{\text{IV}}\text{=O}$ and Ce^{III} . **a. draksharapu, J. Klein, W. Rasheed, C.J. Cramer, L. Que**
- Factors influencing the electronic nature of the active oxidant in a bio-inspired non-heme mononuclear iron catalyst. **S. Kal, S. Iyer, L. Que**
- Modulation of a weakly coupled peroxo-dicopper(II) complex by interaction with alkali metal ions. **L. D'Amore, M. Swart, A. Brinkmeier, F. Meyer**
- Characterization of a novel $\text{Fe}(\text{V})\text{=O}$ species using Mossbauer spectroscopy and Electron Paramagnetic Resonance (EPR) spectroscopy. **R. Fan, J. Serrano Plana, A. Company, W.N. Oloo, L.A. Rueda, K.K. Meier, B. Verdejo, E.V. Garcia-Espana, M.G. Basallote, E.L. Bominaar, Y. Guo, L. Que, M. Costas, E. Munck**
- Roles of $(\text{L})\text{Fe}^{\text{V}}(\text{O})$ and $(\text{L})\text{Fe}^{\text{III}}\text{—OOAc}$ intermediates in bio-inspired C—H and C=C oxidations. Kinetics and spectroscopy. **W.N. Oloo, R. Banerjee, S. Lee, C. Kim, J.D. Lipscomb, L. Que**
- Elucidation of the mechanism of activation of oxygen by iron(II)polypyridylamine complexes in water. **D. Angelone, J. Chen, a. draksharapu, W.R. Browne, M. Swart**
- Elucidation of high-valent species involved in carboxylic acid-assisted nonheme iron catalysis.
- S. Xu, a. draksharapu, W. Ching, L. Que
- HDX-MS reveals metal-specific structural changes important to DNA binding by the cobalt and nickel responsive transcriptional regulator, RcnR. **H. Huang, M.J. Maroney**
- Role of citrate and transferrin in determining Ti(IV) solubility,

bioavailability, and its regulation. **S. Sharma**

- Comparative reactivity studies of peroxomangane(III) intermediates supported by two diazacycloalkane-based tetradentate ligands. **M. Denler, T.A. Jackson, G. Wijeratne**
- O—O bond activation by a series of Mn complexes supported by amide-containing ligands. **J. Parham, G. Wijeratne, T.A. Jackson**
- Metal-Assisted oxygen addition to an Fe(III)-thiolate. **M.N. Blakely, G. Villar-Acevedo, M. Dedushko, W. Kaminsky, J. Kovacs**
- InP based heterostructures: Synthesis, electronic structure, and quantitative comparison of absorption properties. **R. Toufanian, M. Chern, A.M. Dennis**
- Non-Covalent interactions in C-H oxidation reactions by metal-oxos: The curious case of CHD and DHA. **J. Klein, B. Dereli, L. Que, C.J. Cramer**
- Exploring the structure-reactivity relationship of a series of N5-ligated oxomanganese (IV) complexes. **A.A. Massie, M. Denler, T.A. Jackson**
- Tuning the proton-coupled electron-transfer reactivity of Mn(III)-hydroxo complexes via ligand perturbations. **D. Rice, A. Burr, T.A. Jackson**
- Thermodynamics of reactivity of a series of hydroxo-manganese complexes in H atom abstraction. **A. Munasinghe, D. Rice, J. Parham, T.A. Jackson**
- Why are nanoparticulates toxic upon inhalation?. N. Wolfe, **M. Vidmar**

Section A

Venue

Placeholder

ACS Award in the Chemistry of Materials: Symposium in honor of Douglas A. Keszler

Materials Chemistry of Solutions & Solids for a Sustainable Future

J. C. Giordan, S. E. Hayes, B. L. Maddux, *Organizers*

5:30 - 7:30 Film formation from peroxo hexatantalate precursors.

R.H. Mansergh, **L.B. Fullmer, D. Park,**

J.M. Amador, M.D. Nyman, D.A. Keszler

- Enhanced dehydroxylation and interface passivation of solution-processed dielectric metal oxide thin films using forming gas annealing. **J.C. Ramos, F. Luo, B.A. Hammann, D. PARK,**

Y. Huang, S.E. Hayes, E.L. Garfunkel, D.A. Keszler

- Amorphous niobium phosphate thin films from clusters in water. **D. Park, S. Goberna-Ferron,**

D. Fast, M. Dolgos, M.D. Nyman, D.A. Keszler

Aqueous solution-derived lanthanum zirconium oxide thin films on Self-Assembled Monolayers (SAMs). **M.C. Thomas, K.N. Woods, C. Page, Y.J. Chabal**

Solution-processed low-refractive index alumina-based thin films for anti-reflective coatings.

C.K. Perkins, M.T. Gutierrez-Higgins, V. Gouliouk, R. Mansergh, D. Park, J.C. Ramos, C. Nanayakkara, Y.J. Chabal, D.A. Keszler

Improved synthesis of the elusive aluminum hydroxide octamer $[\text{Al}_8(\text{OH})_{14}(\text{H}_2\text{O})_{18}]^{10+}$ cluster.

E. Eitheim, C.K. Perkins, L.B. Fullmer, B. Fulton, R. Colla, A.F. Oliveri, D. PARK, W.H. Casey, M.D. Nyman, T. Forbes, D.W. Johnson, D.A. Keszler

Understanding the effect of counterions on the hydrolysis of aqueous aluminum hydroxo clusters using QM computations. **L. Wills, J. Buchanan, C.K. Perkins, B. Fulton, D.A. Keszler,**

D.W. Johnson, P. Cheong

Reactions of hexatantalate and hexaniobate with hydrogen peroxide. **C.E. Malmberg, L. Wills,**

L.B. Fullmer, M.D. Nyman, P. Cheong

Proton-exchange rates on hydroxide bridges of mineral-like metal hydroxide clusters. **C.R. Fields, A. Oliveri, C. Colla, W.H. Casey, D.W. Johnson**

Solution speciation of amphoteric early transition metal clusters. **D. Hutchison, M. Olsen,**

M.D. Nyman

Tin and alkyltin speciation on aqueous and nonaqueous solutions. **M. Olsen, D. Hutchison, S. Saha, M.D. Nyman, D.A. Keszler**

Characterization of *n*-butylSnOOH for nanopatterning: Radiation behavior. **N. Kenane, D.A. Keszler**

Keszler

Characterization of *n*-butylSnOOH for nanopatterning: Solution precursor and film. **J.M. Amador, J.T. Diulus, M. Li, R.T. Frederick, S. Saha, E.L. Garfunkel, D.A. Keszler, G.S. Herman**

Characterization of *n*-BuSnOOH: Solution precursor identity and film quality. **M. Li, J.M.**

Amador, R.T. Frederick, S. Saha, J.T. Diulus, D.A. Keszler, G.S. Herman, E.L. Garfunkel Characterization of butyl tin photoresists with electron stimulated desorption and temperature programmed desorption. **R.T. Frederick, J.T. Diulus, S. Saha, J.M. Amador, M. Li, D.A. Keszler, E.L. Garfunkel, G.S. Herman**

. Alternative organotin clusters for thin films: Low environmental impacts under simulated environmental conditions. **B.L. Maddux**, F. Wu, S. Saha, B. Harper, D.A. Keszler, S. Harper

. Glass formation in basic halogenides of zirconium and hafnium. **J.A. Sommers**, J.M. Amador, E.C. Fong, D.A. Keszler

. Light emission from an electrical conductor. **V. Gouliouk**, K.A. Stewart, R.G. Manley, D.G. Enicks, J.F. Wager, D.A. Keszler

. Design meets nature: New tetrahedrite superabsorbers. **J. Heo**, D.A. Keszler

. Photochemical reaction coordinates of metal-organic complexes in solution revealed by femtosecond electronic and Raman spectroscopy. **L. Zhu**, S. Saha, Y. Wang, N.D. Rozanov, D.A. Keszler, C. Fang

. Effects of Organic Components on Novel Hybrid Organic-Inorganic Structures. **B. Barraza**, R. Seshadri

. Diaquo ruthenium water oxidation catalysts with a novel biimidazolyl backbone. **J.M. Kamdar**, C.E. Moore, A.L. Rheingold, D.K. Smith, D.B. Grotjahn

. Synthesis of gold nanoparticles using Schiff base derivative of N-acetylisatin with ceftriaxone as reducing and capping agent. **A.j. Abdulghani**

. Landscape of ligandable membrane cysteine and its role in modulating immune response. **E.V. Vinogradova**, K.M. Backus, M. Blewett, B.F. Cravatt

. Correlating redox potential with ⁵¹V NMR chemical shifts for vanadium (V) catecholates. **J.T. Koehn**, P. Chatterjee, C.N. Beuning, A. Waterhouse, T. Lucia, T.E. Polenova, D.C. Crans

. Diverse Array of Nucleophilic Reactivity Featuring Molecular Titanium Nitride Complexes. **L. Grant**, P. Carroll, B. Manor, D.J. Mindiola

. Theoretical and experimental investigation of Zn4Sb3 doped with metal elements. **K. Tsang**, R. Vellaisamy, R. Li

. Synthesis and characterization of 1,3-diphenyl-6-aryl fulvene coordination complexes. **B.J. O'Connell**, S.K. Adas, G.J. Balaich, S.T. Iacono

. Iron (II) pyridinediimine complexes with Lewis acids in the secondary coordination sphere. **K.T. Burns**, M. Delgado, J.M. Ziegler, J.D. Gilbertson

. Binding modes of Ni-CO₂ adducts and their CO₂ activation. **C. Yoo**, Y. Kim, Y. Lee

. Copper(I/II) reconfiguration of ligand conformations: Amplification and control of helicity by a single atom and solvent. **X. Duan**, T.M. Albelda, J.W. Canary

. Effects of carrier ligands on cisplatin analog binding to cysteine and methionine. **A.C. Smith**, K. Williams

. Analysis of S-Au-P bonding in phosphine gold(I) polyfluorothiolates: Backbonding and weak interactions. **G. Moreno-Alcantar**, J.M. Guevara-Vela, H. Torrens

. Synthesis and structural characterization of chelating dinitrosyl iron complexes. **O. Becerra**, L. Li

. Synthetic control of coincidental formation of N-heterocyclic carbene-copper(I) complex within 2D and 3D metal-organic frameworks. **H. Lee**, K. Kim, E. Lee

. Metal-organic framework as the new heterogeneous catalysts for biomass conversion. **v. tangsermvit**, W. Jumpathong, T. Lerdwiryanupap, S. Wannakao, **K. Kongpatpanich**

. Synthesis and systematic study of porphyrin metal-organic frameworks. **T. Pila**, P. Piyakeeratikul, W. Jumpathong, S. Wannakao, **K. Kongpatpanich**

. Synthesis and characterization of transition metal complexes with cyclic boroguanidines. **C.M. Donahue**, S.R. Daly

. Low-symmetry subphthalocyanines as fluorescent probes and precursors for low symmetry phthalocyanines. **K. McAuliffe**, E.R. Trivedi

. Synthesis, characterization, and growth kinetics of LiOH and KOH synthesized surface modified zinc oxide quantum dots. A.D. Mena, D. Francis, **D. McCall-Butler**, **C. Walter**, J. Davis-Gunn, S. Cabrera, A.T. Royappa, P.P. Vaughan, A. Schrock, K.S. Molek

. Missing linker on Zr-based Metal Organic Frameworks (MOFs) as the support for catalytic oxidation reactions. **W. Jumpathong**, S. Wannakao, S. Kaenket, **K. Kongpatpanich**

. CO₂ separation and storage in porphyrin-based Metal-Organic Frameworks (MOFs). **P. Piyakeeratikul**, T. Pila, W. Jumpathong, S. Wannakao, B. Boekfa, **K. Kongpatpanich**

. Synthesis, characterization, and growth kinetics of NaOH and CsOH-synthesized surfacemodified Zinc oxide quantum dots. A.D. Mena, D. Francis, D. McCall-Butler, C. Walter, **J. Davis-Gunn**, **S. Cabrera**, A.T. Royappa, P.P. Vaughan, A. Schrock, K.S. Molek

. Synthesis and x-ray single crystal structure characterization of new platinum(II) complexes with O,N,N,O donor salen-type ligands. **G. Gonzalez Garcia**, Y. Saldaña González, J. López J. , A. González García

. Isomerization in gold(I) compounds with 1,2-bis(diphenylphosphine) ethylene and fluorinated thiolates. **G. Romo**, G. Moreno-Alcantar, H. Torrens

. Versatile synthesis of novel polycyclic ligands. **M. Nozari**, N. Johnson, H. Ji, **A.W. Addison** Molybdenum(IV)oxophthalocyanines for Szilárd-Chalmers production of

Section A

Section A

Venue

Venue

Placeholder

Placeholder

Celebrating 60 Years of the Division of Inorganic Chemistry

Coordination Chemistry: Synthesis & Characterization

D. C. Crans, *Organizer*
5:30 - 7:30

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

. Highlights in inorganic chemistry from the 250 years that preceded the creation of the Division of Inorganic Chemistry. **S.A. Koch**

. Cobalt and copper σ -complexes with a diphosphine-hydrosilane ligand. J. Kim, Y. Kim, **Y. Lee**

. Trends in NMR chemical shifts of d⁰ transition metal compounds. **Z. Xue**, T.M. Cook, A.C. Lamb

. Effect of confinement on the acidity of organic and bio ligands. **J. Salas**, A. Cherem, M.D. Johnson

. Selenium speciation in the Fountain Creek water and effects on fish species diversity. **J. Carsella**, S.J. Bonetti, D.C. Crans, S.J. Herrmann, D.R. Nimmo

. Ruthenium complexes as potential anticancer prodrugs that are activated by low pH and light. **J. Gray**, F. Qu, J.A. Lundeen, N.S. Chambers, J. Park, Y. Kim, J.J. Paul, E.J. Merino, R.H. Schmehl, E.T. Papish

. Group transfer and methylation reactions of a terminally bound zirconium methylenide complex. **T. Kurogi**, P. Carroll, D.J. Mindiola

. Energy transfer from PbS nanocrystals to pentacene. **X. Li**, M. Tang

. Comparison of 2,2'-bipyridine and 1,10-phenanthroline ancillary ligands in ruthenium metal complexes containing the 4,4'-dihydroxy-2,2'-bipyridine ligand. **A.E. Kuhn**, D.J. Charboneau, M.J. Kasher, N.A. Piro, W.S. Kassel, T. Dudley, J.J. Paul

. Synthesis, structure and catalytic applications towards *Cis-β*-ruthenium-salen complexes. **C. Lee**, C. Che

. Synthesis of heterometallic 12-MC-4 complexes with ligand and counteranion substitutions. **G. Van Trieste**, M. Zeller, C.M. Zaleski

. Synthesis and luminescent study of lanthanide aluminum metallacrowns and metallacryptands. **J. Travis**, M. Zeller, C.M. Zaleski

. Synthesis of novel mixed O, N, S donor ligands. **E. Jugovic**, C. Hamaker

. NMR characterization of Ln-Mn-Na 12-metallacrown-4 complexes. C. Atzeri, V. Marzaroli, M. Quaretti, J. Travis, L. Di Bari, **C.M. Zaleski**, M. Tegoni

. Reactivity trends dictated by structure that influence terminal ligand substitution of alkylidynecapped trinuclear molybdenum (IV) clusters. **R.C. Brookins**, J.R. Houston

. Electron donor-acceptor properties of substituted pyridine ligands on fac-tricarbonylruthenium(I) systems. **J.R. Farrell**, G. Kerins, K.L. Niederhoffer, L.A. Grandall, C.J. Ziegler

. Magnetic and sorption properties of porous assemblies based on heteropolynuclear 15metallacrown-5 building blocks. **A. Pavlishchuk**, S. Kolotilov, M. Zeller, S.E. Lofland, **A.W. Addison**

. Synthesis and characterization of multinuclear manganese carboxylate coordination compounds by incorporating the anion of 3-(dimethylamino)-1,2-propanediol. **M. Reagan**, A. Saha

. Synthesis and characterization of novel sulfonamide ligands. **A. Penn**, C. Hamaker

. Syntheses, structures, and electrochemical studies of N,N'-bis(alkylthiocarbamate)butane-2,3diimine Cu(II) complexes as pendant alkoxy derivatives of Cu(ATSM). **N.S. Vishnosky**, M.S. Mashuta, R.M. Buchanan, C.A. Grapperhaus

. Interactions between metal ions and ferrocenoyl-histidine peptide conjugates. **A. Ferranco**, H. Kraatz

⁹⁹Mo. V. Rosecker, P. Weinberger, **J.M. Welch**

. Study of multielectron redox chemistry through multiple bonded bimetallic asymmetric systems. **N. Rodriguez**, D. Portillo, D. Villagran

. Synthesis and characterization of molybdenum bimetallic complexes with non-symmetric formamidate ligands. **I. Cervantes**, D. Villagran

. Diverse electronic structure of ruthenium coordinated in situ generated redox active 1,2-dinitrosobenzene and 2-nitrosoanilido. **P. Ghosh**, G.K. Lahiri

. Novel polycyclic thiones: Synthesis and complexation. **D. Tapu**, **R. Hooper**, **O. Kuykendall**

. Synthesis and titration studies of arylazothioformamide ligands with various metals towards quantifying material purification. **N.A. Johnson**, S.R. Wolfe, K.V. Waynant, J.G. Moberly, M.F.

Roll

. Alterations of synthetic routes result in several new novel copper phenanthroline coordination complexes. **M. Wilk**, S. Scott, K. Reyes, V. Nesterov, M. Omary

. Magnetic exchange between ions of the first transition series in dimeric compounds using naphthazarin as bridging ligand. **E.N. Jimenez-Alvarado**, G. Valle-Bourrouet

. Synthesis and complexation of a new thione ligand. **P. Jean**, B. Hunt, D. Tapu

. Functionalized pyridylphosphine ligands: Synthesis and coordination chemistry with late transition metals. **M. Bezpalko**, W.S. Kassel

. Synthesis and characterization of heterobimetallic complexes supported by substituted trispyridylphosphines. **J. Leonard**, A.K. Frampton, W.S. Kassel

. Synthesis and characterization of saccharinate complexes of dirhodium. **S.C. Haefner**

. Synthesis and characterization of bimetallic ruthenium-platinum molecular cluster complexes with N-heterocyclic carbene complexes. **S. Etezadi**, B. Captain

. Formation of radical anions on the dipyrin-1,9-dione scaffold of heme metabolites. **R. Gautam**, E. Tomat

. Singlet fission-based frameworks. **R. Hernandez Sanchez**, M. Trinh, D. Erdosy, X. Zhu, C.P.

Nuckolls

. Synthesis and characterization of some dinitrosyl iron diphosphine compounds. **M.W. Jones**, V. Acquah, N. Jourabchian, N. Khojandi

Addition reactions of some dinitrosyl iron diphosphine complexes. **R. Manandhar**, B. Alajmi,

M.W. Jones

. Thiopyridazine based copper boratrane chemistry. **S. Holler**, M. Tüchler, F. Belaj, K. Kirchner, N. Mösch-Zanetti

Section A

Venue

Placeholder

F. Albert Cotton Award in Synthetic Inorganic Chemistry: Symposium in honor of Pingyun Feng

Cosponsored by WCC

X. Bu, P. Yang, q. Zhang, D. Zhao, N. Zheng, *Organizers*

5:30 - 7:30

. Constrained Volume self-assembly of organic-inorganic nanocomposites. **r. liu**

. Facile synthesis of nanosheet AuPd/g-C₃N₄ composites for photocatalytic H₂ evolution under visible-light irradiation. **L. Ge**, C. Han

. Photochemical method in preparing atomically dispersed catalysts. **P. Liu**, Y. Zhao, G. Fu, N.

Zheng

. Design of (metallo)porphyrin-based coordination frameworks for electrochemical studies. **Q.**

Lin

. Dichalcogenide ligand exchange on germanium nanoparticles. **K.A. Newton**, A.L. Holmes, S. Kauzlarich, W. Blacklock

. Aromatic guest molecules mediated synthesis of porous homochiral camphorate frameworks.

J. Jin, X. Zhao, X. Bu

. Nanoporous carbon derived from a functionalized metal-organic framework as highly efficient oxygen reduction electrocatalyst. **Y. Wang**, P. Feng

. Applications of heterometallic MOFs in gas adsorption, separation and biodiesel preparation. **Y. Wang**, Q. Zhai, P. Feng

. Chirality in atomically precise noble nanoclusters. **J. Yan**, B.K. Teo, N. Zheng

. Multivariable modular design of pore space partition. **X. Zhao**, E.T. Nguyen, X. Bu, P. Feng Rational tuning of structure type in open framework chalcogenide. **X. Chen**, X. Bu, P. Feng

. Crystallography in MOF: Ordering guest molecules by coordination assisted orientation control. **L. Wang**, S. Cohen

. Electrochemiluminescence behaviors featuring the point defects of supertetrahedral chalcogenide nanocluster. **Y. Liu**

. Metal-free peralkylation of the closo-hexaborate dianion, B₆H₆²⁻. **J. Axtell**

. Synthetic design of homochiral metal-organic frameworks. **E.T. Nguyen**, X. Zhao, X. Bu

. Novel metal organic frameworks through tetrameric magnesium clusters. **A. Hong**, X. Zhao, A. Hong, X. Bu

Section A

Venue

Placeholder

Gabor A. Somorjai Award for Creative Research in Catalysis: Symposium in honor of John E. Bercaw

A. Hazari, N. Hazari, *Organizers*

5:30 - 7:30

. Understanding the mechanism of catalytic upgrading (bio)ethanol to butanol. **H. Aitchison**, D. Wass, R. Wingad

Section A

Venue

Placeholder

Nanoscience

B. G. Trewyn, *Organizer*

5:30 - 7:30

. Synthesis, characterization, and application of dendrimer coated silica nanoparticles as fluorescent chemosensors. **H. Deuermeyer**, A. Luhrs, L.D. Margerum

Ag-TiO₂ hybrid nanoparticles as active photocatalyst for hydrogen evolution. **S.**

Varapragasam, S. Mia, C. Balasanthiran, R.M. Rioux, J.D. Hoefelmeyer

. Gold nanorods with a photoresponsive azobenzene shell via *in-situ* reduction of 4nitrobenzenediazonium tetrafluoroborate. **D.H. Wang**, K. Park, R.A. Vaia, L. Tan

. Lead chalcogenide quantum dots: Measurements on a standardized sample. **A. Marshall**, J.C. Johnson, J. Luther, A.F. Fidler, V.I. Klimov, M.C. Beard

. Advantages of naked Ru⁰ surfaces in catalysis and electrocatalysis. S. Anantharaj, **S. Kundu**

. Toward large-area Surface Enhanced Raman Spectroscopy (SERS) sensors: Fabrication of patterned, nanostructured surfaces. **W. Mihalyi-Koch**, **A. Shadrav**, A. Oh, F. Dawood

. Fabrication of highly nanostructured electrodes. **P. Kharel**, A. Talsania, D. Cahill, F. Dawood

. Carbon-based nanomaterials applications in the photo-triggered release of small molecule bioregulators. **P. Huang**, X. Zhao, X. Dang, N. Zheng, P.C. Ford

. Fundamental differences in the cation exchange behaviors of cadmium- and

lead chalcogenide quantum dots. **X.A. Aguilar**, C. Lin, A.L. Morris, S.E. Benjamin, P.G. Van Patten

. Structurally tailored organic-inorganic perovskites: Vapor phase synthesis and optoelectrical properties for nanowires transistors. **R. Dong**, **J.C. Ho**

. Nanotethering to cadmium selenide for solar applications. **D. Jackson**, M.E. Hagerman, J.D.

Kehlbeck

. Studying the surface effects of PEDOT:PSS on nanoporous LiMn₂O₄. **V. Basile**, B. Lesel, S.H. Tolbert

Section A

Venue

Placeholder

Organometallic Chemistry: Applications to Materials & Polymer Science

N. S. Radu, *Organizer*

5:30 - 7:30

. Single chain polyethylene nanocrystals. **M. Schmitte**, A. Godin, P. Kenyon, M. Krumova, I. Goettker Genannt, S. Mecking

Copolymerization of cyclohexene oxide with carbon dioxide catalyzed by dinuclear iron complex bearing a phenylene-bridged bis(tripodal N₂O₂) ligand. **s. zhan**, Q. Jiang, Z. Song

. Ethylene insertion polymerization in the presence of organic radicals - Exploiting mechanistic insights to influence microstructures. **S. Stadler**, F. Ölscher, I. Göttker-Schnetmann, V. MONTEIL, S. Mecking

. Model studies of catalytic olefin chain growth in the presence of biological impurities. **F.P. Wimmer**, I. Göttker-Schnetmann, S. Mecking

. Remote substituent effects in Ni(II)-catalyzed chain growth catalysis. **E. Schiebel**, T. Wiedemann, I. Goettker Genannt, S. Mecking

. Catalytic upgrading of fatty acids from renewable single cell oils. **J. Zimmerer**, L. Williams,

D. Pingen, S. Mecking

. Development of coordinatively unsaturated, low-valent metal isocyanide MOFs. **A. Arroyave**, D. Agnew, J.S. Figueroa

. N-heterocyclic carbene platinum (II) acetylide for blue Organic Light Emitting Diodes (OLED). **J. Bullock**, A. Salehi, C. Zeman, R. Winkel, F. So, K.S. Schanze

Section A

Venue

Placeholder

Organometallic Chemistry: Applications to Organic Transformations

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

- Synthesis and characterization of organometallic compounds of coinage metals relevant to catalysis. **S. Martínez de Salinas Uzquiza**, Á. Mudarra, M. Pérez-Temprano
- Mechanistic studies on the oxidative addition of aryl halides to COBALT(I) complexes. **M. Perez-Temprano**, J. San Jose, D. Gallego
- Precision measurement of the C(sp³)-H activation kinetic isotope effect in a ruthenium-centered olefin metathesis catalyst via differential ¹³C labeling. **C. Galvin**, A. Johns, R.L. Pederson, J. Cannon, R.H. Grubbs, D.J. O'Leary
- N-Heterocyclic Olefins (NHO) as ancillary ligands in catalysis and their application in transfer hydrogenation reactions. **J. E. A. m. iglesias**, N. GARCIA VILLALTA, L.A. Oro
- Iridium(III) bis-N-heterocyclic carbenes catalyzed transfer hydrogenation reactions. **N. GARCIA VILLALTA**, L.A. Oro, M. IGLESIAS, J. E. A
- Synthesis and reactivity of the aminovinyl carbenes toward alkynes in the Dötz reaction. **R.M. Padilla**, **J. Tamariz**, **F. Delgado**, **A. Feliciano**
- Reactivity of biaryl mono-phosphine complexes. **B.E. Silva**, K. Sukert, H. Henriksen, D.B. Grotjahn

Section A

Venue

Placeholder

Sustainability in Electrocatalytic Fuel & Chemical Production

Cosponsored by CATL

L. A. Berben, J. L. Dempsey,
Organizers

5:30 - 7:30

- Silicon-based photoelectrochemical cell for enzymatic CO₂ conversion. **J. Ko**, E. Son, S. Kuk, C. Park
- Towards formic acid oxidation by surface attached Ni(P₂N₂)₂ complexes. **F. Brunner**, C.P. Kubiak

Section A

Venue

Placeholder

Switchable Catalysts

J. A. Byers, P. Diaconescu, *Organizers*
5:30 - 7:30

- Redox switchable catalysts for the synthesis of block copolymers and crosslinked polymers.
- Application of bulk electrolysis methods to redox-switchable catalysis. **S. Quan**, J. Brosmer, P. Diaconescu
- Switchable di-zinc macrocycle catalysts: From highly active lactide polymerization to block copolymers. **A.A. Thevenon**, C. Romain, M. Bennington, h. davidson, A. White, S. Brooker, C.K. Williams
- Redox switchable copolymerization of cyclic esters and epoxides by a zirconium complex. s. quan, **R. Zhang**, P. Diaconescu
- Investigations into fast switching for the redox-switchable ring-opening polymerization of epoxides and lactides. **J.A. Kehl**, J. Curley, M. Qi, J.A. Byers
- DFT studies of redox switchable copolymerization of cyclic esters and epoxides. **J. Wei**, **P. Diaconescu**
- Ligand effect of a redox-controlled Al-based ROP catalyst. **A. Lai**, P. Diaconescu
- Yttrium and indium alkoxide complexes as redox switchable catalysts. **S. Ro**, A. Laughlin, P. Diaconescu
- Polymerization through redox switchable catalysis. **M. Riffel**, J. Wei, P. Diaconescu
- Redox switchable polymerization reactions. **R. Dai**, P. Diaconescu
- Progress towards parameterizing flow reactor design for the efficient scale-up of photoredox catalysis methods. **T.M. Williams**, A. Sun, C. Stephenson
- Ferrocene-Chelating heteroscorpionate complexes in catalysis. **M. Abubekrov**, P. Diaconescu
- Hydroamination through redox-switchable catalysis. **Y. Shen**, S.M. Shepard, P. Diaconescu

Section A

Venue

Placeholder

Undergraduate Research at the Frontiers of Inorganic Chemistry Bioinorganic Chemistry

A. K. Bentley, C. Nataro, S. R. Smith,
Organizers

5:30 - 7:30

- Iron and Cadmium Binding in Metalloprotein II and Myohemerythrin from *Hediste diversicolor*. **A. Krieger**, B. Russell
- Synthesis and evaluation of alkynyl β-sheet mimetics coordinated to tungsten. **E.C. Pedro**, A.N. Boynton, S.M. Berk, T.P. Curran
- Manganese corrole substituted myoglobin. **J.M. Mason**, K.L. Stone

- Investigating dechlorination using bio-inspired nickel compounds. **E. Gund**, R. Griffin, C. Ye, K.M. Van Heuvelen
- Copper (I) substitution at zinc (II) binding domains: Characterization of speciation and functional studies. **M.L. Stevens**, **M.D. Storlie**, K.E. Splan
- Preparation of synthetic conjugated myoglobin to promote new reactivity. **K.L. Stone**, J. Hua, H. Choudhry, J. Mason
- Tandem C-H functionalizations by combining light-driven biocatalysis and photocatalysis. **V. Alfaro**, **J. Faris**, **M. Melkie**, C. Sulca, T. Banh, M. Kato, L.E. Cheruzel
- Synthesis, characterization and photosensitization in a series of Ru(phen)₂(quo)]⁺ complexes. **F. Delano IV**, A. Koerner, A. Cardillo, R.N. Garner, B.B. Sears
- Synthesis and investigation of novel hydroquinone ring-cleaving dioxygenase model complexes. **N. Porter**, T.E. Machonkin, A. Speelman, P.L. Holland
- Copper binding and reactivity of de novo designed Due Ferri single chain (DFsc) proteins. **B. Van Dyke**, A.J. Reig
- Biophysical characterization and catalytic reactivity of rubrerythrin and symerythrin model proteins. **J. Pellegrino**, **K.A. Bell**, R. Polinski, S. Cimerol, A. Jacobs, E.I. Solomon, A.J. Reig
- Using model proteins to understand the structure-function relationships in 4-histidine/2carboxylate diiron proteins. **C. Phillip**, S. Hawkins, A.J. Reig
- Structure-function relationships in G4DFsc variants containing a 4-His/3-carboxylate active site. **K. OShea**, **J. Dorsheimer**, K. Biernat, A. Jacobs, E.I. Solomon, Y. Wu, W.F. Degrado, A.J. Reig
- Characterization of MnpC, a novel hydroquinone ring-cleaving dioxygenase. **J. Duncan**, E. Altman, T.E. Machonkin
- Molybdenum pyranopterin dithiolene complexes: Synthetic model and investigation in the role of pterin reduction in the molybdenum cofactor. **N. Nguyen**, **B. Williams**, **D. Gisewhite**, **S.J. Nieter Burgmayer**
- Mechanistic investigation of photochemical products from iron-iron hydrogenase model compounds. P. De La Torre, A. Nelson , **C.F. Works**
- Synthesis and characterization of cobalt (II) salen and its possible interactions with persulfide species. A. Holm, V. Suarez, L. Alvarez, **C.F. Works**, J. Fukuto
- Dechlorination abilities of biomimetic compounds. **C. Ye**, R. Griffin, K.M. Van Heuvelen
- Investigating the reactivity of the ligating histidines at the Cu_A site of cytochrome c oxidase. **T. Devlin**, L.M. Hunsicker Wang
- Changes in reduction potential of the [2Fe-2S] cluster of the *Thermus thermophilus* Rieske protein using multiple non-covalent interactions. **R. Shepherd**, L.M. Hunsicker Wang
- Exploring the effect of distal charges on the reduction potential of the Rieske protein from *Thermus thermophilus*. **M. Hogsett**, **J. Munoz**, L.M. Hunsicker Wang
- Metal-organic supercontainers for neurobiological applications. **J.W. Fanta**, Z. Wang, B. Burrell
- Mechanistic investigation of the solvent dependent photochemistry of iron-iron hydrogenase model compounds. B. Jolly, L. Ortiz , **C.F. Works**
- Studying the active site of nickel-acireductone dioxygenase through nickel and zinc analogues: A structural and spectroscopic comparison study. **A.J. Gremillion**, S. Sanchez, S.A. Toledo, V. Lynch, C.L. Dorsey
- Capturing an intermediate of the radical S-adenosyl-L-methionine enzyme lysine 2,3aminomutase. **C. Denler**, A.S. Byer, J.B. Broderick

Section A

Venue

Placeholder

Undergraduate Research at the Frontiers of Inorganic Chemistry Coordination Chemistry

A. K. Bentley, C. Nataro, S. R. Smith,
Organizers

5:30 - 7:30

- Green chemistry in the advanced inorganic laboratory: Mechanochemical synthesis and characterization of homoleptic bis-chelate copper(I) complexes. **D.J. Rabaey**, **D.E. Janzen**
- Synthesis and kinetic studies of a trinuclear tungsten metal cluster. **J. Nunez**, R.C. Brookins, J.R. Houston
- Modifying the bridging anion of LnX₃M 12-metallacrown-4 complexes. **J.J. Reed**, J.C. Lutter,

C.I. Daly, C. Chow, A.H. Davis, A. Nimthong-Roldan, M. Zeller, J.W. Kampf, C.M. Zaleski,

V.L. Pecoraro, T.T. Boron

. Synthesis of a family of chiral aminoalcohols as ligands for titanium and tantalum catalyzed asymmetric hydroamination. A.R. Johnson, C.S. Abelson

. Optimized synthesis of molybdenum scorpionate complexes using microwave irradiation. E. Finney, J. Finney

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

. Axial ligand interactions of cyclometallated Pd(II) complexes: Hemilabile oxathiocrowns vs inert but fluxional thiocrowns. D.E. Janzen, M.A. Bruening, A.A. Mamiya, D.A. da Silva Filho

. Synthesis and characterization of SNS pincer ligand precursors and corresponding zinc(II) and copper(II) complexes. J.R. Miecznikowski, T. Ostrowski, M. Siu, K.A. Bayne, N.A. Bernier

. Synthesis, characterization, and reactivity studies of iron dibromide complexes bearing parasubstituted alpha-diimine ligands. D. Soemardi, S.M. Click, A. Beltran, K.A. Wheeler, H.M. Hoyt

. Boron Schiff-Base complexes as detectors for toxic levels of selenate in water. J. Bennett, L. Jefferies

. Synthesis of a lanthanide complex using $\text{Eu}(\text{NO}_3)_3 \cdot 6\text{H}_2\text{O}$ with tripodal ligand 2-OHnaphthtren (tris[N-(2-hydroxynaphthalidene)-2-aminoethyl]amine). J.M. Armen, P.M. Smith

. Activating carbon dioxide using a cobalt complex supported by a macrocyclic tetraza ligand. A. Amado, F. Li, C. Dong

. Syntheses, characterization, and oxygen reactivity of three coordinate SNS pincer copper(I) pincer complexes. J.R. Miecznikowski, M.R. Smith, M. Siu, N.A. Bernier, J. Jasinski, E. Reinheimer

. Synthesis of a new cationic cobalt(III) coordination complex and its potential applications as an indole ring forming catalyst. R.M. Miller, H.P. Nash, A. Morris

. Synthesis of new Fe and Co PONOP/PNP complexes: Towards the development of a first-row Guerbet catalyst. T.M. Townsend, C.E. Hayes, R. Baker, W.D. Jones

. Excimer and exciplex formation involving $[\text{Pt}(\text{bphen})\text{CN}_2]$ and Ag^+ in solution. E.J. Rourk, J.K. Nagle

Synthesis of europium(III) silicates using microwave-assisted hydrothermal methods. Z.J.

Woessner, P.M. Smith

. Natural oxidation state analysis: Principles and applications. M.K. Heili, M. Nathan, J.S.

D'Acchioli

. Synthesis and reactivity of actinide guanidinate complexes. A. Shiau, N. Settineri, J. Arnold

. Ionothermal synthesis and characterization of two new iron thiophosphates:

$[\text{EMIM}]_2[\text{Fe}(\text{P}_2\text{S}_8)_2]$ and $[\text{PMIM}][\text{FeP}_7\text{S}_{16}]$. S.R. Kang, M.L. Major, J.A. Cody

. Synthesis and characterization of thermotropic copper(II) heteroleptic metallomesogens with 2ethylhexanoate ligands. A. Beltran, T.W. Clayton

. Synthesis and characterization of low-coordinate lanthanide isocarbonyl transition metal complexes for single-molecule magnet applications. A. Burkhard, C. Dickie, M. Nippe

. Synthesis, characterization, and aqueous perchlorate reactivity of ruthenium (II) and iron (II) coordination complexes. K. Trotter, E.B. Hulley, N. Arulsamy

. Synthesis and characterization of hyper-coordinate silicon complexes. K.J. Goosherst, J.M. Fritsch

. Progress toward the synthesis of potential AIE-active silafluorene derivatives. H. Tracy, J.L. Mullin, C.M. Prudente, W. Lin

. Computational results of ADF modelling of AIE-active luminophores. H. Tracy, J.L. Mullin, C.M. Prudente, T.w. Nelson

. Spectral characterization of potential AIE-active diphenylsilafluorene derivatives. J.L. Mullin, H. Tracy, C.M. Prudente, N. Mathewson

. Synthesis, characterization and study of liquid crystalline behavior of novel benzimidazol-8hydroxyquinoline complexes. T.H. Jasim, N. Al Rubaya

Section A

Venue

Placeholder

Undergraduate Research at the Frontiers of Inorganic Chemistry General Posters

A. K. Bentley, C. Nataro, S. R. Smith, *Organizers* 5:30 - 7:30

. IONiC VIPeR workshops: Bringing current literature into the classroom. S. Poland, B.B. Sears,

S.A. Toledo, A.R. Johnson

. IONiC bonding: Building a lattice using attractive forces. A.R. Johnson,

J.L. Stewart, A.K. Bentley, H.J. Eppley, E.R. Jamieson, C. Nataro, B.A. Reisner, S.R. Smith, L.A. Watson, N. Williams

Section A

Venue

Placeholder

Undergraduate Research at the Frontiers of Inorganic Chemistry Organometallic Chemistry

A. K. Bentley, C. Nataro, S. R. Smith, *Organizers*

5:30 - 7:30

. Examination of the relative impact of tris(diisopropylphosphinomethyl)phenylborate and tris(diphenylphosphinomethyl)phenylborate in salts of $[\text{M}(\text{CO})_3(\text{PhBP}_3)]^-$ (M = Cr, Mo, W). S. Senthil, J.T. Stephan, M.D. Storlie, M.L. Swift, V.G. Young, Jr., P.J. Fischer

. Bimetallic complexes of tris(diisopropylphosphinomethyl)phenylborate and tris(diphenylphosphinomethyl)phenylborate. J.T. Stephan, S. Senthil, M.D. Storlie, M.L. Swift, V.G. Young, Jr., P.J. Fischer

. Macrocyclic osmium carbonyl complexes with dicarboxylate ligands. D.M. Marolf, J.E. Johnstone, D.F. Zometa Paniagua, G.L. Powell

. Ligand development for iron catalyzed atom transfer radical polymerization. M.R. Donley, S.E. Jenny, T. Dudley, D.L. Zubris

. New Insights into the reactivity of tris(triphenylphosphine)ruthenium(II) dichloride. M.

Aristov, K.B. Ghiassi, X.B. Powers, M.M. Olmstead, A.L. Balch

. Synthesis and reactivity of bis(NHC)borate titanium(IV) imido complexes. M.G. Bernbeck,

J.A. Ziegler, R.G. Bergman, J. Arnold

. Synthesis and crystal structure of $(\text{dppe})\text{PtH}(\text{SnPh}_3)$. A. Schmiechen, T.A. Mobley, I.A. Guzei
Hydrogenation of carbon dioxide with ruthenium bis(pyridyl)isoindolene complexes. J.L.

Ciatti, J.B. Geri, N.K. Szymczak

. Synthesis and reactivity of $\text{Fe}(\text{TSPE})_2\text{HCl}$ for natural gas purification. B. Han, L.N. Zakharov, J.W. Gohdes

. Diiron carbonyl photochemical carbon monoxide releasing compound or PhotoCORM. C. Stephenson, E. Duran, C.F. Works

. Late transition metal compounds with 1,1'-bis(phosphino)ferrocene ligands. N. Lauricella, S. Hartlaub, C. Ryczek, A. Furneaux, J.D. Melton, N.A. Piro, W.S. Kassel, C. Nataro

. Substitution reactions of compounds containing 1,1'-bis(phosphino)ferrocene ligands. N. Wamser, K. Cabrera, C. Nataro

. Assessing CMPO-based ligands for selective lanthanide extraction from acidic solution. M. Patterson, O. Sode, S.M. Biros, E.J. Werner

. Synthesis and catalytic assessment of palladium complexes bearing bridging and pendant amine bis(phenolate) ligands. E. Collins, B.J. Graziano, B. Wile

. $\text{B}_{12}(\text{OR})_{12}$ Reagents as tunable one-electron oxidants. P. Chong, M. Messina, J.C. Axtell, Y. Wang, B. Upton, B.M. Hunter, S. Khan, J.R. Winkler, H.B. Gray, A. Alexandrova, H.D. Maynard, A.M. Spokoyny

. Synthetic and analytical studies of a series of organic quinone ligands for catalytic purposes.

J.N. Herring, W. Cross Lopez, S. Kruse, S.K. Hurst

. Dibenzo[a,j]xanthylum derivatives: Analytical studies and characterization. W. Cross Lopez,

J.N. Herring, S. Kruse, S.K. Hurst

. Novel phosphorous-based ligands for precious metal catalysts. S. Kruse, J.N. Herring, W. Cross Lopez, S.K. Hurst

. Organophosphate alcoholysis by polymer-supported molybdenum peroxy complexes. L. Miao, L.Y. Kuo

. Computational investigation of hydrophothioate-neurotoxin hydrolysis by monomeric MoO_4^{2-} .

E. Bright, L.Y. Kuo

. Catalytic and electrochemical properties of pyridine substituted imidazolium salts and the corresponding NHC-M complexes.

R.J. Swails, S. Kariofillis, R. Cerbone, A. Conner, M. Sebold

. Synthesis of gold(III) complexes containing phenanthroline- or quinoline-based ligands. K.M.

Gilmore, R.L. Marley, J.E. Thompson, G.R. Donalson, A.R. McCormick, C.P. Owens, S.R. Weller, I. Nizalowski, A.L. Rheingold, D.R. Weinberg

. Comparison of C-H bond cleavage in a series of palladium carboxylate complexes. I.L.

Hunter, J. Jacobson, G.L. Bourne, A.N. Rainsberry, T. Kowalczyk, M.L. Scheuermann

. Synthesis and reactivity of molybdenum carbon dioxide complexes. M.E. Graziani, X. Duan, L.J. Briggs, G.R. Lorz, J.R. Vasta, M.A. Pogash, P.M. Graham

Section A

Venue

Placeholder

Undergraduate Research at the Frontiers of Inorganic Chemistry

Solid State & Materials Chemistry

A. K. Bentley, C. Nataro, S. R. Smith, *Organizers*

5:30 - 7:30

. Synthesis and characterization of metal-organic framework materials for aqueous heavy metal detection. N.S. Morey, **T.E. Bustamante**

. Singlet fission in a hybrid system with CdSe nanocrystals and functionalized chromophores.

D.S. Hamilton, X. Li, M.L. Tang

. Design of Polyethylene Glycol (PEG)-grafted gold nanoparticles for biomedical applications. **J. Grundler**, T. Lafferty, **E. Park**

. Effects of seasonal variation of groundwater composition on gold nanoparticle surface chemistry. **E.R. Carlson**, A.K. Bentley

. Catalytic activity of ultrasmall copper nanoparticles. **A. Kale**, G. Ferko, S.K. St Angelo

. Dye encapsulation in metal-organic frameworks. **B.J. Johnson**, K. Anderson, E. Goyke, K. O'Connor, N. Anderson, N. Beaulieu

. Single step synthesis of Sb/Cu-doped ZnO and ZnS nanostructures on mica and n-GaN/Al₂O₃ substrates by a simple vapor phase transport method. **H. Rivera-Marrero**, T.M. Trad, M.J. Uddin

Synthesis and characterization of phthalocyanine-based heterometallic metal organic frameworks. **B.G. Boe**, D.R. Neu

. Electrochemical characterization of manganese dioxide supercapacitors. **B.T. Hohman**, R.S.

Zickel, A.K. Bentley

. Fabrication of hierarchical nanostructures for surface-enhanced Raman scattering biosensors.

K. Curtin, N. Wu

. Understanding secondary structures of metal organic frameworks via tuning of ligand-ligand interactions. M. Johnson, M.J. Voegtle, **K. Tran**, J. Jones, C. Bauer

. Growth of microporous imidazolate frameworks in mild conditions via polymer-templating. **C. Bauer**, K. Kwong, B. Doyle, H. Kim

. Negative fingerprints development on reducing metal substrates. **N. Zuparova**, L. Mullen, L. Bliss, A. Lafi, H. Abdou, A. Mohamed

. Gold nanoparticle catalysts: Chemical properties and catalytic behavior. **M.N. Pollock**, **C. Peterson**, C. Pursell, B.D. Chandler

. Varying zinc sulfide nanocrystal shape, size, and surface chemistry to

control copper doping via cation exchange. **H.M. Sizemore**, K.N. Heupel, J.L. Jenkins

. Ligand effects on the reactivity and synthesis of bimetallic molecular precursors for semiconductor materials. **J.L. Tennant**, L.J. Maxton, A.W. Holland

. Hydrogenation over metal oxide supported gold nanocatalysts. **M. Huthner**, H. Krause, C. Pursell, B.D. Chandler

. Understanding growth behavior of alumina (Al₂O₃) and boehmite (AlO(OH)) nanoparticles. **M.**

Casillas, F.A. Fasulo, N.S. Bell, T.J. Boyle, L.J. Treadwell, B.A. Hernandez-Sanchez

Deposition & Etching of Nanostructures

Posters

Sponsored by COLL, Cosponsored by INOR

MONDAY MORNING

Section A Venue

Placeholder

ACS Awards in Inorganic Chemistry: Plenary Session

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

J. D. Protasiewicz, *Organizer, Presiding*

8:15 . Copper-Oxygen complexes relevant to enzyme intermediates.

W.B. Tolman

8:50 . Rational development of pincer supported iron complexes for the reversible hydrogenation of carbon dioxide to formic acid and methanol. **N. Hazari**, W.H. Bernskoetter

9:20 . Amazing nonheme high-valent iron-oxo landscape. **L. Que**

9:55 Intermission.

10:10 . Hydrogenase- and ACS-inspired bioorganometallic chemistry. **M.Y. Darensbourg**

10:40 . Crystalline semiconducting and porous materials: Synthesis, properties, and applications.

P. Feng

11:10 . Mechanistic studies of 1-alkene trimerization and polymerization with organotransition metal catalysts. **J.E. Bercaw**

11:40 . Inorganic materials chemistry and innovation. **D.A. Keszler**

Glenn T. Seaborg Award for Nuclear Chemistry: Symposium in honor of David L. Clark

Sponsored by NUCL, Cosponsored by INOR

Multicenter Molecules & Coupled Molecular Assemblies: Synthesis, Characterization & Theory

Synthesis

Sponsored by PHYS, Cosponsored by INOR

LGBT Graduate & Postdoctoral Student Chemistry Research Symposium

Frontiers in Analytical & Physical Chemistry: From Atmospheric to Atomic Discoveries

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

Support & Activator Effects on Metal Mediated Polymerization

Sponsored by PMSE, Cosponsored by CATL and INOR

Light-Driven Chemistry: Photoelectrochemistry & Photocatalysis

Photoelectrochemistry & Photocatalysis

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

MONDAY AFTERNOON

Section A

Venue

Placeholder

Gabor A. Somorjai Award for Creative Research in Catalysis: Symposium in honor of John E. Bercaw

A. Hazari, *Organizer*

N. Hazari, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 . Stoichiometric and catalytic reactions mediated by water-soluble host-guest supramolecular systems. **R.G. Bergman**

2:00 . Organometallic chemist's nightmare: Chemistry in air, water, and heterogeneous environments. **L. Do**, A. Ngo, S. Bose, L. Yang

2:25 . Polymerization catalysts that benefit from dynamic ligand behavior. **J.A. Byers**, N.K. Szymczak, J.A. Kehl, A. Kaur, C.M. Manna, K.T. Tseng, L.V. Hale, A.B. Biernesser

2:50 . Biologically inspired clusters: Synthetic control of structure and effects on reactivity. **T. Agapie**

3:15 Intermission.

3:25 . Metal oxo cubanes as catalytic centers for oxygen evolution. **T. Tilley**, A. Nguyen

3:50 . Versatile redox chemistry of nanoscale cerium oxide. **J.M. Mayer**, D. Damatov, S. Laga, J. Peng

4:15 . One and two dimensional cobalt dithiolene frameworks for artificial photosynthesis. **S.C.**

Marinescu, A.J. Clough, C.A. Downes

4:40 . From single atom based-catalysts to nanoparticles. **E. Bunel**

5:05 . Recent advances in olefin metathesis. **R.H. Grubbs**

Section B

Venue

Placeholder

Celebrating 60 Years of the Division of Inorganic Chemistry Former Young Investigators

M. J. Clarke, D. C. Crans, *Organizers*

J. R. Long, J. D. Protasiewicz, N. Radu, *Presiding*

1:30 Introductory Remarks.

1:35 . Multi-electron redox chemistry: Redox load distributions in cluster cores. **T. Betley**

2:05 . Metals and immunity: Explorations of a biological hexahistidine site. **E.M. Nolan**

2:35 . Plasmon enhanced solar steam generation and desalination. **J. Zhu**

3:05 . Single-molecule magnets based on oligo- and polynuclear lanthanide complexes. E. Mazarakioti, J. Tang, G. Christou, **T. Stamatos**

3:35 Intermission.

3:50 . Filled tetrahedral semiconductors: Solution phase synthesis of low dimensional intermetallics. **J. Vela-Becerra**

4:20 . Graphite-Conjugated catalysis. **Y. Surendranath**

4:50 . Synthesis, characterization, and reactivity of redox active 2,5-diiminopyrrole ligands and complexes. **J.S. Anderson**, A.J. McNeece

5:20 . Responsive chemical tools for COS and H₂S delivery. **M.D. Pluth**

Section C

Venue

Placeholder

Undergraduate Research at the Frontiers of Inorganic Chemistry Solid State & Materials Chemistry A. K. Bentley, C. Nataro, S. R. Smith, Organizers S. Poland, Presiding

1:30 . Synthesis and properties of transition metal carbide buckypaper. **K.E. Madsen**, B.M.

Leonard

1:50 . Super robust and water-soluble gold nanoparticles for biomedicine. **L. Mullen**, L. Bliss, N. Zuparova, B. Atallah, H. Abdou, A. Mohamed

2:10 . Using carboxylate ligand sterics to control copper availability during cation exchange to yield Cu-doped ZnS nanocrystals. **K.N. Heupel**, H.M. Sizemore, J.L. Jenkins

2:30 . Characterization of silver (I) and engineered Silver Nanoparticle (AgNP) binding to apo and metal reconstituted zinc finger peptides. **Z. Amaris**, G.A. Park, M. Eiken, K.E. Splan, K. Wheeler

2:50 Intermission.

3:05 . Coordination compounds and hybrid materials containing the hydtris(3,5-dimethyl-1,2,4-triazolyl)borate ligand. E.T. Roberts, K.L. Salvatore, B.C. Chan, **B.A. Reisner**

3:25 . Synthesis of UO₂-Zircaloy thin films to address pellet-cladding debonding. **B. Klamm**,

R.F. Hess, T.J. Boyle, K. Hattar, R. Dingreville, D. Perales

3:45 . Advances in manganese- and cobalt-based nanostructures for oxygen/hydrogen electrocatalysis. **J.A. Vigil**, T.N. Lambert

4:05 . Understanding titanium and sulfur speciation in titanium trisulfide electrodes using x-ray spectroscopy. **C. Wilson**, V. Doan-Nguyen, J.D.

Bocarsly, A. Lanzirrotti, R. Seshadri

4:25 . Synthesis of quantum dot bioimaging agents to study bacteriophage. **S. Mendoza**, M. McKeown, M. Casillas, C. Stevens, J. Pelowitz, A. McBride, C. Ashley, B.A. HernandezSanchez

Section D

Venue

Placeholder

ACS Awards: Symposium in honor of Lawrence Que Jr. & William B. Tolman

P. L. Holland, M. J. Maroney, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 . Bioinorganic aspects of nitrogen oxide chemistry with heme and/or copper complexes.

K.D. Karlin

2:00 . Synthetic chemistry as a window into biology: Architectural complexity at the molecular level. **A. Borovik**

2:25 . Cleaving and forming C–H bonds by moving protons and electrons. **J.M. Mayer**, J. Darcy, T. Markle, S. Kolmar

2:50 . Oxygen activation and C–H bond cleavage by metalloenzymes and metalloporphyrins. **J.T. Groves**

3:15 Intermission.

3:30 . Bioinorganic spectroscopy: Activating metal sites for biological electron transfer. **E.I. Solomon**

3:55 . Insights into the electronic structure of iron sulfur clusters using two-dimensional x-ray spectroscopy. **S. DeBeer**

4:20 . Bio-inspired bimetallic complexes for activating H₂ and CO₂. **C. Lu**, R. Cammarota, S. Desai, J. Xie, K. Vogiatzis, D. Pahls, L. Gagliardi

4:45 . Tracking mobile zinc in the brain - new probes, new biology. **S.J. Lippard**

Section E

Venue

Placeholder

Inorganic Nanomaterials: Structure & Function in 0, 1 & 2 Dimensions

Financially supported by Chemistry of Materials

K. R. Kittilstved, *Organizer*

E. J. McLaurin, *Organizer, Presiding*

A. Greytak, *Presiding*

1:30 . Chemically tunable 2D layered materials. **K.J. Koski**

2:00 . Solution-Phase approaches to indium nitride nanomaterials: Chemical insights on a new mechanism. Y. Chen, Z. Liu, N.S. Karan, **R. Beaulac**

2:30 . Linking the forward and reverse vapor-liquid-solid mechanisms in metal oxide nanostructures. L. Yu, B.M. Hudak, A.J. Riddle, S. Wang, Y. Chang, **B. Gupton**

3:00 Intermission.

3:15 . Patterns and plasmonics: Nanopatterning of silicon surfaces via directed self-assembly. F. Liu, E. Lubert, B. Olsen, **J.M. Buriak**

3:45 . Responsive and reconfigurable materials from dimensionally confined colloidal nanocrystal assemblies. **B. Helms**, Z. Zhang, E. Goldfine, C. Huang, T. Russell

4:15 . Nanomaterial surfaces in 0, 1, and 2 dimensions: Results from chromatography and functional imaging. **A.B. Greytak**

Section F

Venue

Placeholder

Sustainability in Electrocatalytic Fuel & Chemical Production

Cosponsored by CATL L. A. Berben, J. L. Dempsey, *Organizers* C. A. Caputo, *Presiding*

1:30 . Sustainable solar-to-fuels and solar-to-fertilizer production. **D.G. Nocera**

1:55 . Reducing overpotential and maintaining high rates in nickel electrocatalysts for H₂ production.

M.J. O'Hagan, A.P. Cardenas, A.M. Appel, R. Bullock, E.S. Wiedner

2:20 . Unravelling PCET pathways of the hydride formation step in cobalt complexes relevant to solar fuel production. **N. Elgrishi**

2:40 . Electrocatalytic reduction of CO₂ using cyclopentadienone iron complexes. **R. Francke**,

A. Rosas-Hernández, H. Junge, M. Beller, M. Roemelt

3:05 . Earth-abundant metal complexes with flexible ligand coordination for catalytic proton and carbon dioxide reduction. S. Saund, K. Ng, S. Goldschmid, **V. Thoi**

3:30 Intermission.

3:45 . Variable temperature spectral and electrochemical studies of carbon dioxide reduction by

[Fe₄N(CO)₁₂]-: Mechanistic investigations. **A. Taheri**, L.A. Berben

4:05 . Bioinorganic approaches to solar-to-chemical conversion: Merging molecular catalysis with materials and biology. **C.J. Chang**

4:30 . Catalytic production of hydrogen and reduction of carbon dioxide by dirhodium(II,II) complexes. **C. Turro**, K.R. Dunbar

4:55 . Homogeneous water oxidation and CO₂ reduction: Catalysts and mechanisms. Y. Xie, D.W. Shaffer, D. Szalda, **J.J. Concepcion**

Section G

Venue

Placeholder

F. Albert Cotton Award in Synthetic Inorganic Chemistry: Symposium in honor of Pingyun Feng P. Yang, q. Zhang, D. Zhao, N. Zheng, Organizers X. Bu, Organizer, Presiding

1:30 . Mo-S Complexes based on [MoO(S₂)₂] motif as MoS_x-inspired electrocatalysts for hydrogen production. **Y. Wu**, B. Garrett

1:50 . Compositional, structural, and geometrical design of crystalline porous materials. **X. Bu**

2:10 . Controlled encapsulation of catalysts into metal-organic frameworks. **C. Tsung**

2:30 . Controlling the structures and properties of gold/silver nanoclusters with unconventional protecting ligands. **Q. Wang**

2:50 . Surfactant-thermal method to prepare crystalline inorganic materials. **q. zhang**

3:10 Intermission.

3:40 Crystal engineering of titanium-oxo clusters. **J. Zhang**

4:00 . Stabilization of isolated metal chalcogenide nanoclusters and their electrocatalytic applications for

hydrogen evolution reaction and oxygen reduction reaction. **T. Wu**

4:20 . Beyond multimetallic nanoparticles for catalysis: A general approach to stable high-index faceted multimetallic nanowires. **X. Huang**

4:40 . Metal nanoclusters as a model system for investigating the surface structure and catalysis of metal nanoparticles. J. Yan, L. Ren, P. Yuan, L. Huang, **N. Zheng**

Section H

Venue

Placeholder

Organometallic Chemistry: Applications to Materials & Polymer Science N. S. Radu, Organizer A. Dudnik, Presiding

1:30 . Chiral Phospha[n]ferrocenophanes: New metallopolymers through ring-opening polymerizations. **m. cao**, S. Sadeh, J. Quail, J. Müller

1:50 . Asymmetric hybrid salen/phoshasalen initiators for the iso-selective ring-opening polymerisation of rac-lactide. **C. Coleman**, C.K. Williams, N.J. Long

2:10 . Redox control of aluminum ring-opening polymerization: A combined experimental and DFT investigation. **J. Wei**, **P. Diaconescu**

2:30 . Synthesis of (salfen)In(OPh)(OtBu)₂ catalyst, and redox-swiyachable ring-opening polymerization of ε-caprolactone and other cyclic esters. s. quan, **R. Zhang**, P. Diaconescu

2:50 . Highly robust Pd(II) α-diimine catalysts for olefin (co)polymerization. **S. Dai**, C. Chen

3:10 . Redox-controlled olefin (Co)polymerization catalyzed by ferrocene-bridged phosphinesulfonate palladium complexes. **M. Chen**, C. Chen

3:30 . Supported lanthanide catalysts: Role of the grafting on the stereochemical outcome of different polymerization reactions. **I. Del Rosal**, L. Maron

3:50 . Investigation of a unique mechanism for the production of high molecular weight polyethylene using bis(pyridylimino)isoindolate iron(II) catalysts. **J.A. Kehl**, K.T. Tseng, L.V. Hale, A.B. Biernesser, N.K. Szymczak, J.A. Byers

4:10 . Mechanistic studies of Pd(II)-catalyzed copolymerization of ethylene and vinylalkoxysilanes: Evidence for a β-silyl elimination chain transfer mechanism. **Z. CHEN**, W. Liu, O. daugulis, M. Brookhart

4:30 . Non-chiral lithium aluminate reagents for the determination of enantiomeric excess of chiral alcohols. **R. Garcia**, D. Wright

4:50 . Oligomerization of ethylene using a diphosphine palladium catalyst. **D. Bezier**, O. Daugulis, M. Brookhart
5:10 . Aqueous polyethylene nanocrystal dispersions from catalytic polymerization. **P. Kenyon**, A. Godin, S. Mecking

Section I

Venue

Placeholder

2017 Priestley Medalist: Symposium in honor of Tobin J. Marks Supported Organometallics & Heterogeneous Catalysis

Cosponsored by PMSE

Financially supported by Dow-Dow Corning, ExxonMobil, STRENGTH, Argonne National Lab, Northwestern University

A. Facchetti, T. Lohr, *Organizers*

M. Neurock, *Presiding*

1:30 Introductory Remarks.

1:35 . Tuning nanoparticle alloys to enhance C-H bond activation for the catalytic dehydrogenation of ethane. V. Cybulskis, J.R. Gallagher, H. Tsent, B. Bukowski, Z. Wu, E.C. Wegener, A.J. Kropf, B. Ravel, J.P. Greeley, F. Ribeiro, **J. Miller**

2:05 . Hydrogen and formaldehyde generation from bio-derived alcohols using supported molybdenum-oxo catalysts. **T. Lohr**, A. Mouat, M. Delferro, P.C. Stair, T.J. Marks

2:35 . Integration of the three fields of catalysis: Heterogeneous, homogeneous, and enzyme.

G.A. Somorjai

3:05 . Catalysts synthesized by organometallic surface chemistry. **P.C. Stair**

3:35 Intermission.

3:45 . Surface structural-chemical characterization of supported single-site organometallic catalysts. **M. Delferro**

4:15 . Metallocyclobutane structure influence on the production of propylene via olefin metathesis over surface organometallic chemistry derived catalysts. **C.P. Nicholas**, M. Taoufik

4:45 . Metal-organic Frameworks for Sustainable Catalysis. **W. Lin**

Section J

Venue

Placeholder

ACS Award in Organometallic Chemistry: Symposium in honor of Marcetta Y. Darensbourg

D. Mason, C. G. Riordan, *Organizers*
M. R. Mackiewicz, X. Zhao, *Presiding*

1:30 . Carbene-stabilization of elusive main group oxides. **G.H. Robinson**

1:55 . On the contents of metal-seamed metal organic nanocapsules. **J.L. Atwood**, C. Zheng, A. Rathnayake, R. Patil, K. Sikligar, K. Feaster, C. Barnes, P. Atwood, D.A. Atwood

2:20 . Exploiting the non-innocence of antimony ligands in organometallic catalysis. **F.P. Gabbai**

2:45 . Dinitrosyl Iron Complexes (DNICs): Synthesis and spectroscopic characterization toward unveiling the catalytic roles of DNICs. **W. Liaw**

3:10 . Platinum reagents modified for click chemistry: Towards high-throughput analysis of platinum drug targets. A.D. Moghaddam, K. Plakos, J.D. White, r. cunningham, E. Reister, E. Sutton, M.M. Haley, **V. DeRose**

3:35 Intermission.

3:50 . C-H activation by a discrete superoxonickel complex. **C.G. Riordan**

4:15 . Pyridol derived N-heterocyclic amines and applications in coordination chemistry, catalysis, and medicine. **K.N. Green**, S.M. Brewer, H.M. Johnston, M.E. Burnett

4:40 . Fun with devil's copper and the odd oxidations of sulfur. **P.J. Farmer**, M. Kumar

5:05 . Hydrogenase/epoxide-CO₂ catalysis: Killing two birds with one cat. **D.J. Darensbourg**

Section K Venue

Placeholder

Switchable Catalysts

P. Diaconescu, *Organizer* J. A. Byers, *Organizer, Presiding* B. P. Fors, *Presiding*

1:30 Introductory Remarks.

1:35 . Regulating polymer stereomicrostructures and polymerization activity and chemoselectivity by ion pairs and Lewis pairs. **E.Y. Chen**

2:05 . Externally controlled chemistry: New methods for modulating polymerization and other transformations. **C. Bielawski**

2:35 . Potential applications of switchable catalysts for sustainable energy and water production.

M.A. Reynolds

3:05 Intermission.

3:20 . Photocontrolled Cationic Polymerizations. **B.P. Fors**

3:50 . Switchable polymerization catalysts: Selective block copolymers from monomer mixtures.

C.K. Williams

4:20 . Redox switchable catalysis applied to ring opening polymerization. **P. Diaconescu**

4:50 . Mechanistic trends from computational chemistry for the design of redox switchable catalysts. **T. Cantat**

Section L

Venue

Placeholder

Organometallic Chemistry: Synthesis & Characterization-Early Transition Metals

N. S. Radu, *Organizer*

T. K. Hollis, *Presiding*

1:30 . Extreme π -loading as a design element for accessing imido reactivity: CCC-NHC Ta bis(imido) pincer complex synthesis and reactivity in oxidative amination. T.R. Helgert, J.A. Denny, G.M. Lang, G. Liang, C.E. Webster, **T.K. Hollis**

1:50 . Diphenylacetylene reduction mediated by rare-earth naphthalene complexes supported by a ferrocene diamide ligand. **J.L. Brosmer**, W. Huang, P. Diaconescu

2:10 . Ring-opening reactions of quinoline and isoquinoline with a low-valent titanium alkyl complex. **T. Kurogi**, M. Baik, D.J. Mindiola

2:30 . Probing the stability & reactivity of early first-row transition metal centers in lowcoordinate environments supported by silylarylamido ligands. **I.C. Cai**, T. Tilley

2:50 . Oxidative group transfer reactions on macrocyclic N-heterocyclic tetracarbene chromium complexes. **G. Elpitiya**, D.M. Jenkins

3:10 . Synthesis of benzoylphosphine via insertion of sodium phosphoethynolate (Na[OCP]) into a zirconium benzyne complex. J. Kieser, R.J. Gilliard, H. Grützmacher, **J.D. Protasiewicz**

3:30 . Hydroboration reactivity of niobium bis(NHC)borate complexes. **J.A. Ziegler**, R.G. Bergman, J. Arnold

3:50 . Planar Ti₂P₂ core assembled by reductive decarbonylation of $\text{O}=\text{C}=\text{P}$.

L. Grant, B. Pinter, B. Manor, H. Grützmacher, D.J. Mindiola

4:10 . Computational study of extreme π -loading and imido reactivity in CCC-NHC Ta bis(imido) pincer complexes. **C.E. Webster**, G. Liang, T.R. Helgert, J.A. Denny, G.M. Lang, T.K. Hollis

4:30 . Probing Group 4 mixed ligand (Cp, halide, alkoxide) complexes for multiple bonding character and catalytic activity. **N.C. Boyde**, T.P. Hanusa

Glenn T. Seaborg Award for Nuclear Chemistry: Symposium in honor of David L. Clark

Sponsored by NUCL, Cosponsored by INOR

Multicenter Molecules & Coupled Molecular Assemblies: Synthesis, Characterization & Theory

Experimental Characterization

Sponsored by PHYS, Cosponsored by INOR

LGBT Graduate & Postdoctoral Student Chemistry Research Symposium

Advances in Medicinal & Biological Chemistry: From Therapeutics to Education

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ACS Award in Industrial Chemistry: Symposium in honor of Jane Frommer

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Support & Activator Effects on Metal Mediated Polymerization

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Light-Driven Chemistry: Photoelectrochemistry & Photocatalysis

Mechanistic Studies of Catalysis in Photocatalytic & Photoelectrodes
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Undergraduate Research Posters Inorganic Chemistry

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MONDAY EVENING

Section A

Venue Placeholder Sci-Mix

S. A. Koch, *Organizer*

8:00 - 10:00

. Highlights in inorganic chemistry from the 250 years that preceded the creation of the Division of Inorganic Chemistry. **S.A. Koch**

- . IONiC VIPer workshops: Bringing current literature into the classroom. **S. Poland, B.B. Sears, S.A. Toledo, A.R. Johnson**
- . IONiC bonding: Building a lattice using attractive forces. **A.R. Johnson, J.L. Stewart, A.K. Bentley, H.J. Eppley, E.R. Jamieson, C. Nataro, B.A. Reisner, S.R. Smith, L.A. Watson, N. Williams**
- . Toward large-area Surface Enhanced Raman Spectroscopy (SERS) sensors: Fabrication of patterned, nanostructured surfaces. **W. Mihalyi-Koch, A. Shadrav, A. Oh, F. Dawood**
- . Fabrication of highly nanostructured electrodes. **P. Kharel, A. Talsania, D. Cahill, F. Dawood**
- . Effect of confinement on the acidity of organic and bio ligands. **J. Salas, A. Cherem, M.D. Johnson**
- . Diiron carbonyl photochemical carbon monoxide releasing compound or PhotoCORM. **C. Stephenson, E. Duran, C.F. Works**
- . Probing Pterin reduction dynamics in synthetic molybdenum cofactor models. **A.L. Nagelski, D.R. Gisewhite, B.R. Williams, S.J. Nieter Burgmayer**
- . Synthesis and evaluation of alkynyl β -sheet mimetics coordinated to tungsten. **E.C. Pedro, A.N. Boynton, S.M. Berk, T.P. Curran**
- . Characterization of a novel Fe(V)=O species using Mossbauer spectroscopy and Electron Paramagnetic Resonance (EPR) spectroscopy. **R. Fan, J. Serrano Plana, A. Company, W.N. Oloo, L.A. Rueda, K.K. Meier, B. Verdejo, E.V. Garcia-Espana, M.G. Basallote, E.L. Bominaar, Y. Guo, L. Que, M. Costas, E. Munck**
- . Novel thione based ligands: Synthesis and complexation. **P. Jean, B. Hunt**
- . Natural oxidation state analysis: Principles and applications. **M.K. Heili, M. Nathan, J.S. D'Acchioli**
- . Activation of small molecules by 2-[(dicyclohexylphosphino)ethyl]trimethyl ammonium chloride iridium complexes. **J. Knapp, S.H. Schreiner**
- . Very low-temperature lanthanide and actinide borates from boric acid flux. **A.T. Chemey, S.S. Galley, T.E. Albrecht-Schmitt**
- . Photoelectrochemical mechanism for instability of blue-phosphorescent Ir(III) complexes in electroluminescence devices. **S. Kim, H. Bae, S. Park, J. Kim, J. Kim, Y. Jung, S. Sul, S. Ihn, C. Noh, S. Kim, Y. You**
- . Assessing CMPO-based ligands for selective lanthanide extraction from acidic solution. **M. Patterson, O. Sode, S.M. Biro, E.J. Werner**
- . Nickel telluride as a bifunctional electrocatalyst for efficient water splitting in alkaline medium. **U. De Silva, W.P. Liyanage, J. Masud, M. Nath**
- . Superhard alloys of transition metal dodecaborides: $Zr_{1-x}Y_xB_{12}$, $Zr_{1-x}Sc_xB_{12}$ and $Y_{1-x}Sc_xB_{12}$. **G. Akopov, M.T. Yeung, Z.C. Sobell, C.L. Turner, R.B. Kaner**
- . Acid-labile linker design for targeted delivery and release of platinum-acridine anticancer agents. **H. Wang, M. Yang, U. Bierbach**
- . Modifying the bridging anion of LnX_4M 12-metallacrown-4 complexes. **J.J. Reed, J.C. Lutter, C.I. Daly, C. Chow, A.H. Davis, A. Nimthong-Roldan, M. Zeller, J.W. Kampf, C.M. Zaleski, V.L. Pecoraro, T.T. Boron**
- . Single step synthesis of Sb/Cu-doped ZnO and ZnS nanostructures on mica and n-GaN/Al₂O₃ substrates by a simple vapor phase transport method. **H. Rivera-Marrero, T.M. Trad, M.J. Uddin**
- . Modelling defects in LaMnO₃ for solid oxide fuel cell cathodes. **A.L. Gavin, G.W. Watson**
- . Catalytic and electrochemical properties of pyridine substituted imidazolium salts and the corresponding NHC-M complexes. **R.J. Swails, S. Kariofillis, R. Cerbone, A. Conner, M. Sebold**
- . Solution-processed low-refractive index alumina-based thin films for anti-reflective coatings. **C.K. Perkins, M.T. Gutierrez-Higgins, V. Gouliouk, R. Mansergh, D. Park, J.C. Ramos, C. Nanayakkara, Y.J. Chabal, D.A. Keszler**
- . Discovery of earth abundant catalysts towards the implementation of a hydrogen economy. **T. Soucy, J. Mondschein, J. McEnaney, C. Badding, R. Schaak**
- . Hyp₃Sb for separation of heavy metals. **E.G. Leach, S.M. Biro, J.E. Bender**
- . Crystal engineering of metal-inorganic frameworks from phosphorescent building blocks. **J. Ivy, M.A. Omary**
- . Single chain polyethylene nanocrystals. **M. Schnitte, A. Godin, P. Kenyon, M. Krumova, I. Goettker Genannt, S. Mecking**
- . 3D Macroporous TiO₂@CeO₂ and TiO₂@AuNP composite fabrication and application. **B. Baruah, D. Corella, M. Geiger**
- . Cytocompatible polysaccharide incorporated biomimetic tubules. **K. Punia, M. Bucaro, A. Punia, A. Bykov, K.S. Raja**
- . GeP₃ thin layers: Novel 2D materials revealed by first-principles calculations. **Y. Jing**
- . Organo-oxo tin cluster reactivity: Insight into cluster formation, degradation, and interconversion. **M.C. Sharps, J.E. Hutchison, D.W. Johnson**
- . Graphene-On-Silica, CMOS-integrable, thermal-guiding structures: Applications in Boolean-Logic and neuromorphic computation. **D. Loke, J. Skelton, T. Chong, S. Elliott**
- . Two principles of reticular chemistry uncovered in a metal-organic framework of heterotritopic linkers and infinite secondary building units. **N.R. Catarineu, A. Schoedel, P. Urban, M.B. Morla, C. Trickett, O.M. Yaghi**
- . Integration of oriented anatase TiO₂ electron transport layer into perovskite solar cells to improve carrier separation. **H. Dehnashi, m.L. mayer, A. Yore, Y. Tran, M. Howard, A. Newaz, A.S. Ichimura**
- . Structural design of magnetoelectric multiferroics in garnets. **A.J. Neer, B.C. Melot**
- . Elucidating the effect of fluoride-containing ionic liquids on indium phosphide nanocrystals. **S. Lee, E.J. McLaurin**
- . Vapor-Phase epitaxial growth of aligned nanowire networks of cesium lead halide perovskites (CsPbX₃, X = Cl, Br, I). **J. Chen, Y. Fu, L. Samad, L. Dang, Y. Zhao, S. Shen, L. Guo, S. Jin**
- . Novel synthesis, structure, and enhanced photoluminescence of lanthanide dicyanoaurates containing aurophilic interactions. **T. Hamby, R. Sykora, J. Hendrich, E. Kost**
- . Alterations of synthetic routes result in several new novel copper phenanthroline coordination complexes. **M. Wilk, S. Scott, K. Reyes, V. Nesterov, M. Omary**
- . Precision measurement of the C(sp³)-H activation kinetic isotope effect in a ruthenium-centered olefin metathesis catalyst via differential ¹³C labeling. **C. Galvin, A. Johns, R.L. Pederson, J. Cannon, R.H. Grubbs, D.J. O'Leary**
- . Chirality in atomically precise noble nanoclusters. **J. Yan, B.K. Teo, N. Zheng**
- . Copper binding and reactivity of de novo designed Due Ferri single chain (DFsc) proteins. **B. Van Dyke, A.J. Reig**
- . Ruthenium-catalyzed substitutions of icosahedral dodecaborates. **D.C. Adams, J.A. Dopke, R.J. Staples**
- . Impedance studies of silyl/carbonate electrolyte blends. **M. Treichel, C.A. Ortiz, L.J. Lyons**
- . Metal flux and supercritical fluid syntheses of actinide materials. **W. Potter, T.E. Albrecht-Schmitt, S.E. Latturmer**
- . Structure and reducibility of CeO₂ doped with trivalent cations. **A.K. Lucid, G.W. Watson**
- . Interface-facilitated hydrothermal synthesis of large-area graphene-like carbon nanosheets from toluene. **H. Gao, G. Wang, S. Fan, C. Dong, A. Li, X. Zhu, X. Li**
- . Reactivity of biaryl mono-phosphine complexes. **B.E. Silva, K. Sukert, H. Henriksen, D.B. Grotjahn**
- . Photochemical method in preparing atomically dispersed catalysts. **P. Liu, Y. Zhao, G. Fu, N. Zheng**
- . Efficient ammonia adsorption property of Prussian blue analogues. **A. Takahashi, H. Tanaka, Parajuli, T. Nakamura, K. Minami, Y. Sugiyama, Y. Hakuta, S. Ohkoshi, T. Kawamoto**
- . Synthetic and structural comparisons between first row transition metal dithiolato complexes and group 14 metallocenes. **J. Pratt, P.P. Power**
- . Singlet fission in a hybrid system with CdSe nanocrystals and functionalized chromophores. **D.S. Hamilton, X. Li, M.L. Tang**
- . Cyclopentadienyl pyridazines and oxazines and their applications in energy and advanced electronics. **N.C. Tice, E.M. Collins, C.A. Snyder, D.L. Smith**
- . Remote substituent effects in Ni(II)-catalyzed chain growth catalysis. **E. Schiebel, T. Wiedemann, I. Goettker Genannt, S. Mecking**
- . Vanadium oxide and vanadium oxynitride composite as electrode materials for lithium ion batteries. **W. HUANG, S. Yen, Lee, H. Chiu**
- . Synthesis and catalytic reactions with macroporous botanically templated metal oxides and metal on carbon structures. **N. Black, E.G. Gillan**
- . Exploring electrocatalytic N₂ activation under mild synthetic conditions. **A. Nielander, J. McEnaney, T.F. Jaramillo**
- . Characterizing the kinetic capabilities of supported gold nanoparticle catalysts using benzyl alcohol oxidation. **M.Y. Santos, B.D. Chandler, C. Pursell, A. Tombo**
- . Large-scale synthesis of Sb₂Q₃ (Q = S, Se) nanofibers topotactically converted from ternary metal chalcogenides and their optical and

- transport properties. **H. Lee**, M. Kim, B. Yoo, K. Ahn, I. Chung
- . Electron donor-acceptor properties of substituted pyridine ligands on *fac*-tricarbonylrhenium(I) systems. **J.R. Farrell**, G. Kerins, K.L. Niederhoffer, L.A. Crandall, C.J. Ziegler
- . Toward the synthesis of a new anionic N-heterocyclic carbene and its corresponding metal complexes. **A. Carter**, **A. Mason**, **D. Tapu**, M. Baker, G. Bettler, A. Changas
- . Unusual reactivity of PCP-supported rhenium carboxylates. **A.J. Kosanovich**, W. Shih, O. Ozerov
- . Organophosphate alcoholysis by polymer-supported molybdenum peroxy complexes. **L. Miao**, L.Y. Kuo
- . Optimizing hydrothermal reaction conditions for lanthanide coordination polymer formation: A study of the 1,4-benzenedicarboxylate system. **J. Einkauff**, D.T. de Lill
- . Probing slow magnetic relaxation in a series of mononuclear uranium (v) compounds. **D. Lussier**, J.R. Long, D.K. Shuh
- . Borylated N-Heterocyclic Carbenes(NHCs) - Synthesis and migration studies. **W. Liu**, C. Chiu
- . Electronically versatile benzenedithiolates on electronic and coordination structures of metal complexes: Mimicking the electronic interplay in [FeFe]hydrogenase active site. **Y. Liu**, K. Chu, M.H. Chiang
- . Alternative organotin clusters for thin films: Low environmental impacts under simulated environmental conditions. **B.L. Maddux**, F. Wu, S. Saha, B. Harper, D.A. Keszler, S. Harper
- . Magnetic exchange between ions of the first transition series in dimeric compounds using naphthazarin as bridging ligand. **E.N. Jimenez-Alvarado**, G. Valle-Bourouet
- . Selenium speciation in the Fountain Creek water and effects on fish species diversity. **J. Carsella**, S.J. Bonetti, D.C. Crans, S.J. Herrmann, D.R. Nimmo
- . Characterization of butyl tin photoresists with electron stimulated desorption and temperature programmed desorption. **R.T. Frederick**, J.T. Diulus, S. Saha, J.M. Amador, M. Li, D.A. Keszler, E.L. Garfunkel, G.S. Herman
- High performance CsPbX₃ perovskite quantum dot light emitting devices achieved via solidstate ligand exchange. **Y. Suh**, T. Kim, H. Park, C. Lee, J. Park
- . Synthesis of gold nanoparticles using Schiff base derivative of N-acetylisatin with ceftriaxone as reducing and capping agent. **A.J. Abdulghani**
- . Enhanced dehydroxylation and interface passivation of solution-processed dielectric metal oxide thin films using forming gas annealing. **J.C. Ramos**, F. Luo, B.A. Hammann, D. PARK, Y. Huang, S.E. Hayes, E.L. Garfunkel, D.A. Keszler
- . Novel mesoionic/remote N-heterocyclic carbene ligands and their ruthenium(II) aqua complexes. **T.C. Cao**, D.B. Grotjahn
- . Synthesis and structural characterization of chelating dinitrosyl iron complexes. **O. Becerra**, L. Li
- . Redox switchable copolymerization of cyclic esters and epoxides by a zirconium complex. s. quan, **R. Zhang**, P. Diaconescu
- . Nitrous oxide removal with titanium oxide. **H. Gokturk**
- . Rhodium complexes with N-heterocyclic carbene and triazene ligands as catalysts for alkyne hydrothiolation. **J.P. Camarena-Díaz**, D.B. Grotjahn, A.L. Rheingold, J. Perez-Torrente, R. Castarlenas, L.A. Oro, . Passarelli, M. Parra Hake, V. Miranda-Soto
- . Synthesis, characterization and reactivity of group ten phosphinoferrrocene - carbonyl complexes. **E. Kober**, S.H. Schreiner
- . Towards formic acid oxidation by surface attached Ni(P₂N₂)₂ complexes. **F. Brunner**, C.P. Kubiak
- . Metal-organic frameworks as templates for transition metal clusters. **A. Turkiewicz**, M.I. Gonzalez, L.E. Darago, J.R. Long
- . Crystal structure features and luminescent properties of the copper-doped Ca-Eu apatite. **M. Pogosova**, F. Azarmi
- . Metastable layered metal chalcogenides: From superconductivity to ferromagnetism. **B. Wilfong**, X. Zhou, H.K. Vivanco, E.E. Rodriguez
- . New annulated N-heterocyclic carbenes and their transition metal complexes. **G. Bettler**, **A. Changas**, O.J. Buckner, C. Boudreaux, B. Norvell, D. Tapu
- . Synthesis and reactivity of actinide guanidinate complexes. **A. Shiau**, N. Settineri, J. Arnold Switchable di-zinc macrocycle catalysts: From highly active lactide polymerization to block copolymers. **A.A. Thevenon**, C. Romain, M. Bennington, h. davidson, A. White, S. Brooker, C.K. Williams
- . Synthesis and characterization of heterobimetallic complexes supported by substituted trispyridylphosphines. **J. Leonard**, A.K. Frampton, W.S. Kassel
- . Characterization of a dicopper dihydroxide water oxidation electrocatalyst. **S.J. Koepke**, P.E. VanNatta, A. Shrestha, M.T. Kieber-Emmons
- . Three versatile Pt(II) oxime complexes that display anion sensing, thermochromism, and solvatochromism. **S.O. Elsidieg**, F.R. Fronczek, A.W. Maverick
- . Synthesis and characterization of three cationic, isorecticular layered materials based on neodymium and α,ω -alkanedisulfonates. **A. Kareh**, S. Oliver
- . New route for the formation of SnSe thermoelectric materials with low thermal conductivity. **S. Kundu**, S. Yi, C. Yu
- . Synthesis, crystal structure, and thermoelectric properties of new phosphides BaCu₅P₃ and Ba₄Cu_{11.2}Mg_{2.8}P₁₀. **J. Mazzetti**, J. Wang, K. Kovnir
- . Understanding growth behavior of alumina (Al₂O₃) and boehmite (AlO(OH)) nanoparticles. **M. Casillas**, F.A. Fasulo, N.S. Bell, T.J. Boyle, L.J. Treadwell, B.A. Hernandez-Sanchez
- . Coordination chemistry of the rhodizonate anion with Pb(II) and lanthanides: From understanding complexation to analytical applications. **J.A. Silverman**, E.V. Govor, K. Kavallieratos
- . Design of lanthanide half-sandwich complexes exhibiting single-molecule magnetism. **R. Khoo**, J.R. Long
- . Catalytic upgrading of fatty acids from renewable single cell oils. **J. Zimmerer**, L. Williams, D. Pingen, S. Mecking
- . Environmentally friendly and versatile method for the synthesis of transition metal alloys and their hybrid nanoparticles. **A. Penn**, J. Sharpsteen, H.P. Rathnayake
- . Binding modes of Ni-CO₂ adducts and their CO₂ activation. **C. Yoo**, Y. Kim, Y. Lee
- . Energy transfer from PbS nanocrystals to pentacene. **X. Li**, M. Tang
- . Synthesis, characterization, and application of dendrimer coated silica nanoparticles as fluorescent chemosensors. **H. Deuermeyer**, A. Luhrs, L.D. Margerum **none** . Analysis of S-Au-P bonding in phosphine gold(I) polyfluorothiolates: Backbonding and weak interactions. **G. Moreno-Alcantar**, J.M. Guevara-Vela, H. Torres
- . Photodynamic therapy of cancer using sterically strained ruthenium complexes. R.S. Khnazyer, N. Mansour, S. Mehanna, R.I. Taleb, M. Mroueh, M. ElSibai, **C.F. Daher**
- . B₁₂(OR)₁₂ Reagents as tunable one-electron oxidants. **P. Chong**, M. Messina, J.C. Axtell, Y. Wang, B. Upton, B.M. Hunter, S. Khan, J.R. Winkler, H.B. Gray, A. Alexandrova, H.D. Maynard, A.M. Spokoyny
- . Synthesis of a novel multitopic nonchelating N-heterocyclic carbene. **D. Tapu**, **A. Carter**, **R. Justice**, **R. Hooper**, O. Kuykendall, M. Baker, G. Bettler, A. Changas, A. Mason
- . Synthesis and characterization of magnetic nanocomposites for energy storage applications. **B. Shen**, S. Sun
- . Combined effects of peripheral fluorine and central metal on phthalocyanine properties. **R. Szlag**, M.A. Kaster, E.R. Trivedi
- . Oxidation of an iridium hydride pincer complex by O₂: A DFT study. **J. Williams**, A.M. Wright, K.I. Goldberg, T.R. Cundari
- . Mechanistic insight into nitrite to nitric oxide conversion at copper(I) and copper(II) sites. **Z. Sakhaei**, S. Kundu, J. Donnelly, T.H. Warren
- . Ethylene insertion polymerization in the presence of organic radicals - Exploiting mechanistic insights to influence microstructures. **S. Stadler**, F. Ölscher, I. Göttker-Schnetmann, V. MONTEIL, S. Mecking
- . Redox switchable catalysts for the synthesis of block copolymers and crosslinked polymers. **K.R. Delle Chiaie**, A.B. Biernesser, J.A. Byers
- . Rhenium-oxo and gold corroles: Synthesis, spectroscopy, and application to photodynamic therapy. **R.F. Einrem**, A. Alemayehu, O.A. Gederaas, **A. Ghosh**
- . Metal-free peralkylation of the *closo*-hexaborate dianion, B₆H₆²⁻. **J. Axtell**
- . Design of biotemplated titanium dioxide nanoparticles for potential application as anodes in dye-sensitized solar cells. **A. Reyes-Oliveras**, G. De Jesus-Morales, V. López-Mejías
- . Difluoroboron β -diketonate polyactides as luminescent oxygen sensing materials for wound imaging. **C.A. DeRosa**, S.A. Seaman, A.S. Mathew, C.M. Gorick, Z. Fan, J.N. Demas, S.M. Pearce, C. Fraser
- . Comparative reactivity studies of iridium(I) and rhodium(I) complexes

stabilized by chelating diphosphine ligands. **K. Olsen**, S.H. Schreiner

Landscape of ligandable membrane cysteinome and its role in modulating immune response.

E.V. Vinogradova, K.M. Backus, M. Blewett, B.F. Cravatt

. HDX-MS reveals metal-specific structural changes important to DNA binding by the cobalt and nickel responsive transcriptional regulator, RcnR. **H. Huang**, M.J. Maroney

. Effects of acid strength and position of an intramolecular acidic functional group on the catalytic reduction of CO₂ to CO. **S. Lense**, I.A. Guzei, K. Thao, J. Andersen, M. Schultz

. Facile fabrication of recyclable magnetic oxide@MOF nanocomposites for aerobic oxidation of benzylic C-H bonds. **G. Wang**, S. Fan, H. Gao, J. Wang, D. Jia

. Synthesis and characterization of cationic silver(I) coordination polymers for photoluminescent properties. **E. Soe**, J. Kim, S. Oliver

. Topochemical intercalation and ion-exchange of layered iron sulfides via low-temperature hydrothermal routes. **X. Zhou**, B. Wilfong, H.K. Vivanco, E.E. Rodriguez

. Reversible formation an Fe^{III}-O-Ce^{IV} intermediate from the reaction of Fe^{IV}=O and Ce^{III}. **a. draksharapu**, J. Klein, W. Rasheed, C.J. Cramer, L. Que

. Modulation of a weakly coupled peroxo-dicopper(II) complex by interaction with alkali metal ions. **L. D'Amore**, M. Swart, A. Brinkmeier, F. Meyer

. Tuning the proton-coupled electron-transfer reactivity of Mn(III)-hydroxo complexes via ligand perturbations. **D. Rice**, A. Burr, T.A. Jackson

. Towards broadband-emitting 2D-perovskites LEDs. **P. Carmona Monroy**, D. Solis, E. Perez Gutierrez

. Soft-templating strategies for anisotropic Au nanomaterials and hollow multi-Au@SiO₂ nanosystems. **H. Yoo**

. Exploring biphasic routes to functionalized CdSe nanoparticles for use in solar nanocomposites.

K. Bolduc, **M.E. Hagerman**, J.D. Kehlbeck

. Acid-catalyzed hydroxylation of iodododecaborate. **Z.S. Lincoln**, J.A. Dopke, R.J. Staples

. Synthesis and characterization of energetic nitroformate salts. **A. Baxter**, I. Martin, K.O. Christe, R.M. Haiges

. Crystallography in MOF: Ordering guest molecules by coordination assisted orientation control. **L. Wang**, S. Cohen

. Film formation from peroxo hexatantalate precursors. **R.H. Mansergh**, L.B. Fullmer, D. Park, J.M. Amador, M.D. Nyman, D.A. Keszler

Trends in NMR chemical shifts of d⁰ transition metal compounds. **Z. Xue**, T.M. Cook, A.C.

Lamb

. Diaquo ruthenium water oxidation catalysts with a novel biimidazolyl backbone. **J.M. Kamdar**, C.E. Moore, A.L. Rheingold, D.K. Smith, D.B. Grotjahn

. Correlating redox potential with ⁵¹V NMR chemical shifts for vanadium (V) catecholates. **J.T. Koehn**, P. Chatterjee, C.N. Beuning, A. Waterhouse, T. Lucia, T.E. Polenova, D.C. Crans

. Copolymerization of cyclohexene oxide with carbon dioxide catalyzed by dinuclear iron complex bearing a phenylene-bridged bis(tripodal N₂O₂) ligand. **s. zhan**, Q. Jiang, Z. Song

. Model studies of catalytic olefin chain growth in the presence of biological impurities. **F.P. Wimmer**, I. Götter-Schnetmann, S. Mecking

. Development of coordinatively unsaturated, low-valent metal isocyanide MOFs. **A. Arroyave**,

D. Agnew, J.S. Figueroa

. Synthesis and characterization of organometallic compounds of coinage metals relevant to catalysis. **S. Martínez de Salinas Uzquiza**, Á. Mudarra, M. Pérez-Temprano

. Mechanistic studies on the oxidative addition of aryl halides to COBALT(I) complexes. **M. Perez-Temprano**, J. San Jose, D. Gallego

. Synthesis and Characterization of Cr(0) terminated π-linkers based on linear oligoazulenic frameworks. **N.R. Erickson**, M.V. Barybin

. Heterobimetallic complexation of a mercapto and isocyano functionalized linear 6,6'-biazulenic π-linker: Synthesis, redox behavior, and spectroscopic characterization. **J.C. Applegate**, N.R. Erickson, M.V. Barybin

. Glycoconjugates of organometallic ruthenium-arene complexes. **L. Miller**, **L. Kennington**, L. Wisniewski, M. Burnatowska-Hledin, A.L. Eckermann

. Fluorinated pyrrolic macrocycles for biological imaging: Optical properties and aggregation in solution. **M.A. Kaster**, R. Szlag, K. McAuliffe, E.R. Trivedi

. Synthetic models of Ni-thiolate coordination units in biology. **R.A. Steiner**, T.C. Harrop

. Vanadium-Dependent Haloperoxidase Enzymes: A Review of Mechanism, Structure/Functional Relationships, and Coordination Environments. **K.**

Doucette, C. Wallace, C.C. McLaughlan, D.C. Crans

. Comparison of 2,2'-bipyridine and 1,10-phenanthroline ancillary ligands in ruthenium metal complexes containing the 4,4'-dihydroxy-2,2'-bipyridine ligand. **A.E. Kuhn**, D.J. Charboneau, M.J. Kasher, N.A. Piro, W.S. Kassel, T. Dudley, J.J. Paul

. Synthesis of novel mixed O, N, S donor ligands. **E. Jugovic**, C. Hamaker

. Iron (II) pyridinediimine complexes with Lewis acids in the secondary coordination sphere.

K.T. Burns, M. Delgado, J.M. Ziegler, J.D. Gilbertson

. Synthesis and characterization of multinuclear manganese carboxylate coordination compounds by incorporating the anion of 3-(dimethylamino)-1,2-propanediol. **M. Reagan**, A. Saha

. Formation of radical anions on the dipyrin-1,9-dione scaffold of heme metabolites. **R. Gautam**, E. Tomat

. Coupling of chromophoric dyes with applied bias or microwave heating to increase DSSC photoconversion efficiency. **C.A. Sweet**, **C. Flynn**, C.J. Timpson, C. Murphy

. Reduced copper metal-organic frameworks: A heterogeneous catalyst for click chemistry. **K. Xie**, Q. Fu, P. Webley, G.G. Qiao

. Impact of rare-earth dopants on the catalytic activity of CeO₂ nanoparticles for both CO oxidation and preferential CO oxidation reactions. **J. Yoo**, K. Kim, J. Han, W. Jung

. Mössbauer spectroscopy: Predictive property models from experimental design and statistical learning. **J. Proppe**, M. Reiher

. Acid reactions of model systems of molybdoenzymes. **K. Schwalenstocker**

. Achieving surface sensitivity in soft x-ray spectroscopy: Transient reflectivity of charge transfer dynamics in iron oxide. **A. Cirri**, J. Husek, S. Biswas, L. Baker

TUESDAY MORNING

Section A

Venue

Placeholder

Gabor A. Somorjai Award for Creative Research in Catalysis: Symposium in honor of John E. Bercaw

N. Hazari, *Organizer*

A. Hazari, *Organizer, Presiding 8:30*. Thermodynamic efficiency, chemoselectivity and turnover frequency in chemical and electrochemical catalysis: Synergistic

principles for catalyst development and optimization. **S.S.**

Stahl

8:55. Recent advances in Ti-catalyzed nitrene transfer reactions. **I. Tonks**, E. Beaumier, H. Chiu, Z.W. Davis-Gilbert, X. See, A.C. Wotal

9:20. Selective indium and zinc catalysts for controlled polymerization of cyclic esters. **P.**

Mehrkhodavandi, T. Ebrahimi, L. Chile, A. Kremer, S. Hatzikiriakos

9:45. Selective catalytic trimerization of alkenes. **J.A. Labinger**

10:10 Intermission.

10:25. Cobalt-catalyzed methods for the polyborylation of hydrocarbons.

P.J. Chirik, N. Palmer, S. Krautwald

10:50. Group 4 metal complexes for the formation of block copolymers. **P. Diaconescu**

11:15. Mechanism of formic acid dehydrogenation by a diiridiumtrihydride catalyst. J. Celaje, Z. Lu, E.A. Kedzie, **T.J. Williams**

11:40. Metal-oxos in chemistry and biology. **H.B. Gray**

12:05 Concluding Remarks.

Section B

Venue

Placeholder

Celebrating 60 Years of the Division of Inorganic Chemistry Award Winners

M. J. Clarke, *Organizer*

D. C. Crans, *Organizer, Presiding*

K. Bowman-James, K. N. Raymond, *Presiding*

8:00 Introductory Remarks.

8:05. Synthesis of multinary transition metal chalcogenide nanoparticles for applications in photovoltaics. M. Braun, L. Korala, **A.L. Prieto**

8:35. Probing anisotropy in molecular magnetism. **K.R. Dunbar**

9:05. Learning from computational studies of NMR chemical shifts: The case of a main group atom in transition metal complex. C. Raynaud, S. Halbert, C. Coperet, **O.G. Eisenstein 9:35**. Chemical surprises at the frontier of the periodic table. **J.L. Kiplinger**

10:05 intermission.

10:20. X-ray spectroscopic studies of biological dinitrogen reduction in molybdenum and vanadium nitrogenases. **S. DeBeer**

10:50. Pyridinol Based Ligands for Transition Metal Catalyzed Reduction of CO₂ and Related Substrates: Elucidating the Role of Lewis Acids. **E.T. Papish**, S. Siek, D.B. Burks, C.

Boudreaux, D.L. Gerlach, G. Liang, D.B. Grotjahn, C.E. Webster
11:20 . Technetium, the first radioelement in the periodic table. **A.P. Sattelberger**, E. Johnstone, M.A. Yates, f. poineau, K. Czerwinski
11:50 . Design of azurin that spans the entire 2V range of physiological redox potentials and its application in engineering a copper protein that performs fast and reversible S-nitrosylation. **Y. Lu**, P. Hosseinzadeh, S. Tian, J. Liu

Section C

Venue
Placeholder

Undergraduate Research at the Frontiers of Inorganic Chemistry Bioinorganic Chemistry

A. K. Bentley, C. Nataro, S. R. Smith, *Organizers*

S. A. Toledo, *Presiding*

9:00 . Structural, spectroscopic and reactivity studies of the first structural model of the resting state of Nickel Acireductone Dioxxygenase (Ni-ARD). **D. Ivan**, S.A. Toledo, V. Lynch

9:20 . Protein charge effects on Rieske protein reduction potentials. **K.R. Hoke**, A.L. Watkins, R.J. Quarles

9:40 . Modelling the O-O bond formation step in the oxygen-evolving complex. **E. Hanada**, J. Kovacs

10:00 . Trinuclear ruthenium complexes with diimine ligands: Experimental and computational investigations of biological activity. **F.A. Beckford**

10:20 Intermission.

10:35 . Improved photocatalytic activity of hybrid P450 biocatalysts by tuning the Ru(II)polypyridyl photochemical properties. **H. Shalan**, A. Colbert, T. Nguyen, M. Kato, L.E. Cheruzel

10:55 . Copper transport into the avian oocyte: A second cargo for the vitamin transporter riboflavin binding protein. **S.R. Smith**, M. Benore

11:15 . Photosensitizer-Embedded polyacrylonitrile nanofibers as an antimicrobial non-woven textile. **S. Stanley**, R. Ghiladi

11:35 . Synthesis and conformational analysis of peptides appended to a novel, rigid, cyclic, bimetallic ring system. **T.P. Curran**, A.P. Lawrence, T.S. Murtaugh, W. Ji, N. Pokharel, L.M. Davidson, J.P. Sanderson-Brown, P.R. Handali, V. Nguyen, C. Gober, J. Suitor

11:55 . Rare and unusual square planar copper (I) complexes. **P.A. Cheung**, R. Berger, J.D. Gilbertson

12:15 Concluding Remarks.

Section D

Venue
Placeholder

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

L. M. Berreau, *Organizer*

P. L. Holland, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 . Mechanistic studies of Cu(II)/O₂-promoted oxidative aliphatic carbon-carbon bond cleavage reactions. **L.M. Berreau**

9:00 . Reactivity of mononuclear nonheme cobalt(III)-superoxo complexes. **W. Lee**, C. Wang, K. Yeh

9:25 . Bio-inspired heterodinuclear NiFe catalysts for H₂ production. D. Brazzolotto, L. Wang, M. Gennari, F. Meyer, m. orio, V. Artero, **C. Duboc**

9:50 . Why are O₂ and N₂ so different?. **K.H. Theopold**, F. Dai, E.S. Akturk, Y. Hung, D.C. Cummins, G.P. Yap

10:15 Intermission.

10:30 . Cu(III) as a biological oxidant?. L. Chiang, W. Keown, C. Citek, J.B. Gary, E.C. Wasinger, **T.P. Stack**

10:55 . Modeling nitric oxide signaling chemistry at copper and zinc sites. **T.H. Warren**

11:20 . Studies on the mechanism of Ti-catalyzed nitrene transfer reactions. **I. Tonks**, E. Beaumier, Z.W. Davis-Gilbert, A. Koley, A.J. Pearce, T.A. Wheeler, A.C. Wotal

11:45 . Bioinspired small molecule activation for energy-related catalysis. **F. Meyer**

Section E

Venue
Placeholder

Inorganic Nanomaterials: Structure & Function in 0, 1 & 2 Dimensions

Financially supported by Chemistry of Materials

K. R. Kittilstved, E. J. McLaurin, *Organizers*

B. Guiton, K. J. Koski, *Presiding*

8:30 . Chemistry of nanoconfined water molecules in 1-D metal organic nanotubes. **T. Forbes**

9:00 . Fabrication, characterization and application of carbon nanoparticles for the detection of heavy metal ions in

aqueous media. **A. Wanekaya**, A.M. Simpson, K. Ghosh

9:30 . Micelle encapsulation: A versatile platform for generating multifunctional nanoparticles. **J.O. Winter**

10:00 Intermission.

10:15 . Novel properties and applications of plasmonic metal nanostructures: A case study and recent progress on Hollow Gold Nanospheres (HGNs). **J.Z. Zhang**

10:45 . Synthesis of Core@Shell nanocatalysts with intermetallic interiors. **S.E. Skrabalak**

11:15 . Controlling nanoscopic and atomic segregation of Pt within Pt-Ni rhombic dodecahedra and nanoframes for fuel cell catalysis. **P. Yang**, N. Becknell, Z. Niu

11:45 . Using nanowire arrays as a sensitive tool for understanding copper-antimony anode materials. E.D. Jackson, **A.L. Prieto**

12:15 Concluding Remarks.

Section F

Venue
Placeholder

Emergent Phenomena in the Solid State

B. C. Melot, *Organizer*

E. E. Rodriguez, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 . Understanding the impact of crystal chemistry on the physical properties of garnets. **B.C. Melot**

9:10 . Mixed-Valence and chemical-pressure effects on magnetic properties of ThCr₂Si₂-type pnictides. X. Tan, A. Yaroslavtsev, K. Kovnir, **M. Shatruk**

9:50 . Density functional investigation on the magnetic anisotropy in rare-earth-free metal borides with the Ti₃Co₅B₂-type structure. **Y. Zhang**, B. Fokwa

10:10 . Ground state magnetism in S = 1/2 Li₂MgReO₆ system with orthorhombic crystal structure. J. Milam-Guerrero, C.J. Bloed, P. Nguyen, J.P. Carlo, G. Luke, B.C. Melot, **S. Derakhshan**

10:30 Intermission.

10:50 . Structural and electronic instabilities in electron-doped Sr₃Ir₂O₇: Emergent phenomena at the edge of the spin-orbit Mott state. **S. Wilson**

11:30 . Electron doping a kagome spin liquid. **Z. Kelly**, M.J. Gallagher, T. McQueen

11:50 . Magnetic properties of osmium mixed-metal double perovskites. **C. Thompson**, X. Fu

Section G

Venue
Placeholder

ACS Award in the Chemistry of Materials: Symposium in honor of Douglas A. Keszler

Materials Chemistry of Solutions & Solids for a Sustainable Future

Cosponsored by BMGT[‡], MPPG and PROF[‡]

J. L. Bryant, J. C. Giordan, *Organizers*

S. E. Hayes, B. L. Maddux, *Organizers, Presiding*

8:30 Introductory Remarks.

8:40 . Nonlinear optical borates based oxides for solid state laser frequency conversion in the UV range. **G. AKA**, J. REN, P. LOISEAU

9:00 . Atomic solid state energy scale. **J.F. Wager**, D.A. Keszler

9:20 . Chalcogenide semiconductors as p-type transparent conductors, absorbers and alloys. **J. Tate**

9:40 . Characterization of CSMC resists and other nano-material structures: Results and methods. **E.L. Garfunkel**

10:00 Intermission.

10:30 . Solution-Deposition of disordered RuO₂ nanoskins: An example from the fourth quadrant of electronic materials. **D.R. Rolison**

10:50 . New functional materials as a design problem. **A. Zunger**

11:10 . Creating a one-stop platform for computed XAS and NMR materials data and comparison algorithms on the Materials Project. **K. Persson**

11:30 . Solid-state NMR of thin metal oxide films from prompt inorganic condensation. B.A.

Hammann, Y. Afriyie, M. Kast, C.K. Perkins, P. Plassmeyer, D.W. Johnson, D.A. Keszler, C. Page, S.W. Boettcher, **S.E. Hayes**

11:50 . Metal-oxo clusters from across the periodic table. **M.D. Nyman**

12:10 . Aqueous inorganic coordination clusters: Synthesis, solution speciation, structure, and their use as inks for materials. **D.W. Johnson**

Section H

Venue
Placeholder

Spectroscopic Elucidation of Metalloenzyme Mechanism: Current Successes & Future Challenges

Cosponsored by BIOL

Financially supported by Northwestern U, U of California-Davis

J. A. Telser, *Organizer*

V. DeRose, *Organizer, Presiding*

8:30 . Cytochrome P450 oxidations: A controlled burn of inert organic compounds. **M. Green**

9:00 . Bifunctional peroxidases (KatGs): A challenging family of enzymes for understanding putative evolutionary strategies in fine-tuning the oxidation reactions catalyzed by heme-Trp[•] intermediates and related e⁻ transfer mediated by Trp[•]/Tyr[•]. P.C. Loewen, **A. Ivancich**

9:30 . Mechanistic studies on the radical SAM enzyme CDG synthase. **V. Bandarian**

10:00 . Decoding a secret handshake: Tracking protein-to-protein Cu(I) transfer by rapid x-ray absorption and intrinsic fluorescence techniques. **K.N. Chacon**

10:20 Intermission.

10:30 . How metal ions in the brain tip the toxic balance of the killer prion protein. **G.L.**

Millhauser

10:50 . On the use of Co(II) to elucidate Zn(II) enzyme mechanism. **D.L. Tierney**

11:10 . Aromatic amino acid hydroxylases: Exploring the details of a catalytic cycle with EPR spectroscopy. **J.L. McCracken**

11:30 . Taking snapshots of the water oxidation reaction in photosystem II with X-ray crystallography and X-ray spectroscopy. J. Yano, **V.K. Yachandra**

12:00 . Ammonia binding to the OEC of Photosystem II, what does this tell us about water binding and O-O bond formation?. **R. Britt**

Section I

Venue

Placeholder

2017 Priestley Medalist: Symposium in honor of Tobin J. Marks

Conjugated Polymeric Materials

Cosponsored by PMSE

Financially supported by Dow-Dow Corning, ExxonMobil, STRENGTH, Argonne National Lab, Northwestern University A. Facchetti, T. Lohr, *Organizers* B. M. Savoie, *Presiding*

9:00 Introductory Remarks.

9:05 . Designing responsive piezomaterials from the bottom up: Learning from nonlinear optical materials. **G. Hutchison**, W.S. Horne, C.W. Marvin, H.M. Grimm

9:35 . Polymers and polymer composites for flexible opto-electronic devices. **A. Facchetti**

10:05 . Conjugated polymers and doping strategies for conductive layers and thermoelectric compositions. **H.E. Katz**

10:35 Intermission.

10:45 . Interfacial engineering of two-dimensional nanoelectronic heterostructures. **M. Hersam**

11:15 . Electronic processes, morphologies and structural-functional correlations in low bandgap oligomers and polymers for OPV. **L.X. Chen**

11:45 . Organic polymers for photovoltaics: Small structural differences yield large performance changes. **J.R. Reynolds**

Section J

Venue

Placeholder

Chemistry is Central to Applied Materials

C. J. Chang, *Organizer*

C. R. Bertozzi, M. A. Paley, *Organizers, Presiding*

8:30 . Dynamic MOF SBUs as active sites for small molecule reactivity and catalysis. **M. Dinca**, E. Metzger, R. Comito, C. Brozek, H. Park, C. Hendon

9:05 . Physical chemistry of nanocrystals with the graphene liquid cell. **P. Alivisatos**

9:40 . Mucin-inspired thermoresponsive synthetic hydrogels induce stasis in human pluripotent stem cell colonies. **S.P. Armes**

10:15 Intermission.

10:30 . Interactions at the nano-bio interface. **C.J. Murphy**

11:05 . Computationally guided discovery of metal-decorated metal-organic frameworks active for catalysis. **L. Gagliardi**, V. Bernales, M.A. Ortuno, A. Mavrandonakis, Z. Li, D. Yang, O.K. Farha, C.J. Cramer, B.C. Gates, J.T. Hupp

11:40 . Grain boundary effects in electroreduction catalysis. **M. Kanan**

Section K

Venue

Placeholder

Switchable Catalysts

J. A. Byers, P. Diaconescu, *Organizers* A. J. Boydston, A. M. Spokoyny, *Presiding*

8:30 . Switchable catalysis in precision polymerizations in aqueous and organic media. **M. Sawamoto**

9:00 . Organomimetic boron cluster photosensitizers. **A.M. Spokoyny**

9:30 . Stereocontrol in photochemical reactions. **T.P. Yoon**

10:00 . Switchable catalysis in ATRP. **K. Matyjaszewski**

10:30 . Redox-Switchable iron-based polymerization catalysts. **J.A. Byers**, A.B. Biernesser,

K.R. Delle Chiaie, J.A. Kehl, M. Qi, A.W. Sudyn

11:00 . Factors controlling the activity of Fe-based catalysts for the polymerization of lactide and epoxides. **C.J. Cramer**, B. Dereli, M. Ortuño

11:30 . Redox-mediated metal-free ring-opening metathesis polymerization. **A.J. Boydston**, L. Pascual, T. Kensy, D. Lee, J. Vandenbrande, N. Alrashdi

12:00 . New avenues in synthesis via organic photoredox catalysis. **D.A. Nicewicz**

Section L

Venue

Placeholder

Chemistry of Materials: Nanomaterials

C. G. Lugmair, *Organizer*

R. Beaulac, W. Feng, *Presiding*

8:00 . Quantifying cation exchange of Cd²⁺ in ZnTe: A challenge for accessing type II heterostructures. **M. Enright**, H. Sarsito, B. Cossairt

8:20 . Room-temperature synthesis of metal chalcogenide nanocrystals from N-heterocyclic carbene synthons. **H. Lu**, R.L. Brutchey

8:40 . Design of colloidal semiconductor nanocrystals for enhanced absorption and band edge tuning exceeding 2.0 eV. **D. Kroupa**, M.V. Vörös, N.P. Brawand, B. McNichols, E. Miller, J. Gu, A.J. Nozik, A. Sellinger, G.A. Galli, M.C. Beard

9:00 . Colloidal synthesis of transition metal dichalcogenide nanostructures. **Y. Sun**, Y. Wang, D. Sun, B.R. Carvalho, C. Read, C. Lee, Z. Lin, K. Fujisawa, J.A. Robinson, V.H. Crespi, M. Terrones, R.E. Schaak

9:20 . Design, fabrication and modification of advanced fluorescent polymer based on ordered quantum-dots from nanoscale to large production. **S. Chen**

9:40 . Native phosphine surface ligand exchange on plasma-synthesized indium phosphide nanocrystals. **N.R. Neale**, N.D. Bronstein, L. Wheeler, N.C. Anderson

10:00 . Single-enzyme direct biomimetalization of metal chalcogenides nanocrystals with tunable optical properties. **L. Spangler**, Z. Yang, R. Dunleavy, A. Sadeghnejad, R. Chu, L. Lu, C.J. Kiely, B. Berger, S. McIntosh

10:20 Intermission.

10:35 . Synthesis and characterization of colloidal CsPbX₃ nanowires. **D. Zhang**, Y. Yang, Y. Bekenstein, Y. Yu, N. Gibson, A.B. Wong, S.W. Eaton, L. Dou, S.R. Leone, P. Alivisatos, P.

Yang

10:55 . 2D redox-active superatom frameworks. **A. Champsaur**, C.P. Nuckolls

11:15 . Modulation of electrical and optical properties of tungsten disulfide. **S. Chee**, M. Son, G. Son, H. Jang, M. Ham

11:35 . Chiral semiconductor helices at the mesoscale. **W. Feng**, J. Kim, X. Wang, H.A. Calcaterra, Z. Qu, L. Meshi, N. Kotov

11:55 . Photoredox processes involving colloidal quantum dots: Surface states, structural inhomogeneities, and ultrafast hole extraction. C. Mi, M. Saniepay, P. Dutta, Y. Tang, J.A. McGuire, **R. Beaulac**

12:15 . Synthesis of heterostructured nanocrystals with pre-programmable compositions and spatial arrangements. **X. Li**, R.E. Schaak

Glenn T. Seaborg Award for Nuclear Chemistry: Symposium in honor of David L. Clark Sponsored by NUCL, Cosponsored by INOR

Metalloprotein-Initiated Signaling Transduction Response to Redox Stress

Sponsored by BIOL, Cosponsored by INOR

Multicenter Molecules & Coupled Molecular Assemblies: Synthesis, Characterization & Theory Applications & Devices

Sponsored by PHYS, Cosponsored by INOR

Frontiers in Heavy Element Electronic Structure: A Tribute to Bruce Bursten

Sponsored by NUCL, Cosponsored by INOR

Support & Activator Effects on Metal Mediated Polymerization

Sponsored by PMSE, Cosponsored by CATL and INOR

Light-Driven Chemistry: Photoelectrochemistry & Photocatalysis

Molecular & Bio-Inspired Photocatalysts

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

Deposition & Etching of Nanostructures

Sponsored by COLL, Cosponsored by INOR

TUESDAY AFTERNOON

Section A

Venue			
Placeholder			
Chemistry of Materials: Synthesis & Properties			
C. G. Lugmair, <i>Organizer</i>			
B. Boardman, J. M. Szarko, <i>Presiding</i>			
1:30 . Highly efficient emitters for Organic Light Emitting Diodes (OLEDs) based on intramolecular rotation and spin-state inversion. M. Bochmann , A.S. Romanov, D. Di, L. Yang, D. Credgington, M. Linnolahti			
1:50 . Boron containing perovskite single crystal for thermal neutron detection. M.L. Higgins , F. Ely, M. Quevedo-Lopez			
2:10 . Molecular doping approach for metal oxide photosensitization. D. Jung , L.M. Saleh, Z. Berkson, J. Hwang, M.F. El-Kady, E. Titarenko, Y. Shao, K. McCarthy, A.I. Wixtrom, J. Guo, I.B. Martini, S. Kraemer, E.C. Wegener, J. Ciston, J.L. Brosmer, J.I. Zink, J.T. Miller, X. Duan, R.B. Kaner, B.F. Chmelka, A.M. Spokoiny			
2:30 . Sensitized Eu ^{III} and Tb ^{III} emission by functionalized polycarbonate-based materials. R.A. Tigaa , X. Aerken, A. Fuchs, A. De Bettencourt Dias			
2:50 . Crystal structure effects on the Davydov splitting of electronically active conjugated systems. J.M. Szarko , A. Austin, X. Zhu, F.C. Spano, N. Hestand, M. Zdilla			
3:10 . Broadband white-light emission in two-dimensional layered lead-bromide perovskites. T. Hu, M.D. Smith , E. Dohner, M. Sher, X. Wu, M. Trinh, A. Fisher, J. Corbett, X. Zhu, H. Karunadasa, A. Lindenberg			
3:30 Intermission.			
3:45 . Micropasma-assisted synthesis of GQD-AgNP nanohybrids with enhancing light-matter coupling for SERS-based detection. W. Chiang, K. Lin			
4:05 . Direct polymerization of cobalt chalcogenide clusters for hybrid photovoltaic materials. B. Boardman , D.A. Corbin			
4:25 . Aiming for the heteroatom control in the synthesis of polyoxometalates. L. Vilà Nadal, J. Mathieson, L. Cronin			
4:45 . Luminescent gold(I)-thiophenolate coordination polymers as phase change materials and precursors for the formation of multifunctional nanocomposites. A. Demessence , O. Veselska, N. Guillou, M. Monge, g. ledoux, A. Fateeva, P. Bordet 5:05			
Insulator-to-semiconductor transition in a porous vanadyl Prussian Blue analog upon air exposure. M. Manumpil , C. Leal Cervantes, M.R. Hudson, C.M. Brown, H.I. Karunadasa			
5:25 . Preparation and properties of tetrathiafulvalene radical cation heavy metal (Pb, Bi) iodide hybrid materials. H. Evans , J. Labram, A. Lehner, S. Smock, M.L. Chabinye, R. Seshadri, F. Wudl			
	Section B		
Venue			
Placeholder			
Celebrating 60 Years of the Division of Inorganic Chemistry Recent Officers			
M. J. Clarke, D. C. Crans, <i>Organizers</i>			
B. T. Donovan-Merkert, S. Koch, D. J. Mindiola, <i>Presiding</i>			
1:30 Introductory Remarks.			
1:35 . Bioinorganic systems for artificial photosynthesis. K. Bren , S. Chakraborty, P. Lamberg, B. Kandemir, T. Krauss			
2:05 . Generation and characterization of primary copper(I)-dioxygen adducts. K.D. Karlin			
2:35 . Spectroscopic studies of molecular magnetism. Z. Xue , S.E. Stavretis, D.H. Moseley, A.A. Podlesnyak, C.M. Brown, L.L. Daemen, Y. Cheng, A.J. Ramirez-Cuesta, X. Wang, C.M. Hoffmann, S.O. Diallo, K. Thirunavukkuarasu, Q. Chen, H. Zhou, J. Ludwig, D. Smirnov, Z. Zhu, M. Guo, J. Tang, H. Cui, F. Fei, X. Chen			
3:05 . Coordination chemistry of Fe(II) and Fe(III) MRI contrast agents. J.R. Morrow , P.B. Tsitovich, E. Snyder			
3:35 Intermission.			
3:50 . Synergism of two alkali metals in self-assembly of novel supersized heterobimetallic sandwich compounds. M.A. Petrukhina			
4:20 . Photomechanical Effects from Ruthenium Sulfoxide Polymers. M. Livshits, J. Shin, J. Rack			
4:50 . Visible light-induced solid-state CO-releasing compounds. L.M. Berreau , S. Anderson, M. Larson			
5:20 Excited state reactivity of transition metal complexes. C. Turro			
	Section C		
Venue			
Placeholder			
Organometallic Chemistry: New Ligand Platforms Pincer Ligands			
N S. Radu, <i>Organizer</i>			
O Ozerov, A. Rahman, <i>Presiding</i>			
1:30 . Pyrazine-based gold(III) pincer complexes: Synthesis and Luminescence. J. Fernandez-Cestau , L. Currie, L. Rocchigiani, B. Bertrand, M. Bochmann, T. Penfold			
1:50 . Pincer multifunctionality, together with reduced Fe, cleaves N ₂ . B.J. Cook, C. Chen, A. Hickey, K.G. Caulton			
2:10 . New chemistry of pincer-supported rhenium. A.J. Kosanovich , W. Shih, O. Ozerov			
2:30 . C-H activation and functionalization with PNP rhodium pincers: Stoichiometric reactivity and catalysis. J. Gair			
2:50 . New insight into C-H borylation with iridium pincer complexes. O. Ozerov , L.P. Press, A.J. Kosanovich, C. Lee			
3:10 . Bis-N-heterocyclic carbene pincers as versatile ligand platform for uniquely active ester hydrogenation homogeneous catalysts. R. van Putten , G. Filonenko, L. Lefort, E. Hensen, E. Pidko			
3:30 . Development of new cobalt pincer complexes for catalytic applications. Y. Li, J.A. Krause, H. Guan			
3:50 . Iron pincer complexes with isonitrile ancillary ligands for formic acid and methanol dehydrogenation. N. Smith , N. Hazari			
4:10 . Computational investigation of ester and amide hydrogenation by aliphatic Fe and Ru PNP complexes. Z. Culakova , E. Clot, K.I. Goldberg, O.G. Eisenstein			
4:30 . Hydrogenation of carboxylic carbonyl derivatives (C=O, C≡N) catalyzed by iron and cobalt pincer complexes or particles. H. Dai , J.A. Krause, H. Guan			
4:50 . Synthesis and studies of naphthaquinone and anthraquinone derived iridium Pincer catalysts for the conversion of ethanol to butanol. A. Rahman , W.D. Jones, M. Wiklow-Marnell			
5:10 . Synthesis and characterization of new C ^α C ^β N Pincer-type palladium complexes containing N-heterocyclic carbene ligands. J. Yan , Z. Zhu, Y. Wang, J. Niu, X. Zhu, X. Hao, M. Song			
	Section D		
Venue			
Placeholder			
ACS Award for Distinguished Service in the Advancement of Inorganic Chemistry: Symposium in honor of William B. Tolman			
P. L. Holland, <i>Organizer</i>			
L. M. Berreau, <i>Organizer, Presiding</i>			
1:30 Introductory Remarks.			
1:35 . Nacnac doesn't fall far from the tree: Activation of N ₂ with diketiminate complexes. P.L. Holland			
2:00 . Inorganic chemistry: A salute and a challenge. R. Eisenberg			
2:25 . Nickel-sulfido and nickel-selenido complexes: Preparation, spectroscopy and C-H activation. C.G. Riordan			
2:50 . Greater than the sum of their parts: Heterodinuclear polymerization catalysts. C.K. Williams			
3:15 Intermission.			
3:30 . Innovation and potential career paths in industry. N. Aboeella			
3:55 . Copper transport in methanotrophic bacteria. G.E. Kenney , L.M. Dassama, S.Y. Ro, A.C. Rosenzweig			
4:20 . Factors controlling the activity of Al-based catalysts for the ring-opening transesterification polymerization of caprolactone. C.J. Cramer , B. Dereli, C. Dunbar, J. Freeze, M. Johnson, M. Mandal, D. Marell, H. Vazquez Lima			
4:45 . How is metal covalency reflected in ligand field parameters?. F. Neese , E. Suturina, M. Atanasov			
	Section E		
Venue			
Placeholder			
Bioinorganic Chemistry: DNA, RNA & Inorganic Drugs			
S. A. Koch, <i>Organizer</i>			
J. P. Selegue, A. D. Tinoco, <i>Presiding</i>			
1:30 . Synthesis, characterization and DNA interaction studies of potential anticancer titanium complexes with biologically relevant ligands. M. Mahroof-Tahir , L. Sreerama, Z.E. Mahmoud , A. Al Dawood, E.M. Looli			
1:50 . Inter-duplex distance distributions in metal-modified peptide nucleic acids measured by double electron-electron resonance. A. Sargun , A. Jarvi, S.K. Saxena, C. Achim			
2:10 . Identifying cancer-relevant DNA damage via a charge transfer			

mechanism involving [4Fe4S] cluster proteins. **E. Tse**, J.K. Barton

2:30 . Divalent copper complexes as Influenza A inhibitors. **J.D. Lynch**, N.A. Gordon, K.L. McGuire, S.K. Wallentine, G.A. Mohl, R.G. Harrison, D.D. Busath

2:50 . N-Heterocyclic carbene gold(I) complexes conjugated to DNA-aptamers for targeted drug delivery. **W. Niu**, X. Chen, W. Tan, A.S. Veige

3:10 . Regulating photochemistry and nucleic acid targeting of Ru(II) complexes. **P.C. Glazer**

3:30 intermission.

3:40 . Build-In fluorescent M24L8 octahedral metal organic molecular cages for nuclearpenetrating pH-responsive drug delivery. **Y. Fang**

4:00 . Ruthenium complexes as new pH-dependent switchable metallodrugs. **F. Martinez-Peña**, A.M. Pizarro

4:20 . Expanding the therapeutic potential of the iron chelator deferasirox in the development of aqueous stable Ti(IV) anticancer complexes. **A.D. Tinoco**, S. Loza, A.M. Vázquez, S.C. Perez,

Y. Delgado, K. Gaur, K.I. Rivero, L.J. Negron, T.B. Parks, C. Munet-Colon

4:40 . Low-symmetry boron subphthalocyanines as fluorescent imaging probes and precursors for designer metallophthalocyanines. L. Sejdarasi, K. McAuliffe, R. Szlag, M.A. Kaster, **E.R. Trivedi**

5:00 . Mixed polypyridyl/N-heterocyclic carbene complexes as potential cytotoxic pro-drugs.

J.P. Selegue, R.T. Ryan, J. Mahmoud, P.C. Glazer

5:20 . Targeting ErbB tyrosine kinases with platinum-functionalized small molecule inhibitors.

M. Yang, H. Wu, T.K. West, C.M. Furdui, G.L. Kucera, U. Bierbach

Section F

Venue

Placeholder

Emergent Phenomena in the Solid State

E. E. Rodriguez, *Organizer*

B. C. Melot, *Organizer, Presiding*

1:30 . Structure and magnetic properties of the 3d transition metal formate-chlorides. **K. Kovnir**

1:50 . Site identity and importance in fluorite-related transparent conductors.

K. Rickert, A. Dolgonos, **K.R. Poepplmeier**

2:10 . Adventures in the Ti-Au binary: Iron man and beyond. **E. Morosan**

2:50 . Soft chemical control of iron-based superconductors and related

compounds. **S. Clarke** **3:30** Intermission.

3:50 . Competing orders in the 12 Fe based superconducting family under chemical doping and external pressure. **N. Ni**

4:30 . Hydride route for the synthesis of 122 iron arsenide superconductors. **Y. Zaikina**, M. Kwong, B. Baccam, S. Kauzlarich

4:50 . Layered transition metal chalcogenides based on square lattices as functional materials. X. Zhou, B. Wilfong, H.K. Vivanco, **E.E. Rodriguez**

5:25 Concluding Remarks.

Section G

Venue

Placeholder

ACS Award in the Chemistry of Materials: Symposium in honor of Douglas A. Keszler Chemists Leading the Charge: Chemists Using Business Acumen & Transformative Research to Address Societal Needs

Cosponsored by BMGT[†], MPPG, PRES and PROF[‡]

S. E. Hayes, B. L. Maddux, *Organizers* J. L. Bryant, J. C. Giordan, *Organizers, Presiding*

1:30 . Opening overview: Chemists using business acumen and transformative research to address societal needs. **J.C. Giordan**

1:40 . Importance and value of fundamentally inspired use, use-inspired, and market-informed research. **D.A. Keszler**

2:00 . Science behind oxide transistors for displays. **J.F. Wager**

2:10 . Science behind materials for ink jet printing. **J.E. Abbott**

2:20 . Transformative science behind metal-based EUV photoresists. **S.T. Meyers**

2:30 . Science behind tunneling electronics. **B. Cowell**

2:40 . Interactive panel: Chemists using business acumen and transformative research to address societal needs. **J.C. Giordan**, D.A. Keszler, J.F. Wager, J.E. Abbott, S.T. Meyers, B. Cowell, J.L. Bryant

3:10 Intermission.

3:30 . Opening overview for panel 2: Next generation innovators. **J.C. Giordan**

3:40 . Panel 2: Research to innovation CSMC legacy: Training the next generation. **M. Dolgos**,

J.M. Amador, **J.C. Ramos**, **J.C. Giordan**

4:10 . Office hours with the speakers. **J.C. Giordan**, D.A. Keszler, J.F. Wager, S.T. Meyers, J.E.

Abbott, B. Cowell, M. Dolgos, J.M. Amador, J.C. Ramos, J.L. Bryant

Section H

Venue

Placeholder

Spectroscopic Elucidation of Metalloenzyme Mechanism: Current Successes & Future Challenges

Cosponsored by BIOL

Financially supported by Northwestern U, U of California-Davis

V. DeRose, J. A. Telsler, *Organizers*

J. Stubbe, *Presiding*

1:30 . Multifrequency pulse EPR studies of the water oxidizing complex in photosynthesis. **W. Lubitz**, N. Cox, D. Pantazis, F. Neese

2:00 . Progress in high-field EPR and ENDOR spectroscopy to study the radical transfer in class I ribonucleotide reductases. **M. Bennati**

2:30 . Nuclear resonance vibrational spectroscopy as a tool for the characterization of low frequency modes in iron proteins. **V. Schünemann**

3:00 . Nuclear magnetic spectroscopic elucidation of MhuD mechanism. **M.D. Liptak**

3:20 Intermission.

3:30 . Spectroscopic approaches to understanding sulfur insertion into aliphatic carbon centers in the biosynthesis of lipoic acid. **S.J. Booker**

4:00 . Novel outcomes and mechanisms emerging from dioxygen activation by non-heme-di-iron enzymes. **J.M. Bollinger**, C. Krebs

4:30 . Unprecedented [FeS] cluster in the core of the hepatitis B infection. **M. Pandelia**, C. Ueda

4:50 . Elucidating the mechanism and magnetic properties of di-iron-oxo proteins via computational quantum chemistry. **J.H. Rodriguez**

5:10 . Nuclear Resonance Vibrational Spectroscopy (NRVS) of FeFe hydrogenase: New evidence of enzyme intermediates. **S.P. Cramer**

Section I

Venue

Placeholder

2017 Priestley Medalist: Symposium in honor of Tobin J. Marks

Materials for Energy Conversion

Cosponsored by PMSE

Financially supported by Dow-Dow Corning, ExxonMobil, STREX, Argonne National Lab, Northwestern University A. Facchetti, T. Lohr, *Organizers* J. R. Reynolds, *Presiding*

1:30 Introductory Remarks.

1:35 . Nitrogen fixation at room temperature, pressure in water using light. **M.G. Kanatzidis**

2:05 . Creation of structurally defined two-dimensional assemblies. **V.P. Coticello**

2:35 . Photosensitization of a CO₂ reduction catalyst with red and near-infrared light using rylenediimide radical anions and dianions. N. LaPorte, J. Martinez, C.M. Mauck, B.T. Phelan, R. Young, **M.R. Wasielewski**

3:05 Intermission.

3:15 . New Polymer Chemistries for Solid Battery Electrolytes. **B.M. Savoie**

3:45 . Solution-processed metal oxide materials for large-area flexible electronics and hydrogen energy devices. **M. Yoon**

4:15 . Novel synthetic approaches for efficient semiconducting materials. **A. Dudnik**

Section J

Venue

Placeholder

Chemistry of Materials: Materials for Energy & Catalytic Applications

C. G. Lugmair, *Organizer*

B. Baruah, Y. Zhou, *Presiding*

1:30 . Porous benzoxazoles as oxygenation catalysts: Case of amine self-coupling. S.

Subramanian, H.A. Patel, Y. Song, **C.T. Yavuz**

1:50 . High power factor and enhanced thermoelectric performance of SnTe: Synergistic effect of resonance level and valence band convergence. **K. Biswas**

2:10 . Diffusion of cations in 2D/3D perovskite films made by melt infiltration. **E. Keenan**, J. Hu, J. Zhi, D.B. Mitzi, W. You

2:30 . New 2D hybrid perovskite systems for optoelectronic applications. **C. Lerner**, S.T.

Birkhold, S.P. Harm, I.L. Moudrakovski, L.M. Schoop, P. Mayer, L. Schmidt-Mende, B.V.

Lotsch

2:50 . Stabilization of the metastable perovskite phase of Formamidinium Lead Triiodide

(FAPbI₃) via surface functionalization. **Y. Fu**, J. Zhai, M. Shearer, S. Jin

3:10 . Interfaces and their influence on oxide ion diffusion in ceria. **A.K. Lucid**, G.W. Watson **3:30**

Intermission.

3:45 . Engineering carbon sheets supported iron nanoparticles for direct synthesis of light olefins. **Y. Zhou**, C. Wang, S. Natesakhawat, J. Leske, D. Kauffman, C. Matranga

4:05 . Cotton fabric immobilized ZnO@AuNP for heterogeneous

catalysis. **B. Baruah**, D. Agyeman, S. Baruah

4:25 . Structural informatics: Its role in understanding metal-organic complexes. **S. Vyas**, A. Sarjeant

4:45 . Charge density mismatch synthesis and application to UZM-35, a material containing both 10MR and 12MR pores. **C.P. Nicholas**

5:05 . Advancing marine hydrokinetic energy technology through materials chemistry. **B.A. Hernandez-Sanchez**, M.R. Hibbs, P.B. Savage

5:25 . Hierarchical structured MnO₂ nanoparticle-embedded SiO₂ nanofibrous membranes with flexibility and enhanced catalytic performance. **L. DOU**, X. Wang, R. Zhang, B. Ding

Section K

Venue

Placeholder

Switchable Catalysts **J. A. Byers**, **P. Diaconescu**, **Organizers** **C. Chen**, **B. K. Long**, *Presiding*

1:30 . ROP of β -lactones: From syndiotactic homopolymers to blocky and chemically tunable alternating copolymers. **C. Jaffredo**, R. Ligny, S.M. Guillaume, **J. Carpentier**

2:00 . Cationic indium catalysts for formation and polymerization of functionalized monomers.

P. Mehrkhodavandi, I. Yu, C. Chang, C. Diaz Lopez

2:30 . Exploring the chemical space of redox-switchable catalysts. **N. Fey**, P. Diaconescu

3:00 . Rare-earth metal-based catalysts for ring-opening polymerization of lactide monomers. **J.**

Okuda

3:30 . Lewis acid and redox control in olefin polymerization. **C. Chen**

4:00 . Modulating polyolefin microstructure and composition via redox-active catalysts. **W.C.**

Anderson, J. Kern, S. Roy, **B.K. Long**

4:30 . Design and development of metal-free light controlled polymer systems. **J. Read De Alaniz**

5:00 . Stereo- and temporal switch coordination polymerization of conjugated dienes and styrene. **D. Cui**, B. Liu, C. Yao

Section L

Venue

Placeholder

Organometallic Chemistry: Catalysis

N. S. Radu, *Organizer*

N. J. Deyonker, A. R. O'Connor, *Presiding*

1:30 . Catalytic and mechanistic evaluation of norbornene polymerization initiated by cationic (π -Allyl) group 10 complexes containing dialkylbiaryl phosphine ligands. **A.R. O'Connor**, C. Lee, M. Kunitomo, N.B. Jones, G.L. Heard

1:50 . Palladium-catalyzed hydrophosphorylation of alkynes: Scope, limitation and mechanism.

L. Han

2:10 . Can alkylation of the N-H functionality within M/NH bifunctional Noyori-type catalysts lead to improved activity?. **P.A. Dub**, J.C. Gordon

2:30 . Hydroarylation of olefins with (pyridyl-indole)Pt^{II} complexes. **B.A. Suslick**, A.L. Liberman-Martin, T. Tilley

2:50 . Mechanistic elucidation of Pd-catalyzed reactions using high resolution electrospray ionization mass spectrometry. **K.L. Walker**, L.M. Dornan, M.J. Muldoon, R.N. Zare, R.M. Waymouth

3:10 . Polymer-supported palladium (II) carbene complexes: Catalytic activity, recyclability and selectivity in C-H acetoxylation of arenes. **M.H. Majeed**, **P. Shayesteh**, **R.L. Wallenberg**, **A.R. Persson**, **N. Johansson**, **L. Ye**, **J. Schnadt**, **O.F. Wendt**

3:30 . Mechanism of Pd-catalyzed decarbonylation of esters to linear α -olefins. **M.A. Ortuno**, B.

Dereli, A. John, H.E. Johnson, M.A. Hillmyer, W.B. Tolman, C.J. Cramer

3:50 . Modeling the selectivity of the Pd-based hydroxycarbonylation of pentenoic acids to adipic acid. **B. Pudasaini**, **A. Genest**, N. Roesch

4:10 . Is an exhaustive conformational search necessary for proposing catalytic mechanisms? An investigation of intramolecular Heck catalysis in the formation of coltoic acid derivatives. **N.J. Deyonker**, T. Ling, R.N. Waltman, F. Rivas

4:30 . Solvent influence into the C_{sp2}-X (X= Cl o Br) bond activation of x-pyridine species by neophylpalladacycle: An experimental study. **O. Serrano**

4:50 . Mechanistic study of the bis(trineopentylphosphine)palladium catalyzed Buchwald-

Hartwig amination reaction. **H. Hu**, K.H. Shaughnessy

Glenn T. Seaborg Award for Nuclear Chemistry: Symposium in honor of David L. Clark

Sponsored by NUCL, Cosponsored by INOR

Multicenter Molecules & Coupled Molecular Assemblies: Synthesis, Characterization & Theory Theory & Modeling

Sponsored by PHYS, Cosponsored by INOR

Frontiers in Heavy Element Electronic Structure: A Tribute to Bruce Bursten

Sponsored by NUCL, Cosponsored by INOR

Deposition & Etching of Nanostructures

Sponsored by COLL, Cosponsored by INOR

Support & Activator Effects on Metal Mediated Polymerization

Sponsored by PMSE, Cosponsored by CATL and INOR

Light-Driven Chemistry: Photoelectrochemistry & Photocatalysis

Novel Photocatalytic & Photoelectrode Materials

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

TUESDAY EVENING

Section A

Venue

Placeholder

Bioinorganic Chemistry: DNA, RNA & Inorganic Drugs

S. A. Koch, *Organizer*

5:30 - 7:30

. Elucidation of the cell death pathways induced by aqueous-stable titanium(IV) compounds as potential anticancer agents. **Y. Delgado**, A.D. Tinoco

. Glycoconjugates of organometallic ruthenium-arene complexes. **L. Miller**, **L. Kennington**, L. Wisniewski, M. Burnatowska-Hledin, A.L. Eckermann . Synthesis, characterization, and in-vitro antitumor activity of copper(II) complexes possessing alky-substituted polypyridyl ligands. **J.F. Eichler**, N. Angel, M. Baird, R.M. Khatib

. Functionalised peptidomimetic metallohelices. **h. song**, S. Allison, S. Shepherd, R. Phillips, P.

Scott

. Photodynamic therapy of cancer using sterically strained ruthenium

complexes. **R.S. Khnazyer**, N. Mansour, S. Mehanna, R.I. Taleb, M. Mroueh, M. ElSibai, **C.F. Daher**

. Design, synthesis and characterization of multifunctional platinum-[benz]acridine agents. **X.**

Yao, M.W. Wright, M. Yang, J. Lee, C.M. Furdul, U. Bierbach

. Synthesis, characterization, and binding properties of metal-based G4 intercalators containing a phosphonium tether. **G.M. Marqus**, M. Dixon, M. Powers, C.H. Leung

. Fluorinated pyrrolic macrocycles for biological imaging: Optical properties and aggregation in solution. **M.A.**

Kaster, R. Szlag, K. McAuliffe, E.R. Trivedi

. Rhenium-oxo and gold corroles: Synthesis, spectroscopy, and application to photodynamic therapy.

R.F. Einrem, A. Alemayehu, O.A. Gederaas, **A. Ghosh** Synthesis and application of silver nanoclusters from DNA templates containing Ag(I)mediated base pairs. **J. Léon**, D. Gonzalez-Abradelo, G. Wilde, M. Peterlechner, C. Strassert, J.

Müller

. From cations to clusters: Ag⁺-mediated DNA base pairings and fluorescent silver clusters. **S. Swasey**, X. Chen, A. Karpenko, S.M. Copp, O. Lopez-Acevedo, E. Gwinn

. Acid-labile linker design for targeted delivery and release of platinum-acridine anticancer agents. **H. Wang**, M. Yang, U. Bierbach

. Anticancer properties of organorhenium picolinato and tryptophanato complexes.

M. Stevenson, S. Pramanik, S.K. Mandal

. Cytotoxic properties of organorhenium flufenamato and ibuprofenato complexes on breast cancer cells. **S. Parnell**, S. Pramanik, S.K. Mandal

. Anticancer properties of organorhenium mefenamato and tolfenamato complexes. **T. Hinton**, S. Pramanik, S.K. Mandal

. Chemical biology of Cu(II) complexes with imidazole or thiazole containing ligands: Synthesis, crystal structures and comparative biological activity. **L.A. Tyler**, A. Lewis, M. McDonald, S.

Scharbach, S. Hamaway, K.M. Fox, J. Tanski, L. Cassimeris

Section A

Venue

Placeholder

Bioinorganic Chemistry: Proteins & Enzymes & Model Systems

S. A. Koch, *Organizer*

5:30 - 7:30

• Square planar copper (I) complexes with geometric constraints pertinent to copper proteins. **P. Cheung**, R. Berger, J.D. Gilbertson

• Synthetic models of Ni-thiolate coordination units in biology. **R.A. Steiner**, T.C. Harrop

• Electronic ground state determination of a novel paramagnetic iron(III)-superoxo complex by

Mössbauer spectroscopy, EPR, and DFT. **H. Stout**, S.T. Kleespies, C. Chiang, W. Lee, L. Que, E. Munck, E.L. Bominaar

Electronically versatile benzenedithiolates on electronic and coordination structures of metal complexes: Mimicking the electronic interplay in [FeFe]hydrogenase active site. **Y. Liu**, K. Chu, M.H. Chiang

• Synthesis of novel mononuclear molybdenum(VI) model complexes of neutral tripodal N₃ ligands and study oxygen atom transfer activity. **J. Paudel**, F. Li

• Nitrite reduction by a PDI complex with a proton-responsive secondary coordination sphere. **M. Delgado**, Y.M. Kwon, J.D. Gilbertson

• Probing Pterin reduction dynamics in synthetic molybdenum cofactor models. **A.L. Nagelski**,

D.R. Gisewhite, B.R. Williams, S.J. Nieter Burgmayer

• Increasing the coordination kinetics of the Acetylene Hydratase (AH) model complex via pseudo-hydroxylation. **T. Marshall**, M.A. Cranswick

• Mechanistic insight into nitrite to nitric oxide conversion at copper(I) and copper(II) sites. **Z. Sakhaei**, S. Kundu, J. Donnelly, T.H. Warren

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

• New metal complexes of tridentate N,N,O scorpionate ligands. **S.E. Sherman**

• Chemosensors for Ni(II) employing N/S-based donors. **E. Broering**, T.C. Harrop

• Synthesis and reactivity studies of nickel-selenium complexes. **L. Cordeiro**, G.P. Yap, C.G. Riordan

Section A

Venue

Placeholder

Chemistry is Central to Applied Materials

C. R. Bertozzi, C. J. Chang, M. A. Paley, *Organizers*

5:30 - 7:30

• Self-healing metallogels as the recyclable materials for selective dye adsorption and separation.

C.K. Karan, M. Bhattacharjee

• X-ray powder diffraction structural study of hydroxyapatite derived from edible animal bones from Eastern Colombia. **A. Chaparro**, J.H. Quintana Mendoza, J. Henao

TAAILs - Tunable aryl-alkyl ionic liquids: A new generation of ionic liquids. **T. Strassner**

• Effects of calcination intensity on rutile TiO₂ white pigment production via short sulfate process. **C. TIAN**

• Highly selective Ru/TiO₂ catalysts for HDO of phenolic compound: Effects of support structure and partial substitution of nickel for ruthenium. **S. Husremovic**, R.C. Nelson, B.G. Frederick,

R.N. Austin, A. Mahdavi, S. Ki

• Novel approaches to the chemical syntheses of azamacrocyclic compounds and derivatives. G. Ren, E.J. Parish, Y. Lo, **H. Honda**, T. Wei

• Calcium cobalt hexacyanoferrate cathodes for rechargeable divalent ion batteries. **J. Thiebes**,

P. Padigi, N. Kuperman, G.M. Goncher, D. Evans, R. Solanki

• Graphene-On-Silica, CMOS-integrable, thermal-guiding structures: Applications in BooleanLogic and neuromorphic computation. **D. Loke**, J. Skelton, T. Chong, S. Elliott

• Difluoroboron β-diketonate poly lactides as luminescent oxygen sensing materials for wound imaging.

C.A. DeRosa, S.A. Seaman, A.S. Mathew, C.M. Gorick, Z. Fan, J.N. Demas, S.M. Peirce, C. Fraser

Section A

Venue

Placeholder

Chemistry of Materials

C. G. Lugmair, *Organizer*

5:30 - 7:30

• White light emission of lead(II) metal-organic frameworks. **A. P Peedikakkal**, J.J. Vittal

• Interface-facilitated hydrothermal synthesis of large-area graphene-like carbon nanosheets from toluene. **H. Gao**, G. Wang, S. Fan, C. Dong, A. Li, X. Zhu, X. Li

• Effect of electrodeposition variables on the topography and photoelectron kinetics of zinc oxide nanorods grown on graphene. C. Villarreal, **D. Pirzada**, **A. Wong**, A.K. Mulchandani

• Crystal structure features and luminescent properties of the copper-

doped Ca-Eu apatite. **M. Pogosova**, F. Azarmi

• Structure and reducibility of CeO₂ doped with trivalent cations. **A.K. Lucid**, G.W. Watson Facile fabrication of recyclable magnetic oxide@MOF nanocomposites for aerobic oxidation of benzylic C-H bonds. **G. Wang**, S. Fan, H. Gao, J. Wang, D. Jia

• Polydopamine-induced CaCO₃ mineralization and its application for the synthesis of nanostructured electrocatalysts. **J. Ko**, C. Park

• Molecular origins of superacidity in sulfated MOF-808. **C. Trickett**, C. Yan, T. Popp, J. Jiang,

A. Huq, J.A. Reimer, M.D. Fayer, O.M. Yaghi

• Polytypism in the Nowotny-Juza Compounds: Synthetic and Computational Investigation of Solution Phase I-II-V Semiconductors. **A.A. White**, G.J. Miller, J. Vela Becerra

• Alkali bismuth dichalcogenides: Emerging energy materials for photovoltaics and thermoelectrics. **B. Rosales**, J. Vela-Becerra

• Ge_{1-x}Sn_x/II-VI Core-shell nanostructures: Towards near IR active direct band gap semiconductors. **H. Andaraarachchi**, L. Men, J. Vela-Becerra

• In situ study of carbon dioxide reduction on CuO_x cage via electrochemical method. **S. Chiu**, T. Liao, H. Chen

• Cesium germanium iodide perovskite nanocrystals: Photovoltaics beyond organolead perovskites. **L. Men**, B. Rosales, N. Gentry, J. Vela-Becerra

• 3D Macroporous TiO₂@CeO₂ and TiO₂@AuNP composite fabrication and application. **B. Baruah**, D. Corella, M. Geiger

• Synthesis and characterization of cationic silver(I) coordination polymers for photoluminescent properties. **E. Soe**, J. Kim, S. Oliver

• Organo-oxo tin cluster reactivity: Insight into cluster formation, degradation, and interconversion. **M.C. Sharps**, J.E. Hutchison, D.W. Johnson

• Modelling defects in LaMnO₃ for solid oxide fuel cell cathodes. **A.L. Gavin**, G.W. Watson

• Single molecular Wells-Dawson-like heterometallic cluster for the preparation of multifunctional carbon materials: A T1- and T2-weighted dual mode magnetic resonance imaging agent and drug delivery system. Q. Zhang, **Y. Ling**, Y. Zhou

• Two principles of reticular chemistry uncovered in a metal-organic framework of heterotopic linkers and infinite secondary building units. **N.R. Catarineu**, A. Schoedel, P. Urban, M.B. Morla, C. Trickett, O.M. Yaghi

• Novel approaches to the chemical synthesis of polycyclic electron-donor for nanoelectronic materials study. E.J. Parish, G. Ren, Y. Lo, **H. Honda**, **M. Hsiao**, T. Wei

Size tunable submicro/micro TiO₂-related spheres synthesized by sol-gel process and the applications. **Y. Chen**, K. CHAN, H. Chiu, C. Lee

• Integration of oriented anatase TiO₂ electron transport layer into perovskite solar cells to improve carrier separation. **H. Dehnashi**, **m.L. mayer**, A. Yore, Y. Tran, M. Howard, A. Newaz, A.S. Ichimura

• Environmentally friendly and versatile method for the synthesis of transition metal alloys and their hybrid nanoparticles. **A. Penn**, J. Sharpsteen, H.P. Rathnayake

• Photoelectrochemical mechanism for instability of blue-phosphorescent Ir(III) complexes in electroluminescence devices. **S. Kim**, H. Bae, S. Park, J. Kim, J. Kim, Y. Jung, S. Sul, S. Ihn, C. Noh, S. Kim, Y. You

• Fabrication and application of graphene oxide composite films. J. Shen, Y. Feng, C. Ma, D.

Zhang, Z. Xiao, Z. Hui, **Y. Liu**, **Y. Min**

• In situ one-pot synthetic approach towards multivariate Zr-MOFs. **Y. Sun**, H. Zhou

• Hyperpolarized silicon nanoparticles as biocompatible contrast agents for ²⁹Si magnetic resonance imaging. **H. Seo**, I. Choi, D. Kim, Y. Lee

• Mesoporous aluminosilicate nanoparticles hosting glow discharge plasma reduced silver nanoparticles for desulfurization of liquid hydrocarbon fuels. **J. Hauser**, D. Tran, E. Conley, J. Saunders, K. Bastillo, S. Oliver

• Bottom-up synthesis approach to convert layered metal-organic framework materials into hierarchical porous structures. **Z. Li**, K. HE, W. Han, K. Yeung

• Discovery of earth abundant catalysts towards the implementation of a hydrogen economy. **T. Soucy**, J. Mondschein, J. McEnaney, C. Badding, R. Schaak

• Preparation and structural studies of hexyldecylamine/oleic acid capped ruthenium sulfide nanocrystals. **P.A. Ajibade**

• Synthesis and characterization of three cationic, isoreticular layered materials based on neodymium and α,ω-alkanedisulfonates. **A. Karez**, S. Oliver

• Selective aerobic oxidation of primary alcohols to aldehydes in functionalized mesoporous silica nanoparticles. **D. Singappuli-Arachchige**, J. Manzano, L.M. Sherman, I.I. Slowing

. Crystallizing one-dimensional metal-organic sulfide as cathode material of lithium-ion battery.

Z. Ji, C. Trickett, H. Jeong, A. Schoedel, O.M. Yaghi

. Synthesis and catalytic reactions with macroporous botanically templated metal oxides and metal on carbon structures. **N. Black, E.G. Gillan**

Metal-organic frameworks as templates for transition metal clusters. **A. Turkiewicz**, M.I.

Gonzalez, L.E. Darago, J.R. Long

. Cytocompatible polysaccharide incorporated biomimetic tubules. **K. Punia**, M. Bucaro, A. Punia, A. Bykov, K.S. Raja

. Efficient ammonia adsorption property of Prussian blue analogues. **A. Takahashi**, H. Tanaka,

D. Parajuli, T. Nakamura, K. Minami, Y. Sugiyama, Y. Hakuta, S. Ohkoshi, T. Kawamoto

. Three versatile Pt(II) oxime complexes that display anion sensing, thermochromism, and solvatochromism. **S.O. Elsidieg**, F.R. Fronczek, A.W. Maverick

. Molybdenum sulfide molecular clusters for 2D-materials. **C. Bejger**, J.L. Shott, M. Howington, J. Johnson

. Crystal engineering of metal-inorganic frameworks from phosphorescent building blocks. **J. Ivy**, M.A. Omary

. Nickel telluride as a bifunctional electrocatalyst for efficient water splitting in alkaline medium. **U. De Silva**, W.P. Liyanage, J. Masud, M. Nath

Section A

Venue

Placeholder

Coordination Chemistry: Characterization & Applications

S. A. Koch, *Organizer*

5:30 - 7:30

. Transition metal complexes with triamidoborane-bridged diphosphines: Coordination chemistry, reactivity, and XAS studies. **K. Lee**, C.M. Donahue, A.V. Blake, S.R. Daly

. Scavenging for triiodide *via in situ* crystallization of tripalladium(II)cyclophane molecules in photo-cyclopropanation reactions. **H. Lee**, O. Jung

. Combined effects of peripheral fluorine and central metal on phthalocyanine properties. **R. Szlag**, M.A. Kaster, E.R. Trivedi

. Zr-Based metal-organic frameworks for sustainable energy-related applications. **X. Wang**

. Synthesis, characterization and anticancer studies of tris-dithiocarbamate ruthenium(III) complexes. **P.A. Ajibade**

Coordination complexes with guanidine-type ligands towards cleavage of aryl-heteroatom bonds found in naturally occurring feedstocks. **K.D. Feller**, B. Barry

. Complexes with bisguanidine-type ligands towards insertions into sp²-heteroatom bonds. **J. Bruggen**, B. Barry

. Nanojar reactivity with acidic compounds and their conjugate base ligands. **C.K. Hartman**, G.

Mezei

. Probing slow magnetic relaxation in a series of mononuclear uranium (v) compounds. **D. Lussier**, J.R. Long, D.K. Shuh

. Vanadium-Dependent Haloperoxidase Enzymes: A Review of Mechanism, Structure/Functional Relationships, and Coordination Environments. **K. Doucette**, C. Wallace, C.C. McLauchlan, D.C. Crans

. Coordination chemistry of the rhodizone anion with Pb(II) and lanthanides: From understanding complexation to analytical applications. **J.A. Silverman**, E.V. Govor, K.

Kavallieratos

. Theoretical computations of tunable bimetallic systems. C. Feng, M.B. Pastor, **Q. Zhao**

Section A

Venue

Placeholder

Electrochemistry

B. L. Lucht, *Organizer*

5:30 - 7:30

. Vanadium oxide and vanadium oxynitride composite as electrode materials for lithium ion batteries. **W. HUANG**, S. Yen, . Lee, H. Chiu

. Synthesis, characterization and electrocatalytic performance of binary transition metal borides. **H. Park**, B. Fokwa

. Exploring electrocatalytic N₂ activation under mild synthetic conditions. **A. Nielander**, J. McEnaney, T.F. Jaramillo

. Rutile TiO₂ Nanorod arrays grown on graphite foil as binder-free flexible electrode for sodium ion batteries. **Y. Ching Tai**, M. Yang, H. Chiu, C. Lee

Molecular rectification: Chemical synthesis and characterization of donor-sigma-acceptor molecules. G. Ren, E.J. Parish, **H. Honda**, H. Shyu, T. Wei

. Characterization of a dicopper dihydroxide water oxidation electrocatalyst. **S.J. Koepke**, P.E. VanNatta, A. Shrestha, M.T. Kieber-Emmons

. Electrochemical characterization of selenocystine reactivity at modified gold surfaces. **K. Frommer**, **K. Lynch**, **E. Wiita**, **M.C. Buzzeo**

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

Section A

Venue

Placeholder

Emergent Phenomena in the Solid State

B. C. Melot, E. E. Rodriguez, *Organizers*

5:30 - 7:30 . Structural, magnetic, and electrical properties of Pr₂Fe_{4-x}Mn_xSb₅ (x = 0.5, 1.0). **I.W. Oswald**, S.

Li, B. Lv, J. Chan

. Metastable layered metal chalcogenides: From superconductivity to ferromagnetism. **B. Wilfong**, X. Zhou, H.K. Vivanco, E.E. Rodriguez

. Antimony nets and transition metal sublattices: The structure and properties of Ln₂Fe_{4x}CoxSb₅ (Ln = La-Pr; x < 1.5). **K. Benavides**, S. Li, J.V. Burnett, B. Lv, J. Chan

. Evolution of the magnetic properties in the series M₂FeB₂ (M = V, Nb, Mo, Ta and W). **J. Scheifers**, V. Shukla, B. Fokwa

. Topochemical intercalation and ion-exchange of layered iron sulfides via low-temperature hydrothermal routes. **X. Zhou**, B. Wilfong, H.K. Vivanco, E.E. Rodriguez

. Effect of ionicity on magnetism of K₂MnS₂. **A. Bhutani**, P. Behera, K. Kihlstrom, M. Smylie, U. Welp, W. Kwok, E.E. Rodriguez, A. Huq, D. Shoemaker

. Intercalation chemistry of CoSe and Co_{1-x}Fe_xSe mixed phase.

H.K. Vivanco, B. Wilfong, X. Zhou, E.E. Rodriguez

. Structural design of magnetoelectric multiferroics in garnets. **A.J. Neer**, B.C. Melot

Synthesis and characterization of Hf₃Ru_{5-x}M_xB₂ (M = Fe, Co, Ni) – towards rare-earth-free magnets. **P. Shankhari**, B. Fokwa

. Red, white, and blue: Controlling the luminescence of doped rare-earth oxychloride nanocrystals by ligand selection and compositional modulation. **G.V. Villalpando**, G.R. Watzig, G.A. Horrocks, S. Banerjee

. Properties and design of multifunctional phyllosilicates. **E. Howard**, B.C. Melot

Section A

Venue

Placeholder

Environmental & Energy-Related Inorganic Chemistry

S. A. Koch, *Organizer*

5:30 - 7:30

. Impedance studies of silyl/carbonate electrolyte blends. **M. Treichel**, **C.A. Ortiz**, L.J. Lyons

. Nitrous oxide removal with titanium oxide. **H. Gokturk**

. Synthesis and characterization of magnetic nanocomposites for energy storage applications. **B.**

Shen, S. Sun

. Development of a chemosensor device to aid in combatting the trade of fish caught by cyanide fishing. **C. Flynn**, **C.A. Sweet**, A.R. McCabe, C. Murphy

. Design of biotemplated titanium dioxide nanoparticles for potential application as anodes in dye-sensitized solar cells. **A. Reyes-Oliveras**, G. De Jesus-Morales, V. López-Mejías

. Photophysical studies on homoleptic phenylimidazolinato Ir(III) complexes: Electronic effect of terphenyl groups at the phenylimidazolinato ligand. **S. Kim**, Y. Cho, C. Kim, H. Son, S.O. Kang

. New types of deep blue phosphorescent Ir complexes with sulfonyl group in phenyl unit of phenyl pyridine ligand: Photodynamic studies of sulfonyl group effect and their application to solid-state display. **J. Kim**, Y. Cho, s. yi, C. Kim, H. Son, S.O. Kang

. Iridium photosensitizers for artificial photosynthesis: Design monomeric and bimetallic Ircomplexes and Ir-dendrimers. **Y. Cho**, C. Kim, H. Son, C. Pac, S.O. Kang

. Widely controllable syngas (H₂ + CO) production by a dye-sensitized TiO₂ hybrid system with Re(I) and Co(III) dual molecular catalysts under visible-light irradiation. **J. Lee**, D. Won, W. Jung, H. Son, C. Pac, S.O. Kang

. Role of porphyrin antenna for photocatalytic CO₂ reduction in a hybrid catalyst system: Protection from

photo-bleaching. **D. Won**, J. Lee, H. Son, C. Pac, S.O. Kang

. Photosensitization effects of Ir(III) complexes in selective reduction of CO₂ by Re(I)-complex anchored TiO₂ hybrid catalyst. H. Cheong, S. Kim, Y. Cho, D. Cho, C. Kim, **H. Son**, C. Pac, S.O. Kang

. Photophysical studies on homoleptic phenylimidazole iridium(III) complexes: Electronic effect of planar bulky phenylimidazole ligand. **M. Son**, S. Kim, Y. Cho, J. Kim, s. yi, C. Kim, H. Son, S.O. Kang

. Molecular engineering of squaraine dyes for efficient far-red and near-IR sensitization in photocatalytic CO₂ reduction. **M. Cho**, H. Son, C. Pac, S.O. Kang

. Measuring lithium and fluorine diffusion in electrolytes for use in lithium-ion batteries with PFG-STE NMR. **S.A. Beecher**, L.J. Lyons

. Coupling of chromophoric dyes with applied bias or microwave heating to increase DSSC photoconversion efficiency. **C.A. Sweet**, **C. Flynn**, C.J. Timpson, C. Murphy

. Effect of aliphatic ligand length on triplet energy transfer from PbSe nanoparticles to rubrene.

N. Megerdich, M. Mahboub, M. Tang

. Structure, dynamics, and electrochemistry of psychrophilic cytochromes. **S.J. Barth**, **J. Chou**, **S.K. Lone**, **K.S. Montero**, **G.J. Salerno**, **M.C. Buzzeo**, **J.S. Magyar**

. Bioinspired preparation of melanin-like nanoparticles used for highly nitrogen-doped porous carbon spheres: Enhanced CO₂ capacities and efficient oxygen reduction catalyst. h. kim, M. Kim, m. kang, Y. Sung, **w. yoo**

Section A

Venue

Placeholder

Inorganic Catalysts

S. A. Koch, *Organizer*

5:30 - 7:30

Olefins from biodiesel:

Decarbonylation using a ruthenium catalyst. **B. Benson**, A. John, W.B. Tolman

. Reduced copper metal-organic frameworks: A heterogeneous catalyst for click chemistry. **K. Xie**, Q. Fu, P. Webley, G.G. Qiao

. Study on synthesis and catalytic cracking performance of Y zeolite with sheet-like morphology.

S. Cui, G. Wang, B. Liu

. Copper nanocrystals embedded in metal-organic frameworks for highly selective CO₂ hydrogenation to methanol. **B. Rungtaweeveranit**, J. Baek, G.A. Somorjai, O.M. Yaghi

. Mesoporous cobalt oxide with controlled porosity: Efficient catalyst for peroxide free alkene epoxidation under aerobic conditions. **C. Weerakkody**, S.L. Suib

. Copolymerization of cyclohexene oxide and succinic anhydride using Schiff base Zn complex.

A. Virachotikul, P. Wongmahasirikun, K. Phomphrai

. Synthesis of cyclic poly(ϵ -caprolactone) using tin(II) complex containing soft sidearm initiator.

T. Ungpittagul, K. Phomphrai

. Investigation of ring-opening mechanism using x-ray crystallography. **K. Udomsasporn**, K. Phomphrai

. Cobalt, nickel, and iron Schiff Base complexes for hydrogen production in aqueous solution. A. Graves, O. Taghavi, **W.T. Eckenhoff**

. Synthesis of aluminum complexes supported by salicylaldehyde ligands for the polymerization of cyclic esters. **P. Pisitsoopon**, P. Wongmahasirikun, K. Phomphrai

. Electrochemical generation of hydrogen gas by cobalt porphyrin-based Metal-Organic Framework (MOF) and amorphous polymer. **Y. Wu**

. Studies of a low-valent Molybdenum(VI)-dioxo complex as a deoxydehydration catalyst. **R. Tran**, S.M. Kilyanek

. Novel bi-functional catalyst based on Co₂O₄ core – MnO₂ shell for rechargeable Li-air battery.

Y. Lee, D. KIM, S. HA, S. KIM, **Y. Lee**

. Impact of rare-earth dopants on the catalytic activity of CeO₂ nanoparticles for both CO oxidation and preferential CO oxidation reactions. **J. Yoo**, K. Kim, J. Han, W. Jung

. Aqueous solution palladium catalyzed Suzuki cross coupling reactions: Reaction optimization of base and the effects of base concentration. **T. Olson**, J.G. Parsons

. Effects of acid strength and position of an intramolecular acidic functional group on the catalytic reduction of CO₂ to CO. **S. Lense**, I.A. Guzei, K. Thao, J. Andersen, M. Schultz

. Inverse Frustrated Lewis Pair (FLP) approach for catalytic metal-free hydrogenation of imines.

S. Mummadi, D. Kenefake, R. Diaz, C. Krempner

. Role of water in the selective oxidation of benzyl alcohol over gold nanoparticle supported catalysts. **A. Tombo**, M.Y. Santos, B. Chandler, C. Pursell

. Synthesis and electrochemical evaluation of Ru(II) tridentate carbene complexes. **J.T. Hyde**, **D.P. Harrison**

. Novel thione based ligands: Synthesis and complexation. **P. Jean**, B. Hunt

. Characterizing the kinetic capabilities of supported gold nanoparticle catalysts using benzyl alcohol oxidation. **M.Y. Santos**, B.D. Chandler, C. Pursell, A. Tombo

Section A

Venue

Placeholder

Inorganic Nanomaterials: Structure & Function in 0, 1 & 2 Dimensions

K. R. Kittilstved, E. J. McLaurin, *Organizers*

5:30 - 7:30

. Soft-templating strategies for anisotropic Au nanomaterials and hollow multi-Au@SiO₂ nanosystems.

H. Yoo

. High performance CsPbX₃ perovskite quantum dot light emitting devices achieved via solidstate ligand exchange. **Y. Suh**, T. Kim, H. Park, C. Lee, J. Park

. GeP₃ thin layers: Novel 2D materials revealed by first-principles calculations. **Y. Jing**

. Imaging interactions between dipole emitters and single nanowires. **E. Johlin**, J. Solari, S.A. Mann, J. Wang, T. Shimizu, E. Garnett

. Size control and Sb doping of solution grown two-dimensional Bi₂Se₃ nanoplates. **A.J. Bernard**, Y. Hou, D. Yu, S. Kauzlarich

. Characterization of solution-based exfoliated two-dimensional nanosheets. **K. Pachuta**, A. Sehriroglu, E. Pentzer

Vapor-Phase epitaxial growth of aligned nanowire networks of cesium lead halide perovskites

(CsPbX₃, X = Cl, Br, I). **J. Chen**, Y. Fu, L. Samad, L. Dang, Y. Zhao, S. Shen, L. Guo, S. Jin

. Pt Nanoparticle anchored molecular self-assemblies of DNA: A stable and efficient electrocatalyst for hydrogen generation. S. Anantharaj, **S. Kundu**

. Titanium metal nanowires via electrospun polymer nanocomposite. **H.E. Lacy**, A.S. Ichimura, K. Teh

. Solution growth of lead halide perovskite nanowires for high-performance wavelength-tunable nanowire lasers. **Y. Fu**, H. Zhu, X. Zhu, S. Jin

. Polytypic phase transitions in metal intercalated 2D Bi₂Se₃ nanoribbons. **M. Wang**, K.J. Koski

. Exploring biphasic routes to functionalized CdSe nanoparticles for use in solar nanocomposites.

K. Bolduc, **M.E. Hagerman**, J.D. Kehlbeck

. New route for the formation of SnSe thermoelectric materials with low thermal conductivity. **S. Kundu**, S. Yi, C. Yu

. Mechanism of galvanic replacement reactions for hollow germanium nanoparticles. **X. Qi**, S.

Kauzlarich

. Impact of surface reconstruction on the electronic structure of PbS QD nanocrystals:

Experiment and theory. **C.F. Gervasi**, H.J. Seeley, D.A. Kisilitsyn, T.L. Allen, G. Nazin

. Assembly of CdSe quantum dots and gold nanorods into discrete arrangements with unique optical properties. **B. Szychowski**, M. Daniel

. Towards broadband-emitting 2D-perovskites LEDs. **P. Carmona Monroy**, D. Solis, E. Perez Gutierrez

. Elucidating the effect of fluoride-containing ionic liquids on indium phosphide nanocrystals. **S.**

Lee, E.J. McLaurin

Section A

Venue

Placeholder

Inorganic Spectroscopy

V. C. Popescu, *Organizer*

5:30 - 7:30

. Influence of charge transfer in the photoluminescence of lead-free Ba_{1-x}Ca_xTi_{0.9}Zr_{0.1}O₃ electroceramics. **G. Herrera Pérez**, J.G. Murillo, G. Zaragoza-Galán, G. Tapia-Padilla, A. ReyesRojas, L.E. Fuentes-Cobas

. Characterizing the inner filter effect in quantum dot-polymer composites for use as a displacement sensor. **M.A. Koc**, P. Alivisatos

. Single-molecule investigation of initiation dynamics of an organometallic catalyst. **J. Ng**, S. Upadhyay, A. Marquard, K. Lupo, D. Hinton, N. Padilla, D. Bates, R.H. Goldsmith

. Mössbauer spectroscopy: Predictive property models from experimental design and statistical learning. **J. Proppe**, M. Reiher

none. Measuring of the energy transfer efficiency between plasmon nanoparticles and quantum dots using Sample-Transmitted Excitation Photoluminescence (STEP). **P. Moroz**, M. Zamkov

. Acid reactions of model systems of molybdenozymes. **K. Schwalenstocker**

. Photophysical effects of varying imine based ligands with cuprous halides to form vividlycolored/brightly-phosphorescent coordination polymers. **L.E. Scoggins**,

M. Wilk, Z. Henry, V. Nesterov, M. Omary

. TDDFT studies of earth abundant photocatalysts. **C. Nite**, A.K. Rappe

. Theoretical study of tris(1,3-propanedionato)chromium(III) for insight into Cr(III)-based photocatalysts. **J. Nite**, A.K. Rappe

. Thermal polarized vibrational microspectroscopy of weddellite and whewellite single crystals.

G. Kumi, N. ALJUHAN, A. Obaid

. Mössbauer spectroscopy of iron-selone and iron-thione complexes capable of preventing oxidative DNA damage. **V.C. Popescu**, M. Cohara, J.L. Brumaghim, B. Stadelman

. Reexamination of the red band of CuO: Analysis of the $[16.5] \ ^2\Sigma^- - X \ ^2\Pi_i$ transition of ^{63}CuO and ^{65}CuO . **J.C. Harms**, E.M. Grames, S. Yun, B. Ahmed, J.J. O'Brien, **L.C. O'Brien**

none. Analysis of some new electronic transitions observed using intracavity laser spectroscopy (ILS): Possible Identification of HCuN. **J.C. Harms**, E.M. Grames, J.J. O'Brien, L.C. O'Brien

. XESCA: X-ray emission spectroscopy for chemical analysis. **S. Lee**

Section A

Venue

Placeholder **Lanthanide & Actinide Chemistry**

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

. Actinide mediated C-X activation chemistry. **J.M. Dorhout**, M.J. Monreal, D.E. Morris, B. Scott, K.D. Abney, J.L. Kiplinger

. Very low-temperature lanthanide and actinide borates from boric acid flux. **A.T. Chemey**, S.S. Galley, T.E. Albrecht-Schmitt

. Gas phase chemistry of the Ln(III)-TMGA/TMTGA complexes. **X. Chen**, Q. Li, Y. GONG

. Design and synthesis of tri-substituted benzene compounds used as extractants in nuclear waste remediation. **B.G. Wackerle**, S.M. Biros

. Development of bidentate ligands containing soft donor atoms for actinide chelation. **C.C. Miller**, S.M. Biros, J.E. Bender

. Hyp₅Sb for separation of heavy metals. **E.G. Leach**, S.M. Biros, J.E. Bender

. Synthesis and characterization of (2-methoxyphenyl)diphenylphosphine derivatives for nuclear waste remediation. **E. Christoffersen**, S.M. Biros, J.E. Bender

. Phosphine ligands for the extraction of *f*-block elements: Use in nuclear waste remediation.

A.R. Spyker, S.M. Biros, J.E. Bender

. Novel synthesis, structure, and enhanced photoluminescence of lanthanide dicyanoaurates containing aurophilic interactions. **T. Hamby**, R. Sykora, J. Hendrich, E. Kost

. Optimizing hydrothermal reaction conditions for lanthanide coordination polymer formation: A study of the 1,4-benzenedicarboxylate system. **J. Einkauff**, D.T. de Lill

. Recovery and recycling of Pu-238 in spent nuclear fuel to increase the sustainability of nuclear reactors using extraction and luminescence techniques. **M. Hudson**, G. Deblonde, R.J. Abergel, S.M. Biros

. Design of lanthanide half-sandwich complexes exhibiting single-molecule magnetism. **R.**

Khoo, J.R. Long

Section A

Venue

Placeholder

Main Group Chemistry

T. W. Hudnall, *Organizer*

5:30 - 7:30

. Aluminium carboxylates as precursors for the synthesis of aluminium-oxocages. **T.L. Precht**,

A.J. Peel, D. Wright, A. Wheatley

. Reactivity of an acyclic silylsilylene toward ethylene: Migratory insertion into the Si-Si bond.

D. Wendel, S. Inoue, B. Rieger

. Borylated N-Heterocyclic Carbenes(NHCs) - Synthesis and migration studies. **W. Liu**, C.

Chiu

. Synthesis and characterization of energetic nitroformate salts. **A. Baxter**, I. Martin, K.O. Christe, R.M. Haiges

. Triazenyl radicals stabilized by *N*-heterocyclic carbenes. **J. Back**, E. Lee

. Silylene stabilized boron cations: Synthesis and reactivity studies. **H. Tsai**, C.

Chiu . Acid-catalyzed

hydroxylation of

iodododecaborate. **Z.S.**

Lincoln, J.A. Dopke, R.J.

Staples

. Ruthenium-catalyzed substitutions of icosahedral dodecaborates. **D.C.**

Adams, J.A. Dopke, R.J.

Staples

. Synthesis and characterization of salts derived from 5[chloroalkyl]tetrazoles. **Y.O. Ahmed**, c. gibson, S. Schneider, S. Deplazes

. Synthesis and characterization of new derivatized 1,1-dimethylhydrazinium salts. Y.O. Ahmed, **c. gibson**, S. Schneider, S.F. Deplazes

. Cation exchange and disproportionation chemistry of ammonium and potassium magnesium dodecaborates. **D.M. Schubert**, K. Kluherz, D. Neiner, M. McCray

. Polyphosphazenes as Antibacterial Films. **P. Nance**, P. Wisian-Neilson

. Stabilization of heavier main group analogues by London dispersion force interactions. **R.E.**

Tureski, P.P. Power

Section A

Venue

Placeholder

Organometallic Chemistry: Catalysis

N. S. Radu, *Organizer*

5:30 - 7:30

. Single step access to long-chain α,ω -dicarboxylic acids by catalytic isomerizing hydroxycarbonylation. **V. Goldbach**, L. Falivene, L. Caporaso, L. Cavallo, S. Mecking

. Carbon dioxide hydrosilylation catalyzed by iron. **T. Jurado**, J.J. Garcia

. Robust catalyst for the dehydrogenation of neat formic acid. J. Celaje, Z. Lu, **E. Kedzie**, J. Lo, N. Terrile, T.J. Williams

. Olefin oligomerization catalysis: Ligand design, organometallic chemistry, and catalysis. **T.C. Wambach**, T. Tilley

. Ammonia formation from a bulky triphenolate amine transition-metal nitrido complex. **D. Bae**, E. Lee

. 1,5-Regioisomer of the click reaction: Valuable ligand precursors for new Ru-MIC complexes.

L. Suntrup, S. Hohloch, B. Sarkar

. Computational studies of rhodium-catalyzed hydrogenation and carbon dioxide activation. **M. Trenerry**, M.T. Whited, B.L. Taylor

. Hydrogenation of unsaturated triglycerides via catalytic hydrogen transfer from glycerol. **V. Cherepakhin**, T.J. Williams

. Highly efficient synthesis of *N*-alkylation of aromatic amines with primary alcohols catalyzed by an ionic ruthenium pincer complex. F. Yang, Y. Wang, Y. Ni, X. Cao, S. Lu, **X. Hao**, M.

Song

. Synthesis and electrochemistry of ruthenium 2,2'-bipyridine-6,6'-dicarboxylate catalysts using different

phosphorus ligands. **s. yezdani**, J.M. Kamdar, E.R. Paulson, A.L. Rheingold, D.B.

Grotjahn

. Kinetic investigation of the dehydrogenative borylation of terminal alkynes. **B.J. Foley**, N. Bhuvanesh, O. Ozerov

. Tunable catalysis with dimetal tetraguanidinate paddlewheel complexes. **M. Humphries**, E. Wusterbarth, B.R. Smith, J.T. Njardarson, D.L. Lichtenberger

. Catalytic aerobic oxidation by self-sensitized tellurium containing chromophores. **L. Lutkus**, T.

McCormick eactivity and catalytic studies of transition metal complexes with a triazene ligand functionalized with pyrazole. **L.J. Medrano-Castillo**, M.Á. Collazo-Flores, D. Chávez, D.B. Grotjahn, A.L. Rheingold, V. Miranda-Soto, M. Parra Hake

. Butterfly [2Fe-2S] cluster-based electrocatalysts with fast rates for hydrogen production. **K.E. Clary**, O. In-noi, J.M. Marx, K.J. Haller, D.H. Evans, R.S. Glass, D.L. Lichtenberger

. Rhodium complexes with *N*-heterocyclic carbene and triazene ligands as catalysts for alkyne hydrothiolation. **J.P. Camarena-Díaz**, D.B. Grotjahn, A.L. Rheingold, J. Perez-Torrente, R. Castarlenas, L.A. Oro, . Passarelli, M. Parra Hake, V. Miranda-Soto

. Oxidation of an iridium hydride pincer complex by O₂: A DFT study. **J. Williams**, A.M. Wright, K.I. Goldberg, T.R. Cundari

. Development of novel Pd and Pt catalysts for efficient conversion of methane to methanol. **J.**

Chen, **J. Park**, **M. Klosinski**, R. Giron, Y. Lee, B. Rawal, J. Lee, K.W. Jung

Section A

Venue

Placeholder

Organometallic Chemistry: New Ligand Platforms

N. S. Radu, *Organizer*

5:30 - 7:30

. Highly selective and sensitive colorimetric chemosensor for detection of Co²⁺ in a near-perfect aqueous solution. **M. Kim**, H. Cho, C. Kim

. Colorimetric chemosensor for the sequential recognition of mercury (II) and iodide in aqueous media. **H. Ahn**, S. Hwang, M. Yang, C. Kim

. Simultaneous bioimaging recognition of cation Al³⁺ and anion F⁻ by a

fluorogenic method. **J. Kang**, H. Jeong, D. Yun, C. Kim

. Highly sensitive benzimidazole-based chemosensor for the colorimetric detection of Fe(II) and Fe(III) and the fluorometric detection of Zn(II) in aqueous media. **H. Jang**, J. Chae, A. Kim, C. Kim

. Highly selective fluorescence sensor for Al^{3+} and CN^- in aqueous solution: Biological applications and DFT calculations. **J. Jung**, J. Yun, P. Kim, C. Kim

. Pillarplexes: A metal-organic class of supramolecular hosts. **P.J. Altmann**, A. Pöthig Unprecedented metal-ligand cooperation of a (PPP)Ni scaffold: Formation of P-E bonds (E = N or P). **Y. Kim**, Y. Lee

. First-row metal complexes of poly(guanidiny)aryl ligands. J.E. Allen, L. Wilkinson, W.S. Kassel, **N.A. Piro**

. Solvent free hydrosilylation of tertiary, secondary and primary amides using BIAN

[Bis(Arylimino)-Acenaphthene] based Iron complexes. **A. Saini**, M. Findlater

. Synthesis of a novel multitopic nonchelating N-heterocyclic carbene. **D. Tapu**, **A. Carter**, **R. Justice**, **R. Hooper**, O. Kuykendall, M. Baker, G. Bettler, A. Changas, A. Mason

. New annulated N-heterocyclic carbenes and their transition metal complexes. **G. Bettler**, **A. Changas**, O.J. Buckner, C. Boudreaux, B. Norvell, D. Tapu

. Toward the synthesis of a new anionic N-heterocyclic carbene and its corresponding metal complexes. **A. Carter**, **A. Mason**, **D. Tapu**, M. Baker, G. Bettler, A. Changas

. Synthesis and Characterization of Cr(0) terminated π -linkers based on linear oligoazulenic frameworks. **N.R. Erickson**, M.V. Barybin

. Heterobimetallic complexation of a mercapto and isocyano functionalized linear 6,6'-biazulenic π -linker: Synthesis, redox behavior, and spectroscopic characterization. **J.C. Applegate**, N.R. Erickson, M.V. Barybin

. Novel mesoionic/remote N-heterocyclic carbene ligands and their ruthenium(II) aqua complexes. **T.C. Cao**, D.B. Grotjahn

Section A

Venue
Placeholder
Organometallic Chemistry: Synthesis & Characterization-Late Transition Metals

N. S. Radu, *Organizer*

5:30 - 7:30

. 1,3,6-Trisubstituted fulvene derived *ansa*-metallocene ligands: A new route for the synthesis of *ansa*-ytterbocenes and -samarocenes. **S.K. Adas**, G.J. Balaich

. Cyclopentadienyl pyridazines and oxazines and their applications in energy and advanced electronics. **N.C. Tice**, E.M. Collins, C.A. Snyder, D.L. Smith

. Influence of the dicopper core on the reactivity of copper(I) hydrides. **A.J. Jordan**, P.K. Thompson, C.M. Wyss, J.P. Sadighi

. Unusual reactivity of PCP-supported rhenium carboxylates. **A.J. Kosanovich**, W. Shih, O. Ozerov

. Activation of small molecules by 2-[[dicyclohexylphosphino)ethyl]trimethyl ammonium chloride iridium complexes. **J. Knapp**, S.H. Schreiner

. Comparative reactivity studies of iridium(I) and rhodium(I) complexes stabilized by chelating diphosphine ligands. **K. Olsen**, S.H. Schreiner

. Synthesis, characterization and reactivity of group ten phosphinoferrrocene - carbonyl complexes. **E. Kober**, S.H. Schreiner

. Synthetic and structural comparisons between first row transition metal dithiolato complexes and group 14 metalylenes. **J. Pratt**, P.P. Power

Section A

Venue
Placeholder
Solid-State Inorganic Chemistry

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

5:30 - 7:30

. Large-scale synthesis of Sb_2Q_3 (Q = S, Se) nanofibers topotactically converted from ternary metal chalcogenides and their optical and transport properties. **H. Lee**, M. Kim, B. Yoo, K. Ahn, I. Chung

. Hydrothermal synthesis and characterization of three-dimensional titanium(III) phosphites. **L. Hung**, S. Wang

. Mechanoconglomeration and mechanoracemization of gold(I) complex crystals with optical properties alternation. **M. Jin**, T. Seki, H. Ito

. Synthesis, crystal structure, and thermoelectric properties of new phosphides $BaCu_3P_3$ and $Ba_4Cu_{11}Mg_{2.8}P_{10}$. **J. Mazzetti**, J. Wang, K. Kovnir

. Synthesis and structural evaluation of manganese doped cobalt oxides. **A.R. Thuli**, A.M. Morey

Sol-gel synthesis and characterization of lithium nickel cobalt oxides. **J.J. McCune**, A.M. Morey

. Heat treatment intensity on rutile pigment production from unenriched industrial TiOSO₄ solution via short sulfate process. **C. TIAN**

. Two zinc titanophosphates containing organic linkers in situ metal/ligand reactions. L. Huang, P. Chen, L. Hung, **S. Wang**

. Superhard alloys of transition metal dodecaborides: $Zr_{1-x}Y_xB_{12}$, $Zr_{1-x}Sc_xB_{12}$ and $Y_{1-x}Sc_xB_{12}$. **G. Akopov**, M.T. Yeung, Z.C. Sobell, C.L. Turner, R.B. Kaner

. Metal flux and supercritical fluid syntheses of actinide materials. **W. Potter**, T.E. AlbrechtSchmitt, S.E. Latturmer

. Optimization of the CsCl reduction-oxidation flux synthesis of Cs-Zn-Sb clathrates. **S. Heinrich**, B. Owens-Baird, J. Dolyniuk, K. Kovnir

. Thermoelectric properties of n-type SnSe-based materials. **J. Cha**, K. Ahn, I. Chung

. Tunable optical properties of Sn-based perovskite compounds. **M. Lee**, I. Chung

. Novel light emitting phosphors based on olivine structure type oxide, $CaYGaO_4$. **S.M. Araiza**, K. Slowinska, S. Derakhshan

. Chemical conjugation of rare-earth oxychloride nanocrystals to hybrid organic-inorganic perovskite nanoplatelets for solid-state lighting applications. **F.A. Rodriguez Ortiz**

. Stabilization of GdB_{12} in $Zr_{1-x}Gd_xB_{12}$ under ambient pressure. **G. Akopov**, **Z. Sobell**, M. Yeung, R.B. Kaner

. Using a dataset of magnetic material properties to screen for magnetocalorics. **J.D. Bocarsly**, E. Levin, S. Wilson, R. Seshadri

. Effects of microstructurally induced strain on magnetic properties of biphasic Heusler systems. **E. Levin**, M. Buffon, P. Callahan, J. Stinville, S. Mooraj, D. Gianola, T. Pollock, R. Seshadri

WEDNESDAY MORNING

Section A

Venue
Placeholder
Deposition & Etching of Nanostructures
Cospponsored by COLL[†]
Financially supported by ACS Publications, Strem Chemical H. Fairbrother, A. V. Walker, *Organizers*

L. McElwee-White, *Organizer*, *Presiding*

8:30 Introductory Remarks.

8:35 . Using inherent substrate-dependent nucleation to promote selective-area atomic layer deposition. **G. Parsons**, P. Lemaire, M. Ritz, C.J. Oldham

9:10 . Deposition of ZnO nanostructures on graphene: Application as tin oxide-free photoanodes. **C. Villarreal**, D. Pirzada, A. Wong, A.K. Mulchandani

9:35 . Sustainable manufacturing of functional materials. **C.J. Carmalt**

10:10 Intermission.

10:30 . Cobalt metal thin films: Precursor syntheses, atomic layer deposition, and selective growth. **C.H. Winter**

11:05 . Chemical self-assembly strategies for metal-organic surface structures. J. Kestell, R. Abuflaha, D. Olson, **W.T. Tysoe**

11:30 . New precursor chemistries for ALD of transition metal oxides. **A. Devi**

Section B

Venue
Placeholder
Celebrating 60 Years of the Division of Inorganic Chemistry Young Investigators & Officers

D. C. Crans, *Organizer* M. J. Clarke, *Organizer*, *Presiding* L. M. Berreau, C. Turro, *Presiding*

8:00 Introductory Remarks.

8:05 . Chemical tools for investigating cellular zinc metalloenzymes. **E.L. Que**

8:35 . Engineering molecular materials for applications in energy storage. A. Baumann, D. Burns, **V. Thoi**

9:05 . Nonaromatic tetrapyrrole metal complexes supporting a multielectron redox chemistry for efficient dioxygen activation. **J. Rosenthal**, J. Eddy, T. Qiu

9:35 . De novo design of metalloproteins. **I.V. Korendovych**

10:05 Intermission.

10:20 . Highly stable Metal-organic frameworks with ultrahigh capacitance. **D. Feng**, Z. Bao

10:50 . Coordination chemistry with fullerene-based ligands. **A.L. Balch**, M.M. Olmstead, A. Aghabali, S. Jun

11:20 . Employing novel porphyrinoid ligands to access biomimetic manganese and iron complexes of relevance to O₂-activating heme enzymes. **D.P. Goldberg**, J. Zaragoza, R.A. Baglia, J. Sacramento

11:50 . Lanthanide complexes and materials with sensitized metal-centered luminescence. **A. De Bettencourt Dias**

Bettencourt Dias

Section C

Venue

Placeholder

Frontiers in Heavy Element Electronic Structure

Cosponsored by NUCL D. L. Clark, D. K. Shuh, *Organizers* L. Soderholm, *Organizer, Presiding*

8:30 . Up all night with Bruce: From computations to experiments to real computations & experiments. **G.G. Stanley**

8:50 . Designing activated carbons for Hg removal from coal combustion flue gas. **R. Cayton**

9:10 . Counting electrons: What they don't teach you in general chemistry. **J.S. D'Acchioli**, M.K. Heili, P. Sit, E.D. Speetzen, A. Webster, C. Mueller, D. Cunningham

9:30 . Electronic structure and metal-metal bonding in heterobimetallic and heterotrimetallic complexes of a redox-active metalloligand. **A.F. Heyduk**, M. Wojnar, K.E. Rosenkoetter

9:50 . Bonding with Bruce. **D.L. Clark**

10:10 Intermission.

10:30 . Intriguing aspects of non-innocent ligands in transition metal complexes. **M.B. Hall**

10:50 . Give It some thought: Inorganic chemistry and nanotechnology. **C.J. Murphy**

11:10 . Magnetic circular dichroism and electronic absorption spectra of multiply metal-metal bonded rhenium dimers. **A.P. Sattelberger**, M.L. Kirk, f. poineau, E. Johnstone, K. Czerwinski, D. Habel-Rodriguez

11:30 . Heavy element chemistry in a heterogeneous context. **W.F. Schneider**

11:50 . Excited states of mononuclear and dinuclear complexes and their applications. **C. Turro**

Section D

Venue

Placeholder

Solid-State Inorganic Chemistry

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

S. E. Latturmer, F. Rabuffetti, *Presiding*

8:30 . Lead- and tin-based two-dimensional hybrid organic-inorganic iodide perovskites:

Structure, properties and application in planar solar cells. **L. Mao**, H. Tsai, w. nie, L. Ma, J. Im,

C. Stoumpos, C. Malliakas, M.R. Wasielewski, A.D. Mohite, M.G. Kanatzidis

8:45 . Pressure-induced structural, electronic, and optical evolution of hybrid perovskites. **A. Jaffe**, Y. Lin, C. Beavers, J. Voss, W. Mao, H. Karunadasa

9:00 . Tuning indirect to direct bandgaps in double perovskites. **T. Tran**, J. Panella, J. Chamorro, J.R. Morey, T. McQueen

9:15 . Structure and dynamics of perovskite formamidinium lead iodide: Phase transitions, reentrant properties, persistent molecular motion, and large positive thermal expansion. **D.H. Fabini**, G. Laurita-Plankis, C. Stoumpos, T. Siaw, S. Han, M.G. Kanatzidis, R. Seshadri

9:30 . Trends in the lone pair-induced local off-centering of tin and lead atoms in halide perovskites. **G. Laurita-Plankis**, D.H. Fabini, C. Stoumpos, M.G. Kanatzidis, R. Seshadri

9:45 . Negative thermal expansion and other anomalous properties in mixed metal fluorides with structures related to that of ReO₃: A perovskite with helium on the A-site?. **A.P. Wilkinson**, B. Hester

10:00 . Tuning photochemical and photophysical properties of metallosupramolecular materials. **A. Razgoniaev**, A. Ostrowski

10:15 Intermission.

10:30 . Synthesis of new complex metal hydrides and carbides from ytterbium/lithium flux. M. Dickman, **S.E. Latturmer**

10:45 . *In situ* identification of kinetic factors that expedite inorganic crystal formation and discovery. **Z. Jiang**, A. Ramanathan, D. Shoemaker

11:00 . Dynamic origins of noncentrosymmetry in KNaNbOF₅. **M. Holland**, **K.R. Poeppelmeier**, J. Rondinelli, N. Charles

11:15 . In-situ reduction study of the effect of anion concentration in the Fe-Ga-S system. **R. McAuliffe**, D. Shoemaker

11:30 . Design of piezoelectric heterostructural alloys. **S. Miller**, K. Talley, A.W. Weimer, A.

Zakutayev, S. Lany, C. Musgrave, G. Brennecke, A. Holder

11:45 . Piezoelectrics: Putting the squeeze on new materials. **M. Dolgos**

12:00 . Low-Barrier "H-M-H" molecular rotor. **E. Prack**, C.A.

O'Keefe, J.K. Moore, A. Lai, A.J. Lough, P.M. Macdonald, M.S. Conradi, R.W. Schurko, U.W. Fekl

12:15 . Synthesis of bimetallic trifluoroacetates through a crystallochemical investigation of their monometallic counterparts: The case of (A, A')(CF₃COO)₂.nH₂O (A, A' = Mg, Ca, Sr, Ba, Mn).

B. Dhanapala, N. Mannino, K. Dissanayake, L. Suescun, **F. Rabuffetti**

Section E

Venue

Placeholder

Chemistry of Materials: Nanomaterials

C. G. Lugmair, *Organizer*

B. E. Cohen, F. Rabuffetti, *Presiding*

8:00 . Pnictide precursors for pnictide-based thermoelectric nanomaterials. **A. Das**

8:20 . Syntheses of Zn_{1-x}Cd_xS nanocrystals with tunable band structure for efficient reduction of nitroaromatics in water. **kaur** **8:40** Improved covalent protein labeling and single-molecule optical properties of compact CdSe/CdS quantum dots. **B.E. Cohen**, A. Powers, S. Wichner, A. Yildiz

9:00 . Investigations of using environmentally responsive polymers as capping materials for aluminum nanoparticles. **W. Zeng**, S.W. Buckner, P.A. Jelliss

9:20 . Ultrathin copper based core shell nanowires for high-performance transparent conductors - from synthesis to application. **F. Cui**, P. Yang, L. Dou, Z. Niu, Y. Yu

9:40 . Chemically and structurally flexible hosts for Yb-Er sensitizer-activator pairs. K. Dissanayake, B. Dhanapala, **F. Rabuffetti**

10:00 Intermission.

10:15 . Flexible transparent film heaters based on random networks of silver nanowires:

Synthesis, characterization and integration into devices. **C. Celle**, T. SANNICOLORO, D. TOYBOU, A. CABOS, J. SIMONATO

10:35 . Fabrication of high quality compressible 3D graphene aerogel based on graphene oxide nanobelts and for supercapacitor. T. Fan, Z. Xiao, T. He, Y. Liu, **Y. Min**

10:55 . Expansion of the family of gigantic palladium macrocycles based on {Pd84}. **L. Cronin**

11:15 . Spatially orthogonal chemical functionalization of a hierarchical pore network for catalytic cascade reactions. **C.M. Parlett**, S.K. Beaumont, L.J. Durndell, M. Isaacs, N.S. Hondow, K. Wilson, A.F. Lee

11:35 . Synthesis and characterization aluminum nanoparticles capped by polymerization of acrylic monomers. **C.O. Nyapete**, P.A. Jelliss, S.W. Buckner

11:55 . Synthesis and characterization of *o*-carborane passivated aluminum nanoparticles. **A. Benziger**, S.W. Buckner, P.A. Jelliss

Section F

Venue

Placeholder

Lanthanide & Actinide Chemistry

Cosponsored by WCC

A. De Bettencourt Dias, *Organizer*

R. J. Abergel, K. Kavallieratos, D. A. Penchoff, *Presiding*

8:30 . Terminal Uranium(IV) sulfido and hydrosulfido complexes: Theoretical study of the uranium-sulfur bond. **C. Alvarez Lamsfus**, L. Maron

8:50 . Selective separation of americium from europium using 2,9-bis(triazine)-1,10phenanthrolines in ionic liquids: A new twist on an old story. **N.J. Williams**, J. Dehaut, C.W. Abney, H. Luo, S. Dai

9:10 . Computational prediction of paramagnetic NMR spectra of f-element complexes. **H. Moylan**, J. McDouall

9:30 . Thermochemical and structural predictions of lanthanide- and actinide-containing compounds: A computational perspective. **D.A. Penchoff**, C. Peterson, A.K. Wilson

9:50 Intermission.

10:00 . Actinide coordination with bio-inspired ligands: A bridge between fundamental element chemistry and new therapeutic drug development.

R.J. Abergel, G. Deblonde, I. Captain, P. Agbo, A. Ricano, D. An

10:20 . Controlled synthesis of lanthanide nanomaterials with covalent organic frameworks. **A. Braun**, S. Alayoglu, C. Booth, D. Olive, M. Straub, S.G. Minasian

10:40 . Trivalent f-metal coordination and extraction by tripodal sulfonamide ligands and analogs. E.V. Govor, V.A. Anagnostopoulos, A.N. Morozov, A.M. Mebel, R.G. Raptis, **K. Kavallieratos**

11:00 Intermission.

11:10 . Synthesis and redox non-innocent reactivity of bis(NHC)borate-supported thorium complexes. **M. Garner**, S. Hohloch, L. Maron, J. Arnold

11:30 . Exploring water selective properties and uptake rates of a uranium metal-organic nanotube. **A.S. Jayasinghe**, M. Payne, D. Unruh, T. Forbes

11:50 . Chalcogenide insertion reactivity of a thorium-alkyl complex supported by amidinate ligands. **N. Settineri**, J. Arnold

Section G

Venue

Placeholder

Nanoscience

B. G. Trewyn, *Organizer*

B. A. Hernandez-Sanchez, *Presiding*

8:00 Hyaluronic acid conjugated carbon quantum dots for bioimaging and targeted drug delivery in ophthalmology. **B.B. Karakocak**, J. Liang, P. Biswas, N. Ravi

8:20 . Bacteriophage-conjugated quantum dots as *in vivo* luminescent bioimaging agents. **W.C. Corbin**, M. Casillas, J. Pelowitz, C. Ashley, B.A. Hernandez-Sanchez

8:40 . Bioconjugation chemistry in luminescent gold nanoparticles. **R. Vinluan**, j. Zheng

9:00 . Nanoelectronic signaling approaches for chemical sensing and fundamental investigation of chemical/biological systems. **M. Ding**, Y. Huang, X. Duan

9:20 . Magnetically stimulated release from Medusa particles. B.J. McCormick, M.E. Whitaker, E. Roedern, K. O'Connor, R.R. Shah, S. Pan, J.A. Nikles, C.S. Brazel, **D.E. Nikles**

9:40 . Liquid biopsy for detecting ductal pancreatic adenocarcinoma. **S.H. Bossmann**, H. Wang, M. Kalubowilage, O. Covarrubias Zambrano, A.P. Malalasekera, A.S. Yapa, R. Ortega, Y. Toledo, A. Kasi, S. Williamson, C.T. Culbertson, D.L. Troyer

10:00 Intermission.

10:10 . Synthesis of multifunctional dendronized-gold nanoparticles for bimodal *in vivo* imaging. **A. SAHA RAY**, M.W. Brechbiel, M. Daniel

10:30 . Developing lanthanide doped alkaline earth chalcogenide nanoparticles for scintillators and bioimaging agents. **B.A. Hernandez-Sanchez**, T.J. Boyle, T.N. Lambert, P. Lu

10:50 . Light scattering study on the interaction of poly(N-isopropylacrylamide) and transition metal dications. **L. Fulton**, J. Tsavalas, W.R. Seitz, R.P. Planalp

11:10 . Atomically precise Organomimetic Cluster Nanomolecules (OCNs). **E.A. Qian**, A.I.

Wixtrom, J.C. Axtell, A. Saebi, D. Jung, P. Rehak, Y. Han, E. Hakim Mouilly, D. Mosallaei, S. Chow, M. Messina, J. Wang, A.T. Royappa, A.L.

Rheingold, H.D. Maynard, P. Kral, A.M. Spokoyny

11:30 . Bottom-up synthesis and self-assembly of atomically precise pristine and nitrogen-doped graphene nanoribbons. **A. Sinitskii** **11:50** . Integrating sphere microscopy to quantify losses and limits in nanoscale solar cells. **S.A. Mann**, S. Oener, A. Cavali, J. Haverkort, E. Bakkers, E. Garnett

12:10 . Approaching the hole mobility limit of GaSb nanowires. Z. Yang, **J.C. Ho**

Section H

Venue

Placeholder Organometallic Chemistry: Applications to Organic Transformations N. S. Radu, *Organizer* B. Fraga, *Presiding*

8:30 . Mechanistic understanding of catalyst-controlled and tunable, chemoselective silvercatalyzed intermolecular nitrene transfers. **T. Yang**, J.F. Berry

8:50 . Preparation and characterization of copper(I) diazabutadiene complexes and catalytic applications. **B. Zelenay**, F. Maseras, S. Diez-Gonzalez

9:10 . Synthesis and reactivity of weakly interacting dicopper systems. M.B. Pastor, T. Betley, **Q. Zhao**

9:30 . Synthesis and reactivity of mixed-ligand dirhodium(II) complexes with pendant axial ligands. **A. Darko**, D. Cressy, B. Anderson, W.A. Sheffield

9:50 . Selective *ortho* C-H activation of pyridines directed by Lewis acidic boron of PBP pincer iridium complexes. **W. Shih**, O. Ozerov

10:10 . Mechanistic insight into carbon-sulfur bond formation at cobalt (III). **B.J. Foley**, C. Palit, O. Ozerov

10:30 . Oxidative reactivity of organometallic Ni^{II}, Ni^{III} & Ni^{IV} complexes in the formation of CC bonds. **M.B. Watson**, L.M. Mirica

10:50 . Mechanistic study of an improved nickel precatalyst for the Suzuki-Miyaura reaction of aryl sulfamates: Understanding the role of nickel(I) species. **M. Mohadjer Beromi**, N. Hazari

11:10 . Rational design of improved Pd(II) precatalysts and their application towards new crosscoupling reactions. P. Melvin, **N. Hazari**

11:30 . Mechanistic investigations of palladium(II) precatalysts: Effects of reaction conditions on precatalyst activity in the Suzuki cross-coupling of aryl bromides. **K.L. Barnett**, K.H. Shaughnessy

11:50 . Half-sandwich ruthenium catalysts with enantiopure primary amine-tethered Nheterocyclic carbenes for asymmetric ketone hydrogenation.

K. Wan, M.M. Sung, A.J. Lough, R.H. Morris

12:10 . Asymmetric transfer hydrogenation of ketones by rhodium and iridium complexes of chiral oxazolidine fused N-heterocyclic carbene ligands. B. Ramasamy, **P. Ghosh**

Section I

Venue

Placeholder

2017 Priestley Medalist: Symposium in honor of Tobin J. Marks

Polymerization, Coordination Chemistry & Interfacial Catalysis Cosponsored by PMSE

Financially supported by Dow-Dow Corning, ExxonMobil, STRENGTH, Argonne National Lab, Northwestern University

A. Facchetti, T. Lohr, *Organizers*

M. Delferro, *Presiding*

8:30 Introductory Remarks.

8:35 . Controlling ethylene/ α -olefin selectivity with molecular olefin polymerization catalysts. **J. Klosin**

Klosin

9:05 . Performance polymers in the petroleum additives industry. **N.A. Cain**, J.D. Moore

9:35 . Deactivation and reactivation of methylaluminoxane (MAO) and the derived metallocene catalysts. New insight into MAO active site structure and activation mechanism. **L. Luo**, A. Jain, J. Harlan

10:05 . Recent developments concerning post-metallocene olefin poly/oligomerization catalysts at Mitsui Chemicals. **M. Kondo**, S. Ishii, N. Uehara, Y. Tanaka, K. Michiue, K. Tanaka

10:35 Intermission.

10:45 . Can microdroplets catalyze chemical reactions?. **R.N. Zare**

11:15 . Reactions of C-Au and C-H bonds with polynuclear metal carbonyl cluster complexes.

R.D. Adams, P. Dhull, V. Rassolov, J. Tedder, Y. Wong

11:45 . Sustainable polymers with complete recyclability for a circular economy. **E.Y. Chen**

Section J

Venue

Placeholder

Chemistry is Central to Applied Materials

C. J. Chang, *Organizer*

C. R. Bertozzi, M. A. Paley, *Organizers, Presiding*

8:30 . Hybrid perovskites under pressure: Accessing new properties through lattice compression.

A. Jaffe, Y. Lin, D. Umeyama, C. Beavers, J. Voss, W. Mao, **H. Karunadasa**

9:05 . Densely-functionalized porous polymers for ammonia capture, metal ion separations, and battery applications. G. Barin, S. Demir, J.C. Axelson, M. Aubrey, J.A. Mason, N. Brune, M.K. Taylor, S. Lee, J. Van Humbeck, D.K. Shuh, C.J. Chang, **J.R. Long**

9:40 . Designing molecular materials for quantum applications. J. Zadrozny, C. Yu, M. Graham, M. Fataftah, **D.E. Freedman**

10:15 Intermission.

10:30 . Electrolyte-Mediated assembly of charged nanoparticles. **M. Olvera De La Cruz**

11:05 . Seaweed-Based synthesis of nanostructures for multiple energy storage. **D. Yang**, X. Yao

11:40 . Framework chemistry and its global reach. **O.M. Yaghi**

Section K

Venue

Placeholder

Switchable Catalysts

J. A. Byers, *Organizer*

P. Diaconescu, *Organizer, Presiding* F. Breher, *Presiding*

8:30 . Altering the selectivity of iron-catalyzed hydrocarbon upgrading. **P.J. Chirik**, J. Steves, V. Schmidt

9:00 . Reversible interconversion of CO₂/H₂ and formic acid using Cp*Ir(III) complexes with proton responsive ligands. **E. Fujita**, J.T. Muckerman, Y. Himeda

9:30 . Switchable polynuclear complexes consisting of ambidentate ligands. **F. Breher**

10:00 . Redox catalysis for biomass degradation. **C. Stephenson**

10:30 Intermission.

10:45 . Cerium clusters supported by trimetallic crown ethers as catalysts for alternative copolymerization of cyclohexene oxide and CO₂. **K. Mashima**, H. Nagae, R. Aoki, T.P. Spaniol, J. Okuda

11:15 . One-pot switchable catalytic processes involving the copolymerization of epoxides and carbon dioxide. **D.J. Darensbourg**

11:45 . Supramolecular approach to enzyme mimics. **C.A. Mirkin**

12:15 Concluding Remarks.

Section L

Venue

Placeholder

Bioinorganic Chemistry

S. A. Koch, *Organizer*

D. Wang, Y. Zhang, *Presiding*

8:30 . Study the interactions of biometals with microtubule binding domain of tau protein, contribution to Alzheimer's diseases. **S. Ahmadi**, S. Zhu, R. Sharma, R. Dutta Majumdar, R. Soong, D. Wilson, A. Simpson, H. Kraatz

8:50 . Small biomolecules reactions with carbon disulfide: Pursuing a primary biological target.

M.L. Souza, A. DeMartino, P.C. Ford

9:10 . Biomimetic, catalytic water oxidation by molecular nickel complexes with redox active ligands. **D. Wang**, C. Bruner

9:30 . Building copper active sites in artificial metalloproteins. **S.I. Mann**, T. Heinisch, A. Weitz, T.R. Ward, M.P. Hendrich, A. Borovik

9:50 . Can Fe^{IV}(O)'s swim? The aqueous chemistry of the [Fe^{IV}(O)(TMC)]²⁺ complex. **J. Klein**, A. Shokri, a. draksharapu, J. Prakash, C.J. Cramer, L. Que

10:10 Intermission.

10:20 . Proton management within a [FeFe] hydrogenase model complex. **K. Chu**, M. Chiang, Y. Liu

10:40 . HNO Binding in heme proteins: Effects of iron oxidation state, axial ligand, and protein environment. R. Khade, Y. Yang, Y. Shi, **Y. Zhang**

11:00 . FerricCEST: A low-spin Fe(III) complex as paraCEST MRI contrast agent. **P.B.**

Tsitovich, J.R. Morrow

11:20 . Photoreleasing caged molecules containing nitrile functionality from Ru(II) complexes of the bulky 6-phenyl-2,2'-bipyridine ligand. **S. Saha**, R. Coll, K.L. Fillman, J. Pellois, C. Turro, K.R. Dunbar

11:40 . TypeI/TypeII dual photoreactivity of new promising Ru-polypyridyl thiophene complexes: A theoretical exploration. **m. alberto**, J. Pirillo, N. Russo, C. Adamo

12:00 . Dual targeting redox-active gold(I) N-Heterocyclic carbene complexes: A new approach to cancer treatment. **K. Arumugam**, M. Miles, R. McCall, J. Arambula

Multicenter Molecules & Coupled Molecular Assemblies: Synthesis, Characterization & Theory

Synthesis

Sponsored by PHYS, Cosponsored by INOR

Light-Driven Chemistry: Photoelectrochemistry & Photocatalysis

Spectroscopy & Microscopy of Photocatalytic & PEC Materials

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

WEDNESDAY AFTERNOON

Section A

Venue

Placeholder

Deposition & Etching of Nanostructures

Cosponsored by COLL[‡]

Financially supported by ACS Publications, Strem Chemical

H. Fairbrother, A. V. Walker, *Organizers*

L. McElwee-White, *Organizer, Presiding*

1:30 . Experimental and computational development of single source precursors to tin-doped germanium nanocrystals. **J. Vela-Becerra**

2:05 . Surface chemistry guided nanoparticle deposition in plasmonic hotspots. **J. Millstone**

2:40 . Mechanism based design of precursors for FEBID. **L. McElwee-White**

3:15 Intermission.

3:35 . Nanosoldering carbon nanotube junctions with metal via local chemical vapor deposition for improved device performance. J. Do, D. Estrada, X. Xie, N. Chang, J.A. Rogers, E. Pop, J. Lyding, **G.S. Girolami**

4:10 . Designing high-performance nanoscale catalysts for small molecule reactions: Probing size and composition-dependent electrocatalytic behavior in noble metal-based nanowires. **S.S. Wong**

4:45 . Lanthanide oxides and lanthanide nitrides via vapor phase approaches. **H. Parala**

Section B

Venue

Placeholder

Celebrating 60 Years of the Division of Inorganic Chemistry Members

D. C. Crans, *Organizer*

M. J. Clarke, *Organizer, Presiding*

A. De Bettencourt Dias, P. K. Dorhout, *Presiding*

1:30 Introductory Remarks.

1:35 . Meanderings in atom transfer reaction chemistry, structure, electronic structure and thermochemistry. **J.M. Mayer**

2:05 . Tuning transition metal redox potentials through the incorporation of redox-inactive cations: A route to breaking potential dependent scaling relationships?. A.H. Reath, T. Chantarojsiri, **J.Y. Yang**

2:35 . Understanding the formation of Pd(I) and Ni(I) complexes in cross-coupling reactions. **N. Hazari**

3:05 Intermission.

3:20 . Interplay of inorganic and organic chemistry in catalyst design and performance. **D.B. Grotjahn**

3:50 . Evaluating the cluster-surface analogy with electronically and geometrically flexible macrocyclic ligands. P. Cui, Q. Wang, B. Manor, P. Carroll, **N.C. Tomson**

4:20 . Carbon dioxide reduction with transition metal catalysts composed of pyridines and Nheterocyclic carbenes based chelates. **D.B. Burks**, S. Siek, C. Boudreaux, J.H. Delcamp, E.T. Papish

4:40 . Controlling reactivity of small molecules through confinement. M.D. Johnson, **D.C. Crans**

5:10 Concluding Remarks.

Section C

Venue

Placeholder

Frontiers in Heavy Element Electronic Structure

Cosponsored by NUCL

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

D. L. Clark, *Organizer, Presiding*

1:30 . From a high-valent iron nitride to a low-valent pentad of iron nitrosyl complexes {FeNO}⁶⁻¹⁰ stabilized by a chelating, N-anchored tris-N-heterocyclic carbene ligand. **K. Meyer**

1:50 . Design and properties of photoredox chromophores that are stronger reductants than alkali metals. **M.D. Hopkins**, H.B. Vibbert

2:10 . Layered metal oxide nanosheets as model surfaces for understanding the strong metalsupport interaction. M. Strayer, A.S. Rosas, R. Uppuluri, J.M. Binz, T. Senftle, A. Azizi, R.M. Rioux, M.J. Janik, N. Alem, **T.E. Mallouk**

2:30 . Chemistry of iron complexes toward the synthesis of FeX multiple bonds. **P.T. Wolczanski**, B. Jacobs, S.N. MacMillan, T.R. Cundari

2:50 . Actinides, f-orbitals, and multiple bonds: These are just a few of Bruce's favorite things. **J.L. Kiplinger**

3:10 intermission.

3:30 . Addition of H-X to Mn and Ru amide bonds: Catalysts for formic acid decomposition and the aldehyde water shift reaction. **J.M. Boncella**, A.M. Tondreau, N.H. Anderson, B. Scott

3:50 . New thoughts on the speciation of polychalcogenides in solutions: From lapis lazuli, to the paper industry, to synthetic inorganic chemistry and why my clothes smell so bad. **P.K.**

Dorhout **4:10** . Recent advances in the chemistry of

tris(cyclopentadienyl) rare-earth and actinide metal complexes. **W.J. Evans**

4:30 . Betwixt or between? Inter- and intraligand redox processes in Fe and Co-SNS coordination complexes. **R. Baker**

4:50 . Formation of C(sp³)-N bonds from Rh^{III}-Me and Ir^{III}-Et complexes. T. Stevens, T.R. Cundari, **K.I. Goldberg**

Section D

Venue

Placeholder

Chemistry of Materials: Metal Organic Frameworks

C. G. Lugmair, *Organizer*

A. F. Cozzolino, *Presiding*

1:30 . Reproducible synthesis and high porosity of mer-Zn(Im)₂ (ZIF-10): Exploitation of an apparent double-eight ring template. **J.R. Ramirez**, H. Yang, C. Kane, A. Ley, K.T. Holman

1:50 . Water dynamics in three-dimensional extended lead(II) structures: Multiple single-crystal-to-single-crystal transformations. **R.A. Burrow**, B. Brummelhaus de Menezes

2:10 . Redox doping and electron transport in metal-organic frameworks. **M. Aubrey**, B. Wiers, S. Andrews, T. Sakurai, S. Reyes-Lillo, S. Hamed, C. Yu, J.A. Mason, J. BAEG, F. Grandjean, G.J. Long, S. Seki, J. Neaton, P. Yang, J.R. Long

2:30 . Structural characterization of framework-guest interactions in metal-organic frameworks.

M.I. Gonzalez, R.L. Siegelman, E.D. Bloch, J.A. Mason, M. Kapelewski, W. Queen, S.J. Teat,

K.J. Gagnon, J.R. Long

2:50 . Confinement of inorganic clusters in metal-organic frameworks with coordinating sites.

M.I. Gonzalez, A. Turkiewicz, L.E. Darago, J.R. Long

3:10 . Tuning the adsorption-induced phase change in the flexible metal-organic framework Co(bdp). **M.K. Taylor**, J.R. Long

3:30 Intermission.

3:45 . Pyrazolate-based porphyrinic MOFs with extraordinary stability and catalytic activity for C-H bond halogenation. **K. Wang**, H. Zhou

4:05 . Porphyrin-based metal organic frameworks for electrocatalysis. **a. fateeva**, F. Maillard, B. Abeykoon, J. Tommasino

4:25 . Metal-organic layers for earth-abundant metal catalysis. **Z. Lin, W. Lin, T. Sawano, N.C. Thacker, C. Wang**

4:45 . Metal-organic frameworks nodes for earth-abundant metal catalysis. **P. Ji, K. Manna, Z. Lin, W. Lin**

5:05 . Incorporating p-block catalysts into robust metal organic frameworks. **P. Larson, B. Tahmouresilerd, j. cheney, A.F. Cozzolino**

5:25 . Metal-Organic Frameworks with Tunable Bandgap. **J. Park, D. Feng, Z. Bao**

Section E

Venue

Placeholder

Inorganic Spectroscopy

V. C. Popescu, *Organizer, Presiding*

1:30 . Achieving surface sensitivity in soft x-ray spectroscopy: Transient reflectivity of charge transfer dynamics in iron oxide. **A. Cirri, J. Husek, S. Biswas, L. Baker**

1:50 . Probing molecular magnetism with neutron scattering. **S. Stavretis, D.H. Moseley, A.A.**

Podlesnyak, C.M. Brown, Y. Cheng, L.L. Daemen, A.J. Ramirez-Cuesta, X. Wang, C.M. Hoffmann, S.O. Diallo, Z. Zhu, M. Guo, J. Tang, H. Cui, F. Fei, X. Chen, Z. Xue

2:10 . Design principles for porous materials containing quantum sensors. **J. Zadrozny, A. Gallagher, D. Harris, D.E. Freedman**

2:30 . Probing ion-pairing trends in aqueous polyoxometalate solutions. **D. Sures, K. Kozma, P.I. Molina, S. Serapian, C. Bo, M.D. Nyman**

2:50 . High-valent states in cobalt cubanes and clusters: Relevance to O–O bond formation. **R.G. Hadt, C. Brodsky, D. Hayes, L.X. Chen, D.G. Nocera**

3:10 . Studies of single-molecule magnets by far-IR and Raman in magnetic fields. **D.H. Moseley, S. Stavretis, K. Thirunavukkuarasu, Q. Chen, H. Zhou, J. Ludwig, D. Smirnov, Z. Zhu, M. Guo, J. Tang, F. Fei, H. Cui, X. Chen, Z. Xue**

3:30 . Capturing intermediates of molecular solar fuels catalysts by time-resolved mid-IR spectroscopy. **L. Hammarstrom, R. Lomoth, S. Ott**

3:50 . Light driven activation of O₂ with iron(II) polypyridyl complexes. **J. Chen, a. draksharapu, W.R. Browne**

4:10 . Relativistic effects on the spectra and redox properties of 5d metallocorroles. **A. Ghosh, R.F. Einrem, A. Alemayehu**

4:30 . Systematic study of luminescence rigidochromism on ambipolar polyimine rhenium(I) complexes. **G.A. Salazar-Garza, B. Hua, C.M. Williams, V. Nesterov, M.A. Omary**

4:50 . Role of specific and non-specific interactions in understanding the excited-state processes of transition-metal complex based photodrugs. **B. Dietzek**

5:10 . Advanced ¹⁷O MAS NMR methods to characterise the local environment in complex inorganic systems. **D. Grekov, y. bouhoute, K.C. Szeto, N. Merle, I. Del Rosal, L. Maron, R. Gauvin, M. Taoufik, L. Delevoye**

Section F

Venue

Placeholder

Coordination Chemistry: Characterization & Applications

S. A. Koch, *Organizer*

B. Barry, A. Mukherjee, *Presiding*

1:30 . Dual-modal MR/NIR fluorescent probes for zinc sensing applications. **E. Coakley, N.J.**

Long

1:50 . Coordination chemistry approach for lithium ion batteries. **W. Shi, P. Cheng**

2:10 . Molecular engineering of ruthenium complexes for highly efficient dye-sensitized solar cells. **S. Aghazada, M. Graetzel, M. Nazeeruddin**

2:30 . 1,2,3-Triazole-based chelating ligands under investigation: Tuning the donor strength. **L. Suntrup, F. Stein, B. Sarkar**

2:50 . Development of molecular underground chemical tracers: Coordination chemistry of alkaline earth and transition metal salen-derivative precursors. **T.J. Boyle, J.M. Sears, O. Staples, D. Perales, K. Wyss, J.A. Greathouse, R.A. Kemp**

3:10 Intermission.

3:20 . Understanding reactivities of transition metal compounds with ROS. **A. Mukherjee**

3:40 . Mn(III) in an all O-donor ligand environment with fluorinated alkoxides. **C. Kotyk, J. Henebry, C. Sun, J.L. Steele, Y. Chen, V.F. Oswald, J.W. Bacon, A.L. Rheingold, L. Doerrer**

4:00 . Synthesis and reactivity of redox-active molecular group 13 complexes. **T. Sherbow, L.A. Berben**

4:20 . Dinuclear photoCORMS: Visible/near-infrared light activating CO release. **Z. Li, A.E. Pierri, P. huang, W. Gang, A. Iretskii, P.C. Ford**

4:40 . Design, synthesis and characterization of rhenium(I) tricarbonyl complexes derived from a-diimine coligand for bio-imaging applications. **J. Jimenez, I. Chakraborty, P. Mascharak**

5:00 . Complexes with bisguanidine-type ligands towards oxidative additions across sp²heteroatom bonds. **B. Barry, K. Feller, H. Schickel, J. Bruggen, J. Sanborn, R. Velcheck, J. Norman**

Section G

Venue

Placeholder

Coordination Chemistry: Synthesis & Characterization

S. A. Koch, *Organizer*

T. T. Boron, P. Desrochers, *Presiding*

1:30 . Coinage metal nanoclusters: Characterization and catalytic applications. **A.W. Cook, T.W. Hayton**

1:50 . Temperature-Driven geometric conversion of solid-state polymorphs of a four-coordinate nickel(II) complex. **X.B. Powers, K.B. Ghiassi, J.T. Greenfield, M.M. Olmstead, A.L. Balch**

2:10 . Side-on dioxygen complex of cobalt: Structure, reactivity, and conversion to bimetallic products. **D.E. DeRoshia, B.Q. Mercado, P.L. Holland, K.R. Rodgers**

2:30 . Synthesis and reactivity of imido and nitrido complexes of first row transition metals supported by tris(pyrazolyl)borate ligands. **D.C. Cummins, K.H. Theopold, G.P. Yap**

2:50 . Synthesis and reactivity of new divalent bis(alkoxide) complexes. **T. Hollingsworth, S. Groysman**

3:10 Intermission.

3:20 . Sweeter scorpionates incorporate carbohydrates into functional metal chelates. **P. Desrochers, T. Clements**

3:40 . Cu(II) mixed-ligand polypyridyl complexes with 6-mercaptopurine: Synthesis, characterization and their cytotoxicity evaluations. **J.A. Obaleye**

4:00 . Cytotoxicity studies of ruthenium(II) polypyridine compounds with a β-diketone ligand. **J.A. Obaleye, A.O. Rajee, K.R. Dunbar**

4:20 . Ligand design to support high valent metal oxido/hydroxido complexes. **V. Oswald, A. Borovik**

4:40 . Anion effect on aluminum hydroxide cluster synthesis. **E. Eitrheim, C.K. Perkins, B. Fulton, T. Forbes, D.A. Keszler**

5:00 . Controlling single-molecule magnetic behavior of two families of metallocrowns by modifying lanthanide choice or structural components. **T.T. Boron, J.C. Lutter, C.I. Daly, C. Chow, A.H. Davis, A. Nimthong-Roldan, M. Zeller, J.W. Kampf, T. Mallah, C.M. Zaleski, V.L. Pecoraro**

Section H

Venue

Placeholder

Environmental & Energy-Related Inorganic Chemistry

S. A. Koch, *Organizer*

M. Fieser, A. I. Nguyen, *Presiding*

1:30 . Modeling the dissolution of transition metal oxide nanomaterials. **S.E. Mason, J. Bennett**

1:50 . Understanding the mechanisms of CO₂ adsorption enhancement/degradation in all silica zeolites under wet conditions. **W. Jeong, J. Kim**

2:10 . Photochemistry of a direct contact core-shell tandem photocatalyst for overall water splitting. **M.A. Melo, F.E. Osterloh**

2:30 . Bioinspired electrocatalytic CO₂ reduction using first-row transition metal catalysts. **E. Nichols, C.J. Chang**

2:50 . Tunable, site-isolated Co₃O₄ oxygen-evolution catalysts in porous frameworks. **A.I. Nguyen, K.M. Van Allsburg, M. Terban, M. Bajdich, J. Oktawiec, M.S. Ziegler, J.P.**

Dombrowski, K.V. Lakshmi, W. Drisdell, J. Yano, S. Billinge, T. Tilley

3:10 . Aluminum doped SrTiO₃ nanocrystals as photocatalyst for overall water splitting under sunlight. **Z. Zhao, F.E. Osterloh**

3:30 Intermission.

3:40 . Cationic dirhodium(II,II) complexes as dual action electrocatalysts for H⁺ and CO₂ reduction. **S. Witt, C. Turro**

4:00 . Progress towards catalytic ammonia splitting. **M.R. Smith**

4:20 . Rational design of ruthenium(II) chromophores: Towards efficient photocatalytic proton reduction. **R.S. Khnazyer, K. El Roz, F.N. Castellano**

4:40 . Catalytic decarbonylation of fatty acid esters. **M.E. Fieser, A. John, L.A. Mitchell, B. Benson, L.T. Hogan, A.M. LaPointe, W.B. Tolman**

5:00 . Synthesis of Ni₂P nanoparticles supported r-GO composites for hydrodesulphurization applications. **V. Tzitzios, M. Kartsiotis, V. Pillai, T. Anjana, G. PAPA VASSILIOU, T. Karagiannis, S. Al Hassan**

5:20 . Electrochemical evaluation of Ru(II) carbene complexes for CO₂ reduction. **D.P.**

Harrison, J.T. Hyde, D. Chisner

Section I

Venue

Placeholder

2017 Priestley Medalist: Symposium in honor of Tobin J. Marks

Catalysis: Characterization, Computations, & Reactivity

Cosponsored by PMSE

Financially supported by Dow-Dow Corning, ExxonMobil, STREM, Argonne National Lab, Northwestern University A. Facchetti, T. Lohr, *Organizers* M. Stalzer, *Presiding*

1:30 Introductory Remarks.

1:35 . Oxidative water splitting with molecular, heterogenized and heterogeneous iridium catalysts. A. Bucci, I. Corbucci, L. Fagiolari, G. Menendez Rodriguez, G. Bellachioma, C. Zuccaccia, **A. Macchioni**

2:05 . Cascade synthesis of nanoparticle-polymer composites. **M.A. Firestone, B.S. Ringstrand, D.J. Williams, H.D. Magurudeniya, A. Joshi**

2:35 . DMF-stabilized single-nano-sized metal nanoclusters as catalyst for cross-coupling reactions. **Y. Obora**

3:05 Intermission.

3:15 . Preparation of deuterated drugs through novel catalysis: Synthesis, purification, and preclinical data. **G.Y. Li**

3:45 . Mechanistic insights into catalytic conversion methane and light alkanes over supported catalysts. **M. Neurock**

4:15 . DFT approach for the investigation of single-site supported catalysts. **A. Motta, M. Delferro, T. Lohr, T.J. Marks**

Section J

Venue

Placeholder

Organometallic Chemistry: Catalysis

N. S. Radu, *Organizer*
T. J. Williams, *Presiding*

1:30 . Highly electrophilic iridium species supported on a sulfated metal oxide for catalytic H/D incorporation. **R. Klet, M. Delferro**

1:50 . Reactivity of *para*-benzoquinones with ^{ipr}PCPIrH₄: In search of new hydrogen acceptors.

M. Wilklow-Marnell, W.W. Brennessel, W.D. Jones

2:10 . Selective conversion of neat glycerol to lactic acid using a prolific catalyst. **I. Demianets, Z. Lu, T.J. Williams**

2:30 . Platinum-catalyzed ligand-directed C-H functionalization reactions. **S. Huo, D.C. McAteer, E. Javed**

2:50 . Synthesis of 2-alkynoates and 2-ynamides via palladium(II) catalyzed oxidative carbonylation. **N.L. Hughes, Q. Cao, C. Brown, M.J. Muldoon**

3:10 . Mechanistic Studies on Palladium-Catalyzed Aminocarbonylation of Aryl Halides. **J. Wang, J.F. Hartwig**

3:30 . Theoretical study of (hetero)aromatic fluorination catalyzed by palladium. **P. Fleurat-Lessard, M. Ponce Vargas, J. Roger, C. Testa, J. Guilbaud, N. Pirio, J. Hierso**

3:50 . Room temperature conversion of CO₂ to methanol with nickel catalysis. **Z. Lu, T.J. Williams**

4:10 Relative thermodynamics of nickel hydride and formate complexes. **N.A. Eberhardt, J.A. Krause, H. Guan**

4:30 . Computational study of dinuclear nickel catalyzed alkyne cyclotrimerization. **D. Kwon, D. Ess**

4:50 . Synthesis of xanthene-bridged bis(iminopyridine) di-nickel complexes toward alkyne cyclotrimerization. **R. Hollingsworth, R.L. Lord, S. Groysman**

Section K

Venue

Placeholder

Organometallic Chemistry: Synthesis & Characterization-Late Transition Metals

N. S. Radu, *Organizer*
L. Geary, V. M. Iluc, *Presiding*

1:30 . σ-Complexes of cobalt and copper. **Y. Lee**

1:50 . Organometallic cationic dicopper complexes: Synthesis, mixed-valence, reactivity, and their role in catalysis. **M.S. Ziegler, K.V. Lakshmi, T. Tilley**

2:10 . Using dispersion forces to isolate low-valent high-oxidation state copper complexes. **C. Wagner, L. Tao, E.J. Thompson, T.A. Stich, J. Guo, J.C. Fettinger, L.A. Berben, R. Britt, S. Nagase, P.P. Power**

2:30 . C[∧]C*-cyclometalated mesoionic NHC ligands in phosphorescent platinum(II) complexes.

J. Soellner, T. Strassner

2:50 . Adaptable chelating diphosphine ligand for the stabilization of elusive palladium and platinum alkylidenes. **B. Barrett, V.M. Iluc**

3:10 . C[∧]C* cyclometalated ruthenium NHC complexes. **D. Schleicher, T. Strassner**
3:30 . Reactivity of nickel complexes bearing a HN(CH₂CH₂P^{Pr})₂ ligand. **N.P. Nambukara Wellala, J. Luebking, J.A. Krause, H. Guan**

3:50 . Enhanced photoluminescence quantum yields through excimer formation. **P. Piermaria, T. Strassner**

4:10 . Synthesis of luminescent gold(III) cyclometalated complexes. **A.N. Sulicz, A. Maity, T. Gray**
4:30 Structural and electronic characterization of early stage Magnus-type organocobalt intermediates in the Pauson-Khand reaction via x-ray absorption spectroscopy. **L. Geary**

4:50 . Delocalised chains and rings of ferrocenes. **L.E. Wilson, T. Albrecht, N.J. Long**

5:10 . Selective C8-metalation of various purine nucleosides. **F. Kampert, E.F. Hahn**

5:30 . Oxidation chemistry of palladium complexes with the smallest steric N-heterocyclic carbene, I Me (I Me = 1,3-Dimethylimidazole-2-ylidene). **E. Lee**

Section L

Venue

Placeholder

Main Group Chemistry T. W. Hudnall, Organizer T. Perera, Presiding

1:30 . Antimony(III) secondary bonding interactions for anion binding. **J. Qiu, A.F. Cozzolino**

1:50 . Novel reactivity of N-heterocyclic carbenes toward one-electron oxidants. **E. Lee**

2:10 . Synthesis and photochemistry of N,N'-diamidocarbene – Supported Sb(V) and Bi(III) chloro complexes for solar fuel production. **T.A. Perera, T.W. Hudnall**

2:30 . Stable N-heterocyclic carbene adducts of diphosphorus and carbon monoxide. **R.J. Gilliard, R. Suter, Z. Benko, H. Grützmacher, J.D. Protasiewicz**

2:50 . Using N-Heterocyclic Olefin (NHO) ligands to advance concepts in main group chemistry. **E. Rivard, C. Hering-Junghans, M. Lui, N. Paisley**
3:10 . Synthesis and characterization of stable emissive radicals and biradicals derived from singlet carbenes. **R.N. Arias, C. Barragan, T.W. Hudnall**

3:30 . Flexible nature of the carbodiphosphorane, C(PPh₃)₂, and its reactivity towards main group alkyl complexes. **P. Quinlivan, G. Parkin**

3:50 Intermission.

4:00 . Hydrostannylation reactions of low valent tin(II) hydrides, [ArSn(μ-H)]₂ (Ar = Ar^{Pr^{iv}} or Ar^{Pr^{ib}}, Ar^{Pr^{iv}} = C₆H₃-2,6-(C₆H₃-2,6-ⁱPr₂)₂ Ar^{Pr^{ib}} = C₆H₃-2,6-(C₆H₂-2,4,6-ⁱPr₃)₂) with acyclic and bicyclic olefins. **s. wang, M. McCrea-Hendrick, C.A. Caputo, C. Weinstein, J.C. Fettinger, P.P. Power**

4:20 . Sterically encumbering N-heterocyclic tetrylenes and their reactivity. **C. Weinstein, Y. Zhu, G. Bertrand**

4:40 . Amido and alkyl complexes of magnesium, calcium and strontium containing highly fluorinated Tp' ligands. **N. Romero, Q. Dufrois, C. Dinioi, M. Etienne**

5:00 . Synthesis of Lewis acid-stabilized calcium imides. **B.M. Wolf, C. Maichle-Mössmer, R. Anwander**

5:20 . Reactions of terphenyl stabilized tin(II) hydrides: Ar^{Pr^{iv}}SnH and Ar^{Pr^{ib}}SnH {Ar^{Pr^{iv}} = C₆H₃-(C₆H₃-2,6-ⁱPr₂); Ar^{Pr^{ib}} = C₆H₃-(C₆H₂-2,4,6-ⁱPr₃)₂} with alkynes. **M.L. McCrea-Hendrick, s. wang, J.C. Fettinger, P.P. Power**

Multicenter Molecules & Coupled Molecular Assemblies: Synthesis, Characterization & Theory

Experimental Characterization

Sponsored by PHYS, Cosponsored by INOR

Light-Driven Chemistry: Photoelectrochemistry & Photocatalysis

Devices, Assemblies & Hybrid Processes

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

THURSDAY MORNING

Section A

Venue

Placeholder

Bioinorganic Chemistry Proteins & Enzymes & Model Systems

S. A. Koch, *Organizer*

L. E. Cheruzel, S. A. Toledo, *Presiding*

8:00 Determination of differential orbital covalency of heme active sites by L-edge spectroscopy.

M.L. Baker, B.K. Alpert, H. Cho, E. Denison, W.B. Doriese, J.W. Fowler, K.J. Gaffney, J. Gard, B. Gao, G. .

Hilton, K.D. Irwin, Y.I. Joe, C. Kenney, J. Knight, T. Kroll, S. Lee, D. Li, R. Marks, M. Miniti, K. Morgan, R.A. Mori, H. Ogasawara, G. O'Neil, D.

Schmidt, D. Sokaras, D.S. Swetz, Y. Song, C.J. Titus, J. Ullom, T. Weng, C. Williams, J.J. Yan, B.A. Young, D. Nordlund, E.I. Solomon

8:20 . Selective substrates C-H functionalization with light-driven P450 enzymes. **L.E. Cheruzel**

8:40 . Unleashing a pendant base by reduction-induced hemilability in $[\text{NiN}_2\text{S}_2\text{Fe}(\text{NO})_2]^{+/0}$ complexes. **P. Ghosh**, S. Ding, C. Hsieh, R.B. Chupik, N.S. Bhuvanesh, M.B. Hall, M.Y. Darensbourg

9:00 . Model complexes of NiSOD and the factors that influence Ni redox cycling. **P.T. Truong**, T.C. Harrop

9:20 . Cu(II) coordination differences in the amyloid-beta protein binding models GHK and

DAHK result in varied conditional inter-peptidic metal exchange rate constants. **C.N. Beuning**,

B. Mestre, C. Hureau, D.C. Crans

9:40 . Hemilabile bridging thiolates as proton shuttles in bioinspired H_2 production electrocatalysts. **S. Ding**, P. Ghosh, A.M. Lunsford, N. Wang, N. Bhuvanesh, M.B. Hall, M.Y. Darensbourg

Darensbourg

10:00 Intermission.

10:10 . Interplay of copper and iron in NO release from Dinitrosyl Iron Complexes (DNICs).

R.B. Chupik, D. Bruggeman, M. Maurice, J.A. Denny, M.Y. Darensbourg

10:30 . Origins of the catalytic proficiency of cytochrome-based artificial metalloenzymes. **M. Garcia-Borras**, G. Jimenez-Oses, K.N. Houk

10:50 . Expanding our understanding of Nickel-Acireductone Dioxxygenase (Ni-ARD) through a family of structural analogues of the resting state of the enzyme. **S.A. Toledo**, D. Ivan, A. Sanchez, A.J. Gremillion, S. Sanchez, J.D. Green, V. Lynch

11:10 . Alkane hydroxylation catalyzed by nickel(II) complexes: Effect of ligand photoelectronic factors and solvent coordination on nickel(II) spin state and catalytic activity. **M. Palaniandavar**, S. Muniyandi

11:30 . Structure-function relationships of Mn-containing super oxide dismutases (SOD) studied via quantum mechanical computational methods. **J.H. Rodriguez**

11:50 . Merged heme and non-heme manganese co-factors for a dual anti-oxidant surveillance in photosynthetic organisms. **M. Bonchio** Section B

Venue

Placeholder

Coordination Chemistry: Synthesis & Characterization

S. A. Koch, *Organizer*

L. Pan, L. Yang, *Presiding*

8:30 . Structural flexibility, luminescence, and aurophilic interactions in crystals of the binuclear complexes $\text{Au}_2(\text{Ph}_2\text{P}(\text{CH}_2)_n\text{PPh}_2)_2\text{X}_2$ ($n = 2-6$, $\text{X} = \text{chloride}$ and thiocyanate). **K.R. England**,

K.B. Ghiassi, M.M. Olmstead, A.L. Balch

8:50 . Water soluble cationic zinc lysine hydrochloride compound for spontaneous coating of ZnO on biomaterial surfaces. **L. Pan**

9:10 . Luminescence and rearrangement of small poly-gold phosphine complexes. **D.T. Walters**, R. Babadi, X.B. Powers, K. Ghiassi, M.M. Olmstead, A.L. Balch

9:30 . Designing and crystallographic characterization of trinuclear Cu(II) and dinuclear Zn(II) clusters. **M. Shahid**, F. Sama

9:50 . First report of anagostic interaction in heteronuclear polyoxovanadate-Cu complex with highly selective sensing towards nitro explosives: X-ray, theoretical and TRF investigations. **M. RAIZADA**, **Z.A. Siddiqi**

10:10 Intermission.

10:20 . Synthesis and characterization of copper complexes with Cu^ICu^I , $\text{Cu}^{I.5}\text{Cu}^{1.5}$ and $\text{Cu}^{II}\text{Cu}^{II}$ core structures supported by a flexible dipyrrolylamide ligand. **L. Yang**, E.P. McMoran

10:40 . Binding modes and thermodynamics of iron and vanadium with amidoxime ligands. **B. Parker**, Z. Zhang, J. Arnold, L. Rao

11:00 . Using the terminal metal-oxo bond as a reporter of electron donation from bicyclic guanidinate ligands to mid transition metals. **J. Olson**, D. Swenson, L. Messerle

11:20 . Dual cavity tetracarboxamide host for anion and metal ion binding. **J. Lohrman**, H. Telikepalli, V.W. Day, K. Bowman-James

11:40 . Light harvesting through photoswitchable molecules. **A. Rajput**, A.F. Cazzolino

Venue

Placeholder

Electrochemistry

B. L. Lucht, *Organizer, Presiding*

N. R. Neale, *Presiding*

8:00 . Boron cluster-based ionic liquids for reversible electrodeposition. **R. Dziedzic**, S. Lee, J. Kleinsasser, B.D.

Section C

Venue

Bosley, R.A. Kemp, T.L. Peng, V. Lavallo, **A.M. Spokoyny**

8:20 . Effect of surface ligands on CoP for the hydrogen evolution reaction. **D. Ung**, B. Cossairt

8:40 . Molecular surface modification of semiconductor photoelectrodes – A viable water splitting strategy?. **N.R. Neale**, L.E. Garner, J. Gu, K.X. Steirer, J. Young, N.C. Anderson, E.M. Miller, J.A. Turner, A. Sellinger, T.G. Deutsch

9:00 . High frequency resistivity: Determining fundamental photoelectrode properties in a complex world. **N.C. Anderson**, N.R. Neale

9:20 . Redox-active deep eutectic solvents. **J.C. Goeltz**, L.N. Matsushima, D.G. Jones

9:40 . Quantum mechanical screening of single-atom bimetallic alloys for the selective reduction of CO_2 to C_1 hydrocarbons. **M. Cheng**, E.L. Clark, H.H. Pham, A.T. Bell, M.P. Head-Gordon

10:20 . Semiconductor-to-metal transition in rutile TiO_2 induced by tensile strain. **E. Benson**,

E.M. Miller, S. Nanayakkara, B.A. Gregg

10:40 . Deoptimizing the oxygen reduction reaction on doped amorphous TiO_2 coatings for corrosion inhibition. M. Groenenboom, R. Anderson, D. Horton, S. Policastro, **J.A. Keith**

11:00 . Electrochemical detection of doxorubicin and salinomycin. **J.A. Nikles**, B.J. McCormick, S. Pan, D.E. Nikles

11:20 . Fluorescence spectroelectrochemistry of integrated anthraquinone-polyether macrocycles. **A.G. Sykes**

11:40 . Electroreduction pattern of quinone units in pillar[5-n]arene[n]quinones. **M. Rashvand Avei**, A.E. Kaifer

12:00 . Electro-thermochemical Cycling Process for High-Yield Ammonia Synthesis from N_2 and H_2O at Atmospheric Pressure. **J.M. McEnaney**, A.R. Singh, J.A. Schwalbe, J. Kibsgaard, J.C. Lin, M. Cargnello, T.F. Jaramillo, J.K. Nørskov

Section D

Venue

Placeholder

Solid-State Inorganic Chemistry

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

J. Brgoch, K. Kovnir, *Presiding*

8:30 . Decoupled electronic and phonon transport in complex chalcogenides: A substructure approach. **K. Biswas**

8:45 . Thermoelectric performance of Zintl phase $\text{Yb}_{2-x}\text{Eu}_x\text{CdSb}_2$ exhibiting low thermal conductivity. **J. Cooley**, P. Promkhan, S. Gangopadhyay, D. Donadio, S. Kauzlarich

9:00 . Stabilization of extraordinary off-stoichiometric Bi_2Te_3 for enhancing n-type thermoelectric performance. **I. Chung**

9:15 . Synthesis, structure, and properties of new Si-As framework compounds. **K. Woo**, J. Dolyniuk, K. Kovnir

9:30 . High-throughput experimental approach to find new transition metal ternary chalcogenides. **A. Bhutani**, A. Narayan, J.N. Eckstein, L.K. Wagner, D. Shoemaker

9:45 . Crystal chemistry and magnetism of complex compounds with Zn-P frameworks. **K. Kovnir**

10:00 . $\text{Mg}_{0.5}\text{B}_5\text{C}$ carbaboride as Mg-ion intercalation cathode with redox active anions by firstprinciples calculations. **V. Poltavets**, J.D. Davis, M. Johannes

10:15 . Elucidating the mechanism of high-rate and high-capacity lithium-ion intercalation in bulk complex transition metal oxides. **K.J. Griffith**, A. Forse, J.M. Griffin, C.P. Grey

10:30 Intermission.

10:45 . Developing persistent luminescent phosphors for use in point-of-care diagnostics. **J. Brgoch**, E. Finley, A. Cobb

11:00 . Design and synthesis of novel rare earth kagome materials: Applications in geometric magnetic frustration. **M.B. Sanders**, R.J. Cava

11:15 . Development of a low-temperature solvothermal route to a variety of novel iron chalcogenides. **J.T. Greenfield**, K. Kovnir

11:30 . Synthesis and low-temperature properties characterization of superconducting Ni_{1-x}Bi .

K.M. Powderly, S.M. Clarke, A.J. Rettie, C. Malliakas, D.E. Freedman

11:45 . Rapid Microwave Preparation of New Earth Abundant Magnetocaloric Materials. **J. Grebenkemper**, J.D. Bocarsly, E. Levin, R. Seshadri

12:00 . *In situ* and real-time monitoring of mechanochemical ZIF8 synthesis via gas pressure measurements. **I. Brekalo**, C. Mottillo, K.T. Holman, T. Friscic

12:15 . Mechanistic insights into the chemical and electronic properties of dielectric materials exposed to chemical warfare agents and their structural analogs. **J.R. Soliz**, A.L. Tang, W.O. Gordon, A. Balboa, A.J. Hauser, S.R. Padovani

Section E

Venue

Placeholder

Inorganic Catalysts

S. A. Koch, *Organizer*

M. T. Kieber-Emmons, X. Zhao, *Presiding*

8:30 . Reactivity of the $\text{Mo}_2\text{O}_2\text{S}_4(\text{DMF})_3$ complex with cyanide and catalytic conversion of cyanide to thiocyanate. **S.G. Suman**, J. Gretarsdottir, R. Bjornsson

8:50 . Electro- and photolytic hydrogen production catalyzed by molecular Co complexes with pentadentate ligands in aqueous solution. **X. Zhao**, P. Wang, Y. Sun, L. Duan, M. Long, D. Reese, A. Bah, C. James, G. Liang, C.E. Webster

9:10 . Alcoxysilanes production from silica and dimethylcarbonate promoted by alkali bases: A

DFT investigation of the reaction mechanism. **V. Butera**, Y. Choe, N. Fukaya, J. Choi, K. Sato

9:30 . Dehydrogenation of ammonia borane through the third equivalent. **X. Zhang**, **L. Kam**, T.J. Williams

9:50 . Synthetic approaches for cyclic biodegradable polyesters using ligated tin(II) complexes.

K. Phomphrai, P. Piromjitpong, P. Wongmahasirikun

10:10 Intermission.

10:20 . Synthesis and characterization of cyclic polyester: Effect of alkoxy side chains on Schiff's base ligand of tin(II) complexes. **P. Wongmahasirikun**, K. Phomphrai

10:40 . Rh and Pt nanoparticles stabilized by phosphine functionalized silica for selective hydrogenation reactions. **C. Claver**, J. Llop, C. Godard, M. Taoufik

11:00 Efficient and selective oxidation of sulfur mustard using singlet oxygen generated by a pyrene-based metal-organic framework. **Y. Liu**, C.T. Buru, A. Howarth, J. Mahle, J. Buchanan, J.B. DeCoste, J.T. Hupp, O.K. Farha

11:20 . Electrocatalytic water oxidation by a dicopper dihydroxide precatalyst reveals dinuclear intermediates. **M.T. Kieber-Emmons**, S.J. Koepke, P.E. VanNatta, A. Shrestha

11:40 . Highly controllable syngas (H_2 + CO) production through immobilized dual molecular Re(I)/Co(III) catalyst on a ternary TiO_2 hybrid system. **J. Lee**, D. Won, W. Jung, **H. Son**, C. Pac, S.O. Kang

Section F

Venue

Placeholder

Lanthanide & Actinide Chemistry

Cosponsored by WCC

A. De Bettencourt Dias, *Organizer*

J. F. Corbey, S. Demir, L. S. Natrajan, *Presiding* **8:30** . Solution synthesis and CO_2 reactivity of a rare Sc^{2+} complex, $[\text{Sc}(\text{NR}_2)_3]^{1-}$ (R = SiMe₃). **D. Woen**, G. Chen, J.W. Ziller, T.J. Boyle, F.U. Furcher, W.J. Evans

8:50 . Synthesis, structure, and reactivity of complexes containing +2 ions of late lanthanide metals in tris(silylamide) coordination environments, $\{\text{Ln}[\text{N}(\text{SiMe}_3)_2]_3\}^{1-}$. **A. Ryan**, J.W. Ziller, W.J. Evans

9:10 . Metalation of C-H bonds by $\text{Cp}^*_2\text{Y}(\mu\text{-Me})_2\text{MMe}_2$ (M = Al, Ga). **M. Bonath**, C. MaichleMössmer, R. Anwander

9:30 . Radical-Bridged Lanthanide Single-Molecule Magnets with High Blocking Temperatures. **S. Demir**, J.R. Long

9:50 Intermission.

10:00 . Synthesis and reactivity of organometallic divalent lanthanide compounds using a tris(aryloxide)mesitylene ligand. **C. Palumbo**, D.P. Halter, M.E. Fieser, H.S. La Pierre, J.W. Ziller, M. Gembicky, K. Meyer, W.J. Evans

10:20 . Binding preferences of uranyl with cyclic imide dioximes: A theoretical investigation.

D.A. Penchoff, C. Peterson, G.K. Schweitzer, D.M. Jenkins, R.J. Harrison

10:40 . Structural exploration of trivalent f element-containing species of interest for liquidliquid extraction processes. **J.F. Corbey**, B.K. McNamara, B.M. Rapko, J.M. Schwantes **11:00** Intermission.

11:10 . Optical spectroscopic foray into the redox chemistry of the early actinides. **M. Andrews**,

S. Woodall, A. Swinburne, J. Lloyd, A. Ward, S. Botchway, **L.S. Natrajan**

11:30 . Synthesis and magnetic characterization of trinuclear, radical-bridged lanthanide singlemolecule magnets. **C.A. Gould**

11:50 . Hydroypyridinonate ligands: From iron(III) to berkelium(IV) chemistry. **G. Deblonde**, D. An, P.B. Rupert, R.K. Strong, R.J. Abergel

Section G

Venue

Placeholder

Organometallic Chemistry: Catalysis

N. S. Radu, *Organizer*

H. Guan, S. M. Kilyanek, *Presiding*

8:30 . Palladium POCOP-pincer complexes: Catalysis in reduction of CO_2 with boranes. **A. Adhikary**, J.A. Krause, **H. Guan**

8:50 . Using stopped-flow kinetics as a mechanistic probe for the insertion of carbon dioxide into metal-hydride bonds. **J. Heimann**, N. Hazari

9:10 . Role of LiCl in generating soluble organozinc reagents. **C. Feng**, D. Cunningham, **Q. Easter**, S. Blum

9:30 . Filling the gap: Exploration of organoactinide catalysts with amine boranes reveal highly active catalysts and unique structural motifs. **K. Erickson**, B. Scott, P. Dub, J.L. Kiplinger

9:50 . Catalysis, carbon-hydrogen, and carbon-carbon bond activation with PNP Pincersupported group 3 and lanthanide alkyl complexes. **D.S. Levine**, T. Tilley, R.A. Andersen

10:10 . Unexpected proton transfer mechanism in the racemization of lactic acid catalyzed by lactate racemase: A DFT study. **B. Qiu**, **X. Yang**

10:30 . Mechanism based oligomerization catalysis for upgrading α -olefins to produce specialty fuels and chemicals. **T.N. Gunasekara**, M.M. Abu-Omar

10:50 . Mechanistic studies of the deoxydehydration of polyols by group VI transition metal catalysts. **S.M. Kilyanek**, R. Tran, K.A. DeNike

11:10 Isolation of key intermediates in Mo-catalyzed hydrosilylation. **K. Mandla**, J.S. Figueroa

11:30 . Proton and electron transfer by redox-active aluminum complexes for small molecule reduction. **E.J. Thompson**, T. Sherbow, L.A. Berben

11:50 . Norbornenyl-Acyl-Rhodium(III) complex as a likely intermediate in the catalytic hydroacylation of norbornadiene. **M.A. Huertos**

Section H

Venue

Placeholder

Chemistry of Materials: Metal Organic Frameworks

C. G. Lugmair, *Organizer*

P. Deria, M. C. So, *Presiding*

8:30 . Novel magnetic composite materials: Metal-organic frameworks as hosts for molecular nanomagnets. **D. Aulakh**, J. Pyser, X. Zhang, A. Yakovenko, K.R. Dunbar, M. Wriedt

8:50 . Molecular mechanisms of spin crossover in the $\{\text{Fe}(\text{pz})[\text{Pt}(\text{CN})_4]\}$

MOF upon guest adsorption. **H. Pham**, F. Paesani

9:10 . Multifunctional MOFs materials platform for biomedical applications. **D.F. Sava Gallis**,

L.E. Rohwer, M.A. Rodriguez

9:30 . Control over electronic delocalization and conductivity in mixed-valence semiquinoid frameworks. **M.E. Ziebel**, L.E. Darago, J.R. Long

9:50 . Topology-Dependent photophysical properties of zirconium-based metal-organic frameworks. **P. Deria**

10:10 . Porous metal-organic magnets exhibiting high temperature magnetic ordering. **L.E. Darago**, D. Reed, M. Aubrey, E.D. Bloch, J. Zadrozny, J.S. Miller, J.R. Long

10:30 Intermission.

10:45 . Interrogation of charge transport by gas sorption in metal-organic frameworks. **M. Aubrey**, M. Kapelewski, J. Melville, J.R. Long

11:05 . Isolation of metalloporphyrin dioxygen adducts in metal-organic frameworks. **A. Gallagher**, D. Harris, J. Anderson, M. Kely **11:25** Ultra-sensitive detection of mycotoxins by a luminescent metal-organic framework. **Z. Hu**, W.P. Lustig, J. Zhang, C. Zheng, H. Wang, S.J. Teat, Q. Gong, N. Rudd, J. Li

11:45 . Uptake mechanism, diffusion, and binding energetics of chemical warfare agent simulants within MOFs. **C.H. Sharp**, J. Abelard, A. Plonka, Q. Wang, A. Frenkel, W. Guo, C.L. Hill, D. Troya, J.R. Morris

12:05 . Preliminary electrochemical studies on effects of linker length and metal nodes on redox hopping in layer-by-layer assembled metalloporphyrin metal-organic framework-like thin films. **M.C. So**, K. Hara, J.T. Hupp, O.K. Farha

Section I

Venue

Placeholder

Chemistry of Materials: Nanomaterials

C. G. Lugmair, *Organizer*

S. Fischer, J. A. Mason, *Presiding*

8:00 . Design and synthesis of $\text{WO}(\text{OR})_3\text{L}$ complexes as precursors for chemical vapor deposition of WO_3 thin films. **X. Su**, D.C. Bock, T.J. Anderson, L. McElwee-White

8:20 . Quantitative control of metal doping in TiO₂ nanocrystals. **S. Mia**, S. Varapragasam, C. Balasanthiran, J.D. Hoefelmeyer

8:40 . Exploring metal oxide nanostructure synthesis mechanisms using *In situ* TEM. **L. Yu**, R. Han, H. Djieutedjeu, A. Patel, B.S. Guiton

9:00 . Insights into solution-processed metal oxide thin film formation mechanisms through investigations of non-thermal energy sources for annealing. **E. Cochran**, D. PARK, M. Kast, P. Plassmeyer, C. Page, D.W. Johnson, D.A. Keszler, S.W. Boettcher

9:20 . Structure of sub-nm oxides synthesized by atomic layer deposition: From isolated cations to bulk-like structure. **A. Yanguas-Gil**, T. Wu, J. Elam

9:40 Intermission.

9:55 . Precise control over the morphology and dopant distribution in colloidal metal oxide nanocrystals. **A. Singh**, D.J. Milliron

10:15 . Nanoparticle treated filters for sequestration of radioactive analytes. **S. Hunyadi Murph** **10:35** DNA-mediated assembly of stimuli-responsive colloidal crystals. **J.A. Mason**, C. Laramy, C. Lai, M. Obrien, Q. Lin, V.P. Dravid, G.C. Schatz, C.A. Mirkin

10:55 . Exploring the morphology transition from Li/Na {U₂₄Pp₁₂} to Na/K {U₂₄Pp₁₂} uranyl peroxide nanocluster. **Y. Gao**, M. Dembowski, J. Szymanowski, W. Yin, S. Chuang, P.C. Burns, T. Liu

11:15 . Shape control of multi-layer lanthanide-doped NaYF₄ nanocrystals by exploiting the shell growth dynamics. **S. Fischer**, A. Alivisatos

11:35 . Control and quantification of local polarity in nano-confined systems. **D. SingappuliArachchige**, J. Manzano, L.M. Sherman, I.I. Slowing

11:55 . Morphology, electropinnability, and crystalline phase study of SiO₂/TiO₂ composite ceramic nanofibers using sol-gel chemistry. **F. Huang**, B. Motealleh, C.J. Cornelius

Section J

Venue

Placeholder

Chemistry of Materials: Materials for Energy & Catalytic Applications

C. G. Lugmair, *Organizer*

E. G. Gillan, M. B. Ross, *Presiding*

8:30 . Translation of ligand-centered hydrogen evolution reaction activity and mechanism from homogeneous to solid surfaces. **W. Zhang**, R.M. Buchanan, C.A. Grapperhaus

8:50 . Monitoring surface species during carbon dioxide reduction using in situ Raman spectroscopy. **M.B.**

Ross, Y. Li, C. Dinh, E. Sargent, P. Yang

9:10 . Method for the solution deposition of efficient chalcogenide hydrogen evolution reaction electrocatalysts. **C. McCarthy**, R.L. Brutchey

9:30 . Synthesis and catalytic reactions with 3d and 4d phosphorus-rich metal phosphides. **E.G. Gillan**

9:50 . Comparison and structural modulation of cobalt amino porphyrin complexes for electrochemical reduction of CO₂. **M. Abdinejad**, H. Kraatz, X. Zhang

10:10 Intermission.

10:25 Comparative electrocatalytic activities of bimetallic oxides and carbides of iron, nickel and cobalt with tungsten and molybdenum as the second transition metal. **Y.N. Regmi**, B.M. Leonard

10:45 . Molecular Ni-complex containing tetrahedral nickel selenide core as highly efficient electrocatalyst for oxygen evolution reaction in alkaline medium. **M. Nath**, J. Masud, P. Kyritsis

11:05 . Chemistry of chromium carbide mono and bimetallic systems: Synthesis and electrocatalytic activity. **B.M. Leonard**, C. Wan, S. Schmuecker

11:25 . Novel catalytic materials for energy and environment investigating transition metal chalcogenides for efficient oxygen evolution electrocatalysis: The effect of covalency and lattice directionality. **M. Nath**

Section K

Venue

Placeholder

Coordination Chemistry: Characterization & Applications

S. A. Koch, *Organizer*

K. V. Waynant, *Presiding*

8:30 . Water-soluble thiophene-based fluorescent mercury-sensors. **A.K. Shigemoto**, C. Virca,

A. Thompson, J. Dayton, T. McCormick

8:50 . Coordination chemistry approaches for rational vanadium(IV) qubit design. **C. Yu**, M. Graham, J. Zdrozny, D.E. Freedman

9:10 . ¹H Relaxometric approach to determining the thermodynamic and kinetic stabilities of Mn(II) complexes. **D.W. Laorenza**, T.D. Westmoreland

9:30 none . [MoO(S₂)₂L]¹⁻ (L = picolinate or pyrimidine-2-carboxylate) Complexes as MoS_x inspired electrocatalysts for hydrogen production in aqueous solution. **B. Garrett**, C.M. Hadad, Y. Wu

9:50 Intermission.

10:00 . Synthesis, properties, and reactivity of d³ terminal-oxo molybdenum and tungsten complexes. **H.B. Vibbert**, M.D. Hopkins

10:20 . Anion-Incarcerating nanojars: Solution and solid-state characterization and selective extraction of anions from water. **G. Mezei**, B. Ahmed

10:40 Pentadentate and hexadentate pyridinophane ligands support reversible Cu(I)/Cu(II) redox couples. **A. Wessel**, L.M. Mirica

11:00 . Mono vs dual metal catalysis. **A. Poater**

11:20 . Rational catalyst design of first-row d⁸ complexes for the electrocatalytic reduction of CO₂. **A. Ostericher**, M. Reineke, C.P. Kubiak

11:40 . Tripodal pyrazole ligands and analogs for selective ammonium and actinide extraction and sensing. **T.M. Jonah**, L. Mathivathanan, S. Kandel, R.G. Raptis, K. Kavallieratos

12:00 . Coordination studies of arylazothioformamide ligands with transition metals in varying oxidation states for removal of trace metal impurities. **K.V. Waynant**, N.A. Johnson, S.R. Wolfe, J.G. Moberly, M.F. Roll

Section L

Venue

Placeholder

Organometallic Chemistry: Applications to Materials & Polymer Science

N. S. Radu, *Organizer*

C. E. Knapp, *Presiding*

8:30 . Preparation of multiblock copolymers via step-wise addition polymerization of L-lactide and trimethylene carbonate. **M. Abubekerov**, J. Wei, P. Diaconescu

8:50 . Copper ligand and anion effects on the kinetics of photo-induced copper(I) catalyzed azide-alkyne cycloaddition polymerizations. **B. El-Zaatar**, S. Cole, C.J. Kloxin

9:10 . Application of amino and imino pyridine iron(II) catalysts in atom transfer radical polymerization. **S.E. Jenny**, L.M. Thierier, M.R. Donley, L.M. Round, N.A. Piro, W.S. Kassel, D.L. Zubris

9:30 . Optimization of iron-loaded nanoparticles for T₁-weighted MRI contrast enhancement.

T.B. Ditre, Y. Li, Z. Wang, Y. Huang, Y. Xie, M. Botta, J.D. Rinehart, N.C. Gianneschi

9:50 . Porous flexible Cu₂(pzdc)₂(L) [pzdc = 2,3-pyrazinedicarboxylate; L = 1,3-bis(imidazol-1yl)benzene or 1,3-bis(4-pyridyl)propane] pillared-layer structures. **R.R. Arrieta-Perez**, J.N. Primera-Pedrozo, M.E. Marciano-

Gonzalez, J. Exley, J.A. Hogan, D.L. Jan, A.J. Hernandez

10:10 . Nitrogen-doped Polycyclic Aromatic Hydrocarbons (PAHs) *via* titanocene-mediated dinitrile coupling. **G.R. Kiel**, T. Tilley **10:30** Intermission.

10:35 . Block copolymers synthesized by redox-switchable catalysis. **S. Quan**, P. Diaconescu

10:55 . Co-supported tandem catalysts for production of linear low density polyethylene. **D. Aluthge**, A. Sattler, J.E. Bercaw, J.A. Labinger

11:15 . Designer copper precursors and their use in functional materials. **C.E. Knapp**, S.P. Douglas, E.A. Metcalf

11:35 . Cationic iridium(III) complexes bearing 2-aryl substituted oxazolo[4,5f][1,10]phenanthroline (N^N) ligands: Synthesis, crystal structure, photophysics and application for reverse saturable absorption. **X. Zhu**, W. Sun

11:55 . Reversible electropolymerization of nickel azobispyridine complexes based on redox mediated ligand exchange. **N. Clayman**, A. Rudenko, R.M. Waymouth

THURSDAY AFTERNOON

Section A

Venue

Placeholder

Coordination Chemistry: Synthesis & Characterization

S. A. Koch, *Organizer*

L. Cronin, J. M. Sears, *Presiding*

1:30 . Solving topological puzzles in tetramethylcyclam-supported oxoiron(IV) chemistry. **J. Prakash**, G. Rohde, L. Que

1:50 . Synthesis, electronic structure and reactivity of square-planar open shell iridium imido complexes. **M. Kinauer**, S. Schneider

2:10 . Assembling complex inorganic clusters using a programmable networked one-pot reaction array. **L. Cronin**

2:30 . Synthesis and reactivity of six-membered N-heterocyclic thiones and selones. **J.J. Flanagan**, D. Rabinovich

2:50 . Exploration of M[SNS]₂ (M = Mo, W) as redox-active metalloligands in heteromultimetallic systems. **M. Wojnar**, A.F. Heyduk

3:10 Intermission.

3:20 . Ligand-based redox chemistry in transition metal complexes of linear oligopyrroles. **R. Gautam**, E. Tomat

3:40 . Scandium salt dehydration for recycling efforts. **J.M. Sears**, T.J. Boyle, F.A. Fasulo

4:00 . Single-molecule magnetism in a series of two-coordinate ML₂ transition

metal complexes. **P. Bunting**, J.R. Long

4:20 . Electronic conductivity and magnetic ordering in mixed-valence $M(1,2,3\text{-triazolate})_2$ ($M = \text{Cr}^{\text{III/IV}}$, $\text{Fe}^{\text{II/III}}$) metal-organic frameworks. **J.G. Park**

4:40 . Deconvoluting the relative oxidation states in hexanuclear cobalt clusters. **R. Hernandez**

Sanchez, A. Champsaur, D. Paley, B. Choi, M.L. Steigerwald, C.P. Nuckolls

Section B

Venue

Placeholder

Inorganic Catalysts

S. A. Koch, *Organizer*

C. J. Stromberg, *Presiding*

1:30 . Hierarchical structured TiO_2 nanofibrous membranes with enhanced flexibility and photocatalytic activity. **M. Zhang**, J. Song, B. Ding

1:50 . Computational investigations of ruthenium with promoters for Fischer-Tropsch processes. **E.N. Brothers**, S. Moncho, B.G. Janesko

2:10 . Steric, electronic, and geometric effects on the ring opening transesterification polymerization mechanism for sustainable poly(lactones) with aluminum and zinc alkoxide catalysts. **D.E. Stasiw**, A.M. Luke, T. Rosen, M. Mandal, C.J. Cramer, M. Kol, W.B. Tolman

2:30 . First principles study of sulfenamido-olefin ligands in the rhodium-catalyzed addition of arylboronic acids to ketones. **P. Miro**, R. Recio, I. Fernandez

2:50 . Electrochemical Reduction of CO_2 Catalyzed by $\text{Re}(\text{pyridine-oxazoline})(\text{CO})_3\text{Cl}$ Complexes. **J. ngang**

3:10 Intermission.

3:20 . One-pot synthesis of Pt nanoparticles supported by Graphene Nanoribbons with enhanced catalytic performance towards 4-nitrophenol reduction. **D.A. Martinez**, S. Wang, W. Chiang

3:40 Important role of the electrode surface in the electrochemical reduction of CO_2 by Nicyclam. **A. Zhanaidarova**

4:00 . Copper tungstate microcrystals as photocatalyst for water oxidation under visible light. **Z. Wu**, F.E. Osterloh

4:20 . Ultrafast dynamics of cyano functionalized $[\text{FeFe}]$ -hydrogenase model compounds. **C.J. Stromberg**, E.J. Heilweil

4:40 . Selective H_2 or formate production from CO_2 and water:

Mechanistic insights achieved from ligand design. **N.D. Loewen**, L.A. Berben

Section C

Venue

Placeholder

Lanthanide & Actinide Chemistry

Cosponsored by WCC

A. De Bettencourt Dias, *Organizer*

E. Borbas, J. H. Farnaby, A. F. Martins, *Presiding*

1:30 . Highly axial magnetic anisotropy in a N_3O_5 dysprosium(III) coordination environment generated by a merocyanine ligand. P. Selvanathan, B. Le Guennic, S. Rigaut, K. Bernot, L. Norel

1:50 . Series of Dy^{3+} single-molecule magnets with terminal alkoxide ligands that promote large barriers to magnetic relaxation. **L.E. Darago**, J.R. Long

2:10 . F-element complexes with phosphinimide ligands: Probing metal-ligand covalency using ^{31}P NMR Spectroscopy. **S. Younger-Mertz**

2:30 . Excitation- and emission-based multiplexing with near infrared-emitting luminescent lanthanide complexes using red-light excitation. R. Xiong, **E. Borbas**

2:50 Intermission.

3:00 . Investigating the subtle variations in uranyl and neptunyl oxo reactivity through the characterization of crown ether complexes. **M.C. Basile**, E.R. Cole, T. Forbes

3:20 . Using bandgap tuneable capped nanoparticles to sensitize emissive Ln^{III} ions. **R.A. Tigaa**,

G.J. Lucas, S. Silva-Hernandez, J.H. Monteiro, A. De Bettencourt Dias

3:40 . Imaging L-lactate by CEST using paramagnetic shift reagents. **A.F. Martins**, L. Zhang, **A. Sherry**

4:00 Intermission.

4:10 . Synthesis of multi-metallic lanthanide and actinide complexes from organometallic building-blocks. **J.H. Farnaby**

4:30 . Spectroscopic and computational characterization of $\text{Eu}(\text{III})$ -oxalate precipitation processes. **W.C. Isley**, S. Kathmann, Z. Wang, G.B. Hall, S. Chatterjee, E.J. Bylaska, T. Meadows, G.J. Lumetta

4:50 . Synthesis and redox behavior of uranium amidinate complexes. **M. Straub**, S. Hohloch, S.G. Minasian, J. Arnold

Section D

Venue

Placeholder

Main Group Chemistry

T. W. Hudnall, *Organizer*

J. D. Hoefelmeyer, T. Hudnall, *Presiding*

1:30 . Lewis acidic antimony: Application as a non-innocent ligand for the activation of platinum catalyst. **D. You**, H. Yang, F. Gabbai

1:50 . Fluorescent frustrated Lewis pairs for the coordination and functionalization of small molecules. **Z.M. Heiden**, I.A. Kieffer, R.J. Allen

2:10 . Amphiphilic molecules with (quinolin-8-yl) groups on electrophiles. J. Son, S.R. Tamang,

J.I. Fostvedt, **J.D. Hoefelmeyer**

2:30 . Reactivity of Verkade's superbases with various strong Lewis acids. **S. Mummadi**, D. Unruh, C. Krempner

2:50 . Synthesis and application of novel polyhalides. **B. Schmidt**, K. Sonnenberg, F. Redeker, R. Brückner, S. Riedel

3:10 . Solvent-free mechanochemical s-block chemistry: When synthesis and reactivity don't follow the rules. N.R. Rightmire, N.C. Boyde, **T.P. Hanusa**

3:30 Intermission.

3:40 . Direct aromaticity link between Hückel's rule and *closo* boron hydride clusters. **J. Poater**, M. Solà, F. Teixidor, C. Viñas

4:00 Ultrashort beryllium-beryllium distances in molecular clusters. **X. Wang**

4:20 . Boron-based donor-spiro-acceptor compounds as TADF emitters. **A. Lorbach**

4:40 . Synthesis and characterization of polyborofluorenes, a novel boron doped variant of polyparaphenylene. **I.A. Brettell-Adams**, P. Rupar

5:00 . Novel antimony-containing heterocycles synthesized via a Zr-transfer strategy. **A.M. Christianson**, F.P. Gabbai, E. Rivard

5:20 . Cationic N-phosphoramidine ionic liquids. **J.R. Klaehn**, J.S. McNally, N. Arulsamy,

H.W. Rollins, E.J. Dufek

5:40 . Solid, stable, soluble, and stoichiometric oxidizing agents: Hydrogen peroxide and di(hydroperoxy)alkane adducts of phosphine oxides. **J. Blumel**

Section E

Venue

Placeholder

Organometallic Chemistry: Catalysis

N. S. Radu, *Organizer*

J. M. Camara, *Presiding*

1:30 . Cationic palladium(II) complexes for the catalytic Wacker-type oxidation of styrenes to ketones using O_2 as the terminal oxidant. H. Chai, Q. Cao, L.M. Dornan, **M.J. Muldoon**

1:50 . Imparting nobility to first-row metal-hydrides: Unusual anionic Ni-H stabilized by Lewis acidic metal supports and their role in catalytic carbon dioxide hydrogenation. **R. Cammarota**, C. Lu

2:10 . In Situ infrared spectroscopy study of iron-catalyzed transfer hydrometallation. **J.A. Rogers**, B.V. Popp

2:30 . Metallocenes adsorbed on silica and activated carbon: Solid-State NMR and catalysis. **J. Blumel**, K.J. Cluff

2:50 . Synthesis of aziridines at low alkene loadings catalyzed by a chromium(III) tetracarbene complex. **C. Keller**, A. Cramer, G. Elpitiya, J. Kern, S. Roy, D.M. Jenkins

3:10 . Bio-inspired design and computational prediction of iron, manganese and cobalt complexes with pendant amines for the hydrogenation of CO_2 to methanol. **X. Chen**, X. Yang

3:30 Mechanistic study of cyclotrimerization of alkynes via a two-coordinate iron complex. **R. Witzke**, T. Tilley

3:50 . Mechanism of Wacker-type oxidation of terminal olefins with cationic Pd(II) complexes using hydrogen peroxide. **L.M. Dornan**, K.L. Walker, R.M. Waymouth, M.J. Muldoon

Section F

Venue

Placeholder

Chemistry of Materials: Metal Organic Frameworks

C. G. Lugmair, *Organizer*

C. McGuirk, *Presiding*

1:30 . Polymer/Metal-organic-framework composite nanoparticle for gas separation: Rational design and theoretical analysis of core-shell structure. **K. Xie**, Q. Fu, P. Webley, G.G. Qiao

1:50 . Methane adsorption in a flexible iron metal-organic framework with intrinsic heat management. **J. Oktawiec**, J.A. Mason, M.K. Taylor, M.R. Hudson, J. Rodriguez, J. Bachman, M.I. Gonzalez, A. Cervellino, A. Guagliardi, C.M. Brown, P. Llewellyn, N. Masciocchi, J.R. Long

2:10 . Cooperative and reversible chemisorptive capture of carbon

disulfide in diamine-appended metal-organic frameworks. **C. McGuirk**, R.L. Siegelman, P.J. Milner, J.R. Long

2:30 . Computing adsorption properties of structurally deformed metal organic frameworks using a feature space map. **W. Jeong**, D. Lim, S. Kim, A. Harale, M. Yoon, M.P. Suh, J. Kim

2:50 . Enhancing the uptake of oxygen in metal-organic frameworks. **J.B. DeCoste**, T.M. Tovar, I.O. Iordanov, A.M. Ploskonka, G.W. Peterson

3:10 . Thermodynamically directed method to tether alkylamine into metal-organic frameworks for CO₂ capture. **H. Li**, H. Zhou

3:30 Intermission.

3:45 . Record selectivity for olefin/paraffin separations in a metal-organic framework. **M. Kapelewski**, J. Bachman, J.R. Long

4:05 . CO₂ capture enhancement in InOF-1 *via* the bottleneck effect of confined ethanol. **I. Ibarra**

4:25 . Water stable Metal-Organic Frameworks (MOFs) for CO₂ capture. **D. Zhao**

4:45 . Cooperative, adsorbate-induced spin transitions for efficient carbon monoxide separations in an Fe(II) metal-organic framework. **D. Reed**, B. Keitz, J.R. Long

5:05 . Trapping gases in metal organic frameworks with a selective surface molecular barrier layer. **K. Tan**, S. Zuluaga, E. Fuentes, E. Mattson, H. Wang, J. Li, T. Thonhauser, Y.J. Chabal

5:25 . Increased CO₂ adsorption in heterobimetallic MOFs obtained by post-synthetic transmetalations of HKUST-1. **J.M. Veleta**, R. Arrieta, M. Baeza, E. Barajas, K. Castañeda, C. Castañon, Z. Garcia, D. Villagran

Section G

Venue

Placeholder

Chemistry of Materials: Nanomaterials

C. G. Lugmair, *Organizer*

S. M. Noimark, L. J. Treadwell, *Presiding*

1:30 . Dimerization of organic dyes on luminescent gold nanoparticles for ratiometric pH sensing. **S. Sun**, x. ning, J. Zheng

1:50 . Molecular layer deposition of ultrathin manganese oxide hybrid materials for catalysis applications. **D.S. Bergsman**, J.G. Baker, N. Yang, C. MacIsaac, A. Strickler, M. Lillethorup, S.F. Bent

2:10 . Application of chiral tetrahedral Au nanoparticles in enantiomeric separations of chiral

drugs. **N. Shukla**, D. Yang, Y. Zhao, A.J. Gellman

2:30 . Synthesis and characterization of hollow Mn₃O₄ nanoparticles as anode materials for lithium ion batteries. **S. Varapragasam**, C. Balasanthiran, A. Gurung, Q. Qiao, R.M. Rioux, J.D. Hoefelmeyer

2:50 . Multi-walled carbon nanotube-polymer composite coatings for optical ultrasound generation. **S.M. Noimark**, R. Colchester, S. ourselin, I. Papakonstantinou, I.P. Parkin, A. Desjardins

3:10 . Photonic medicine: Large area self-assembly of curcumin derivatives into microsphere resonators emitting visible/near-infrared light with cavity size dependent decay lifetime. **D. Venkatakrishnarao**

3:30 Intermission.

3:45 . Synthesis of N, P co-doped amorphous carbon dots and their toxicological impact on *Shewanella oneidensis* MR-1 bacteria. **B. Zhi**, M.J. Gallagher, B.P. Frank, T. Curry, T.A. Qiu,

A.C. Mensch, Z. Rosenzweig, H. Fairbrother, R.J. Hamers, C.L. Haynes

4:05 . Synthesis of nanoinks using novel precursors for advanced Direct Write applications. **L.J.**

Treadwell, T.J. Boyle, N.S. Bell, A. Cook, D. Woodard, M.V. Parkes

4:25 . Biocompatible and water-soluble gold-carbon nanoparticles. B. Atallah, I. Shehadi, M. Naggari, **A. Mohamed**

4:45 . Surface functionalized metal-oxo polymer nanobeads as potential T₁ MRI contrast agents with dual reporting capability and specific targeting. **V. Dahanayake**, W.J. Hickling, O. Rodriguez, C. Albanese, S.L. Stoll

5:05 . Investigation of nanosized metal oxides for thermal water splitting at reduced temperatures. **G. Larsen**, K. Coopersmith Lawrence, S. Hunyadi Murph

5:25 . Cell-based targeted delivery of mesoporous silica nanoparticles loaded with a T1-contrast agent to 4T1 tumors. **H. Wang**, T.B. Shrestha, J. Covarrubias, A.P. Malalasekera, S.O. Wendel, J. Yu, P. Thapa, M. Pyle, D.L. Troyer, S.H. Bossmann

Section H

Venue

Placeholder

Chemistry of Materials: Materials for Energy & Catalytic Applications

C. G. Lugmair, *Organizer*

V. Doan-Nguyen, J. L. White, *Presiding*

1:30 . Utilization of magnesium silicide as a reactive precursor for the facile synthesis of Si@Ge and Si@C composite electrodes for lithium-ion batteries. j. ahn, m. kang, D. Lee, h. kim, Y.

Sung, w. yoo

1:50 . Investigation of the reversible lithium insertion into anti-NASICON Fe₂(WO₄)₃. **G. Barim**, B.C. Melot, R.L. Brutchey

2:10 . Transition metal polysulfide chalcogenides as electrode materials for Li-ion batteries. **V.**

Doan-Nguyen, K. Subrahmanyam, M. Butala, J.A. Gerbec, S. Islam, K. Kanipe, C. Wilson, M.

Balasubramanian, K. Wiaderek, O. Borkiewicz, K.W. Chapman, P. Chupas, M. Moskovits, B.

Dunn, M.G. Kanatzidis, R. Seshadri

2:30 . Effect of nanostructuring on hydrogen storage properties of complex metal hydrides confined inside nanoporous carbons. **J.L.**

White, V. Stavila, B. Wood, T. Heo, L.E. Klebanoff,

E. Majzoub, M. Allendorf

2:50 . Manganese oxide nanomaterials for electrocatalysis and energy storage. **T.N. Lambert**, J.A. Vigil, J. Duay, M. Kelly

3:10 Intermission.

3:25 . Nb₂N₅/Nb₂O₅-rGO composites as pseudocapacitive anode materials for high power lithium ion batteries. **Y. Yan**, C. Lai, S. Robbenolt, B. Dunn, S.H. Tolbert

3:45 . Modelling La₂NiO₄ for solid oxide fuel cell cathode applications. **A.L. Gavin**, G.W.

Watson

4:05 . Mechanisms and motivations for superionic conductivity in polyborane solid electrolytes from *ab initio* molecular dynamics. **B. Wood**, J. Varley, K. Kweon, P. Shea, V. Stavila, T.J. Udovic

4:25 . Thermodynamics and kinetics at interfaces of metal hydrides for hydrogen storage. **S.**

Kang, T. Heo, P. Shea, K.G. Ray, T. Ogitsu, S. Bonev, B. Wood

Section I

Venue

Placeholder

Organometallic Chemistry: New Ligand Platforms

N. S. Radu, *Organizer*

D. R. Manke, M. P. Marshak, *Presiding*

1:30 . Structure-activity relationship of ruthenium metathesis catalysts in ethenolysis of cyclic olefins. **P. Engl**, C. Santiago, A. Fedorov, C. Coperet, M.S. Sigman, A. Togni

1:50 . Blue phosphorescent zwitterionic Ir(III) complexes featuring weakly coordinating ligands. **K. Kirlikovali**, J.C. Axtell, P.I.

Djurovich, D. Jung, V. Nguyen, B. Munekiyo, A.T. Royappa,

A.L. Rheingold, A.M. Spokoyny

2:10 . Caviplexes: Metal-Organic platforms for supramolecular recognition. **A. Pöthig**, P.J. Altmann

2:30 . Influence of the phenylazopyridine ligand on the reactivity and electronic structure of (cyclopentadienyl)cobalt complexes. **E. McLoughlin**, K.M. Waldie, R. Sarangi, R.M.

Waymouth Synthesis, structure and reactivity of homo- and heterobimetallic complexes. **A. Nicolay**,

T. Tilley

3:10 . Homoleptic organolanthanide compounds supported by a bis(dimethylsilyl)benzyl ligand.

K. Boteju, A. Ellern, A.D. Sadow

3:30 . *m*-Terphenyl substituted β-diketonate ligands support coordinatively unsaturated metals.

M.P. Marshak, E.S. Akturk, R.N. Seals

3:50 . Modular synthesis of tris(aryl)tren ligands and their reactivity. V. Mdluli, **D.R. Manke**

4:10 . Probing the π-acceptor/σ-donor ratio of 2-isocyanoozulen ligands as possible rivals of polyfluorinated organic isocyanides. **M.D. Hart**, J.J. Meyers, T. Nakakita, Z. Wood, N. Gerasimchuk, M.V. Barybin

4:30 . Studies of protonation preferences in bifunctional late-metal organometallics: Applications to heterolytic C-H activation. **E.B. Hulley**, W. Christman, T. Morrow, N. Arulsamy

4:50 . Influence of fluorescent dye containing ligand scaffolds on metal complex reactivity. **Z.M.**

Heiden, N.R. Treich

Section J

Venue

Placeholder

Organometallic Chemistry: Synthesis & Characterization-Late Transition Metals

N. S. Radu, *Organizer*

Z. Assefa, D. C. Lacy, *Presiding*

1:30 . Chemistry of gold(III) pincer complexes: Structure and reactivity Au-H and Au-CO complexes. **M. Bochmann**, J. Fernandez-Cestau, A. Pintus, L. Rocchigiani, P. Budzelaar

1:50 . Synthesis, x-ray crystallography, spectroscopic and cytotoxicity studies of Au(I) complexes of tris(4-methoxy-

3,5-dimethylphenyl)phosphine (MDMPP), bis (2-methoxyphenyl) phosphine (MPP) and further structural studies on higher coordinate Au(I) phosphine complexes.

Z. Assefa, K. Brown, G. Agebeworvi, M. Kanipes-Spinks, C. Rorie

2:10 . Homo- and heterobimetallic dicarbene complexes featuring unsymmetrical bis-NHC ligand. **M. Böhrer**, E.F. Hahn

2:30 . Synthesis and reactivity of Ir^{III} complexes bearing NHC/imidazolyl chelate ligands. **T. Tan**, E.F. Hahn

Reactivity and dynamics of unsaturated cobalt *m*-terphenyl isocyanide complexes. **C. Chan**, J.S. Figueroa

3:10 . Synthesis and reactivity of pincer-supported cobalt complexes.

L.M. Guard, D.E. Linn, D.M. Heineke

3:30 . Metal-metal bonds from halide-bridged group 11 metal cations. **J.P. Sadighi**, C.M. Sato, J. Bacsá

3:50 . Splitting water with an organomanganese tetramer. **D.C. Lacy**

4:10 . Active site installation on a low valent iron cluster. **M.J. Drance**, J.S. Figueroa

4:30 . Bonding in group 8 silylene complexes. **P. Smith**, T. Tilley

4:50 . Rhenium β-diketiminates: Chemistry at the oxo moiety and in low-valent terminal oxo complexes.

T.D. Lohrey, R.G. Bergman, J. Arnold

5:10 . Frustrated Lewis pairs as ligands for late-transition metal complexes: Probing interactions in the coordination sphere. **B.R. Nichols**, J.L. Petersen, B.V. Popp

Section K

Venue

Placeholder

Chemistry of Materials: Synthesis & Properties

C. G. Lugmair, *Organizer*

B. A. Kilos, L. Vilà Nadal, *Presiding*

1:30 . Composition manipulation of germanium nanocrystals via microwave-assisted colloidal synthesis.

K. Tabatabaei, S. Kauzlarich, B. Nolan, H. Lu, X. Zhang, R.L. Brutchey, K. van Benthem

1:50 . Study of Pt(II) precursors for focused electron beam induced deposition of Pt nanostructures. **H. Lu**, J.A. Spencer, Y. Wu, H. Fairbrother, L. McElwee-White

2:10 . Long route from hexagonal-AMn³⁺O₃ to AMn²⁺O_{2.5}. **M. Olivier**, T. Pussacq, M. Huvé, f. tessier, H. kabbour

2:30 . Introducing dimensionality to the archetypical Mn₁₂ single-molecule magnet: A family of

[Mn₁₂]_n chains. **C. Lampropoulos**, S.A. Corrales, J.M. Cain, K.A. Uhlig, T. Jenkins, M.

Garnero, D. Pistey, R. Thomas, E. Williams

2:50 Thermolytic molecular precursor methods to germanium-doped single-sites on silica. **J.P. Dombrowski**, T. Tilley, A.T. Bell

3:10 . Beyond thioureas: Highly monodisperse CdS nanocrystal syntheses via thiocarbonates, thiocarbamates, and thioureas. **L. Hamachi**, I. Jen-La Plante, G. Cleveland, J.S. Owen

3:30 . Synthesis and characterization of MCrX₂ nanoparticles: Phase and morphology control. **H.A. Dalafu**, S.L. Stoll

3:50 Intermission.

4:05 . Simple method to predict the electronic spin configuration of Fe(II) tris-diimine complexes. H. Phan, J. Hrudka, **M. Shatruk**

4:25 . Non-covalent interactions in superatomic crystals. **J.L. Shott**, M. Freeman, N. Saleh, D.S.

Jones, C. Bejger

4:45 . Water confinement properties of a metal-organic nanotube. **M. Payne**, A.S. Jayasinghe, D.

Unruh, T. Forbes

5:05 . Synthesis and characterization of magnesium oxychloride as a fire resistant construction material. **R.F. Gochez**, C.L. Kitchens

5:25 . Industrial outlook on the development of cost effective SiO₂ mesoporous cellular foams technology.

B.A. Kilos, A.M. Kelly-Rowley, S. Matteucci, C.L. Tway, K. Mabe, H. Clements

5:45 . Centimeter-sized epitaxial h-BN as a flexible & transferrable template for heteroepitaxial growth of semiconductor thin films. **H. Oh**, K. Chung, J. Jo, Y. Tchoe, H. Yoon, H. Lee, S. Kim, M. Kim, B. Sohn, G. Yi

Section L

Venue

Placeholder

Nanoscience B. G. Trewyn, *Organizer* **E. Jöhlín**, *Presiding*

1:30 . Monocrystalline nanopatterned films made by nanocube assembly and chemical welding. B. Sciacca, A. Berkhout, M. van Huis, B. Brenny, A. Polman, **E. Garnett**

1:50 . Graphene oxide membranes with strong stability in aqueous solutions and controllable lamellar spacing. **J.**

Hu, Y. Xi, Z. LIU, R. XIE, X. JU, W. WANG, L. CHU

2:10 Photovoltage, effective bandgap and photochemical charge transfer in nanoscale transition metal (Cu, Fe, Mn, Ni) doped SrTiO₃ photocatalysts. **X. MA**, F.E. Osterloh

2:30 . Semiconductor nanocrystals with compact fluorinated shells. **P. Xia**, M.L. Tang

2:50 . 3D Nanostructure imaging via multi-energy deconvolution SEM. **E. Jöhlín**, M. de Goede, B. Sciacca, F. Boughorbel, E. Garnett

3:10 . Opportunities and limitations for nanoscale photovoltaics to surpass the Shockley-Queisser limit. **S.A. Mann**, R. Grote, R.M. Osgood, A. Alu, E. Garnett

3:30 Intermission.

3:40 . Metal halide perovskite nanowire arrays for photodetection with significantly improved stability. **Z. Fan**, L. Gu, M. Tavakoli, A. Waleed

4:00 . Exploring of the scope of polyarylboranates. **M.W. Lee**, T. Wang

4:20 . Efficiency of magnetic induction heating for single crystal iron oxide nanoparticles. R.R. Shah, T.P. Davis, A.L. Paulson, C.S. Brazel, **D.E. Nikles**

4:40 . Elucidation of synthesis and characterization of non-precious nanoscale mixed metal oxides for green chemistry catalysis. **A.M. York**, C.A. Cadigan, R.M. Richards

5:00 . Carrier selective contacts for nanowire solar cells. **S. Oener**, A. Cavalli, J. Haverkort, E.

Bakkers, E. Garnett

5:20 . TERS: Nanoscale Raman characterization of 0-1- and 2D materials. **A. Krayev**, M. Chaigneau