Western New York Inorganic Symposium 2026

August 21st Schedule of Events

All events will be held in Goergen Hall at the University of Rochester River Campus

8:30 – 9:00 AM: Coffee/Snacks and Poster Set-Up (Munnerlyn Atrium)

9:00 – 11:10 AM: Student Talks Session #1 (Moderator: **Luis De Jesús Báez**; Goergen 101)

9:00 AM–9:05 AM	Opening Remarks
9:05 AM–9:30 AM	*A pair distribution function study of local distortions within low-to-high entropy lanthanum-based perovskite oxides*
	Jordan Scalia (De Jesus Baez)
9:30 AM–9:55 AM	*Counter-ion and solvent impacts on proton-coupled electron transfer in polyoxovanadate-alkoxides*
	Becca Walls (Matson)
9:55 AM–10:20 AM	*Incorporating phenolate pendants and bound water in Fe(III) MRI probes*
	Anwita Roy (Morrow)
10:20 AM–10:45 AM	*Ni_2-imido bispincer platforms: cooperative reactivity enabled through substrate addition across a Ni_2N unit*
	Kritika Gour (Besson)
10:45 AM–11:10 AM	*Indium oxidation states and reactivity*
	Millie Trusler (Lancaster)

11:15 AM – 12:00 PM: Poster Session #1 (odd # posters; Munnerlyn Atrium)

12:00 PM – 1:00 PM: Lunch (Munnerlyn Atrium)

1:00 PM – 1:45 PM: Poster Session #2 (even # posters; Munnerlyn Atrium)

1:50 PM – 3:55 PM: Student Talks Session #2 (Moderator: Jon Kephart; Goergen 101)

1:50 PM–2:15 PM	*Coordination chemistry of manganese(III) acetate and the acid-triggered access to reactive $\{Mn^{III}_x\}$ intermediates from manganese(III) acetate*
	Ankita Kumari (Lacy)
2:15 PM–2:40 PM	*Mechanistic investigations of iron-catalyzed reductive N-heterocycle formation*
	Jair Powell (Driver)
2:40 PM – 3:05 PM	*Synthesis and reactivity of iminopyridonate nickel complexes*
	Hailemariam Mitiku (Kennedy)
3:05 PM-3:30 PM	*Adapting metal-organic frameworks for high-throughput experimentation*
	Daniel Nakamura (Milner)
3:30 PM-3:55 PM	*Ironing out heterolytic C-H activation: organometallic structures and dynamics by 2D NMR*
	Heather Arnold (Wolczanski)

3:55-4:10 PM: Break/Snack and Poster take-down (Munnerlyn Atrium)

4:10 – 4:20 PM: Closing Remarks & Student Prizes (Munnerlyn Atrium)

ABSTRACTS FOR ORAL PRESENTATIONS

A Pair Distribution Function Study of Local Distortions Within Low-to-High Entropy Lanthanum-Based Perovskite Oxides

Presenter: Jordan Scalia (Luis De Jesús Báez)
Department of Chemistry, University at Buffalo, Buffalo NY

Abstract. High-entropy materials (HEMs) and oxides (HEOs) have recently gained interest within the materials community due to their increase in phase stability while either retaining or expanding on properties of interest. The proliferation of these properties are attributed to the synergistic interplay between the "four core effects" in HEMs: high entropy effect, cocktail effect, sluggish diffusion, and severe lattice distortion. Out of all these effects, severe lattice distortion provides a direct window into the stability of crystal phases within HEOs and, more importantly, how the other 'core effects' influence the evolution of phases. Unfortunately, due to HEOs having five or more principal elements, it is not trivial to deconvolute these severe lattice distortions with common structural characterization techniques such as powder X-ray diffraction (PXRD). This highlights the need to explore alternative pathways to understand how distortions impact the underlying properties of a given material. In trying to address this limitation, we combined X-ray absorption spectroscopy (XAS) and Pair Distribution Function (PDF) analysis to help dissect local distortions across unit cells. Thus, we identify the characteristics and origin of distortions with increased entropy in relation to oxidation state changes and atomic position of the atoms. As a system, we chose a perovskite family with the general formula $LaBO_3$, where the B-site atom comprises first-row transition metals starting with Ni. This allows us to follow changes from the optimized octahedral conformation in relation to increasing entropy as a measure of distortion within the material. We observed the evolution of B-site distortions to be regulated by a combination of J-T distortions, ionic radii, and overall changes within the unit cell in relation to configurational entropy and the chemical nature of the B-site element.

Counter-Ion and Solvent Impacts on Site-Dependent Tunneling in POV-alkoxides

Presenter: Madelyn (Becca) Walls (Ellen Matson)
Department of Chemistry, University of Rochester, Rochester NY

Abstract. Proton coupled electron transport (PCET) mechanisms dictate many transformations at metal oxide materials. To model these materials, we have employed polyoxovanadate-alkoxide Lindqvist clusters as a soluble model of extended material-substrate interactions. A previous report from our group reports a 10-fold rate enhancement of PCET to the bridging oxido site of a polyoxovanadate-alkoxide, as compared to PCET to the terminal vanadyl site, despite similar thermodynamic and kinetic barriers. As such, we investigated H-atom tunneling effects, a common factor in basic asynchronous PCET pathways, via analysis of the variable temperature kinetic isotope effects, revealing more extensive tunneling observed at the bridging oxido site. To further understand the rate enhancement observed at the bridging oxido, the relationship between solvation and counter-cation coordination is investigated; wherein significant rate enhancement is observed for the

alkali cation derivative, yet transitioning to a more basic solvent (i.e., MeCN to DMF) disrupts the H-bonding network, preventing H-atom tunneling. Herein, this work provides insights into methods for modulating tunneling effects in metal oxides via solvation and counter-ion identity.

Incorporating phenolate pendants and bound water in Fe(III) MRI probes
Presenter: Anwita Roy (Janet Morrow)
Department of Chemistry, University at Buffalo, Buffalo NY
Abstract. Designing molecular Fe-based T1 MRI probes in water requires simultaneous control of oxidation state, spin state, inner-sphere solvation, and aqueous solubility. Pyridyl pendants commonly stabilize Fe(II) states used in redox-responsive probes or as paraSHIFT agents, whereas phenolate donors shift Fe(III)/Fe(II) potentials negative and favor high-spin Fe(III), whose slower electronic relaxation is advantageous for T1 contrast. Building on our previous experience in aqueous iron coordination chemistry, we designed pentadentate TACN complexes with only two phenolate pendants, preserving an inner-sphere water ligand while a noncoordinating sulfonate in [Fe-CREST] improves hydrophilicity without increasing metal denticity. Variable-temperature 17O NMR analyzed by Swift–Connick methods, together with pH-dependent relaxivity, indicates that proton exchange involving the Fe(III)-bound water contributes to relaxation, distinguishing [Fe-CREST] from classical systems dominated by whole-water exchange and extending proton-exchange concepts established for Gd(III) macrocycles to a Fe(III) scaffold. [Fe-CREST] remains intact in physiologically relevant bicarbonate/phosphate/ascorbate media containing apo-transferrin. Preliminary in-vivo studies show that the complex produces measurable T1 contrast in mice and undergoes rapid renal clearance, demonstrating how pendant-controlled aqueous coordination chemistry can balance Fe(III) stability, inner-sphere water, proton relaxation, and in vivo compatibility.

Ni_2-Imido Bispincer Platforms: Cooperative Reactivity Enabled Through Substrate Addition Across a Ni_2N Unit
Presenter: Kritika Gour (Claire Besson)
Department of Chemistry, Binghamton University, Binghamton NY
Abstract. Transition metal imido complexes are renowned for their capacity to undertake challenging 1,2 additions owing to the high basicity of the imido moiety. Access to transition metal imidos is often limited to the addition of organic azides to metal precursors, hindering the design of molecular constructs incorporating imido units. Bimetallic bispincer complexes, 1 and 2, are presented, which are anchored by a central imido moiety supported by pyridyl imine donors, forming highly planarized Ni2N-aryl cores. Complex 2, which also features a Ni—Ni σ-bond, is able to engage in cooperative substrate cleavage of main group hydrides via a formal 1,2 addition to generate paramagnetic Ni2–amido–hydrido complexes 3-BPin and 3-SiPh2H. The 1,2 addition products feature a geometric distortion from the planar core noted in 2, resulting in the destabilization of the Ni—Ni bond to generate a formally S = 1 state. The complexes have been characterized through x-ray diffraction,

spectroscopic studies, and DFT calculations. Catalytic hydrofunctionalization with 2 and 3-BPin support of the 1,2 addition is an on-cycle process in catalysis.

Indium Oxidation States and Reactivity Across Heterobimetallic

Presenter: Millie Trusler (Kyle Lancaster)
Department of Chemistry and Chemical Biology, Cornell University, Ithaca NY

Abstract. Heterobimetallic complexes featuring a main group metal paired with a transition metal enable cooperative tuning of each metal site and have the potential to exhibit unique reactivity modes. In prior work we showed how changing inner-sphere coordination at Ni in a $[Sn\text{-}Ni]^{2+}$ bimetallic hydroboration catalyst modulates the catalytic rate across several orders of magnitude. We now extend our work to heterobimetallic systems consisting of a transition metal, Co or Ni, paired with the 5p metal In. Electronic structure calculations will be presented that showcase varied oxidation states these In centers, with complexes that range from indium (I) to indium (III), with some showing the stabilization of an electronically indium (II) center. Starting from stable In(I) – Ni(0) complexes, the activation of alkyl halides ranging from iodo to fluoro compounds has been demonstrated. Through the investigation of intermediary species and the kinetics of the two-step reaction, the mechanism by which this occurs can begin to be understood.

Coordination Chemistry of Manganese(III) Acetate and the Acid-Triggered Access to Reactive $\{Mn_{IIIX}\}$ intermediates from Manganese(III) Acetate.

Presenter: Anikita Kumari (David Lacy)
Department of Chemistry, University at Buffalo, Buffalo NY

Abstract. The trinuclear cluster of manganese (III) acetate (1) is widely employed in synthetic carbon functionalization reactions, yet its coordination chemistry and solution-state properties are not well studied. This is primarily due to the low solubility of 1, even when coordinated with pyridine and related neutral N-donor ligands. We overcome this challenge by synthesizing a family of well-defined and soluble Mn(III) acetate complexes with neutral pnictogen-oxide ylide (PnO) donors (pyridine-N-oxide, triphenylphosphine oxide, and trimethylamine-N-oxide). These complexes were synthesized from 1 or mononuclear Mn(III) halide precursors and exhibit diverse structural motifs including trinuclear closely resembling 1, linear chain and higher-nuclearity clusters. Higher solubility enabled investigation of the solution state properties especially of the trinuclear Mn(III) acetate clusters. Critically, we unequivocally demonstrated that acid promotes cleavage of trinuclear cluster into mononuclear MnIII species that can be trapped through coordination with PnO ligands. This was established through synthesis of the known complex $MnCl_3(OPPh_3)_2$ and a new PnO-stabilized "$Mn(OTf)_3$" complex. We were also able to capture substrate-bound intermediates derived from 1 under reaction conditions by inclusion of PnO ligands in cyclization reactions between α-methylstyrene (AMS) with acetylacetone (Hacac). These findings provide new insight into the

coordination and solution-state chemistry of Mn(III) acetate and the formation of mononuclear species under conditions relevant to carbon functionalization reactions.

Mechanistic investigations of iron-catalyzed reductive N-heterocycle formation
Presenter: Jair Powell (Driver)
Department of Chemistry, University of Rochester, Rochester NY
Abstract. This presentation examines four iron-catalyzed reductions of nitroarenes, aryl N,O-heterocycles, or nitroalkenes to afford various N-heterocycles, using silane as the terminal reductant. Experiments were performed that provided insight into the mechanisms of these reactions. The resulting data were used to determine their rate equations, activation parameters, and the presence of any kinetic isotope effects. This, in turn, helped elucidate details of the catalytic cycles and their turnover-limiting steps, demonstrating how changes in the structure of the different N-aryl starting materials, as well as how using non aryl nitroalkene starting materials affect the identity of the reaction's turnover-limiting step.

Synthesis and Reactivity of Iminopyridonate Nickel Complexes
Presenter: Hailemariam Mitiku (Rose Kennedy)
Department of Chemistry, University of Rochester, Rochester NY
Abstract. Pyridones have grown to be an important class of ligands both in the biological and precious metal-catalyzed (de)hydrogenative processes typically involving a metal–ligand cooperative mechanism. The tautomerism of pyridones, through which they adopt various coordination modes, is a key enabling factor. However, this versatility can render pyridone-based single-component (pre)catalyst development challenging because of complex speciation. To overcome these limitations, we have designed modular multidentate pyridone ligands with tunable steric and electronic properties for supporting first-row transition metals. Here, I will describe the synthesis and isolation of pyridone-supported nickel complexes across multiple oxidation states, with particular emphasis on dinuclear nickel complexes; the respective electrochemical, spectroscopic, and structural analysis will be discussed. Finally, multimetallic cooperative reactivity of dinuclear nickel complexes with alkyl(pseudo)halides will be discussed in the context of the Suzuki cross-coupling.

Adapting Metal-Organic Frameworks for High-Throughput Experimentation
Presenter: Daniel Nakamura (Philip Milner)
Department of Chemistry and Chemical Biology, Cornell University, Ithaca NY
Abstract. Gaseous reagents represent inexpensive, atom economic building blocks for organic synthesis, but are difficult to incorporate into high-throughput batch chemistry. Metal-Organic frameworks are a promising approach, but their insoluble natures pose a significant challenge for

HTE. Here, we introduce a non-destructive method of shaping MOFs for the rapid delivery of fluorinated gasses in a high throughput manner.

Ironing Out Heterolytic C-H Activation: Organometallic Structures and Dynamics by 2D NMR
Presenter: Heather Arnold (Peter Wolczanski)
Department of Chemistry and Chemical Biology, Cornell University, Ithaca NY
Abstract. Activation of C-H bonds with first-row transition metals remains a significant challenge due to weaker metal-carbon bond strengths and reduced orbital overlap compared to their second- and third-row counterparts. Precious metals are expensive, which has led to the ongoing desire to develop 1st row complexes with simpler, less expensive ligands that can be more readily implemented. Heterolytic C-H activation presents a promising way to achieve similar reactivity in base metal systems. The dynamic interconversion of four organometallic species and their reaction pathways were elucidated through a series of 2D NMR experiments, providing insight into the reactivity and transformation pathways of this system. Additionally, a similar system undergoes a secondary C-H activation at the ligand backbone, providing further insight into the reactivity of iron systems that promote heterolytic C-H activation.

Poster No.	Name, Institution	Title
1	Alec Hegg & Marina Zapesochny, Cornell U.	Synthetic approaches towards magic-sized transition metal oxides
2	Alexander Ruhren, Binghamton U.	Modular TM(II)Tp_2 complexes for post functionalization
3	Asmita Sikdar, U. Rochester	Mechanistic investigations of iron-catalyzed reductive N-heterocycle formation
4	Augustine Obeng, SUNY Buffalo	Atomic orbital energy matching vs overlap in actinide-ligand dative bonding
5	Baela Ferrigno, U. Rochester	Electrocatalytic proton reduction with modified molybdenum chalcogenide clusters
6	Benyu Zhou, Cornell, U.	Development of Sn-Rh Bimetallics as Hydrogenation Platforms
7	Devaleena Kalita, SUNY Buffalo	Chemical tuning of layered Chalcogenides: phase control in MoS_2 and mixed-chalcogen engineering in VS_xSe_y
8	Dilmi Witharana, U. Rochester	Ligand and leaving group interplay in nickel-catalyzed amide cross-coupling
9	Eric Jang & Ethan Brott, U. Rochester	Origins of diastereoselectivity in electrochemical oxidative cyclization–migration reactions of aryl amines
10	Hania Guirguis, U. Rochester	Alkali metal salts influence kinetics and thermodynamics of electron transfer and hydrogen atom uptake
11	Hannah Gorski, U. Rochester	Understanding mechanisms of long-lived charge transfer from CdSe QDs for improved photocatalytic HER
12	Hashini Sithari, U. Rochester	Synthesis and characterization of ternary thiospinel nanocrystals
13	Jessica Navaro Vega, U. Rochester	Ni-catalyzed, light-mediated decarbonyative thioetherification
14	Jin Hyeok Yoon, U. Rochester	Copper pyridonate mediated Chan—Evans—Lam coupling
15	John Noel Maape, SUNY Buffalo	Concerted metal-halogen atom transfer (MXAT) from manganese(III) chloride: mechanism and

		applications in stereoselective dichlorinations and in lignin model degradation
16	Jonah Wuloh, Binghamton U.	Molecular assembly of functionalized Co(II) spin centers for tunable magnetic communication
17	Justin Hao, U. Rochester	Synthesis and reactivity of iron(III)–halide complexes supported by tris(amidate)amine ligands
18	Liam Almekinder, Cornell U.	Photocatalysis using main group metal-organic frameworks
19	Lincorn Murithi, Binghamton U.	Fe(II) spin-crossover complexes for stimuli-responsive molecular junctions
20	Michael Vullo, Cornell U.	Gonna be golden: non-aqueous cathodic corrosion of metal surfaces into discrete nanoclusters
21	Morgan Hern, U. Rochester	Synthesis and Reactivity of a Highly Fluorinated Ferrous Complex
22	Lucy Huffman, U. Rochester	Photochemical Reactivity of a High-Spin Fe(IV)-oxo
23	Nadeeshan Gunarathna, U. Rochester	Coordination environment and ligand identity effects on the electronic and magnetic properties of lanthanide and actinide complexes
24	Quentin Kunath, SUNY Buffalo	Exploring the role of hydroxyl groups for improved water interactions in paramagnetic Fe(II) and Fe(III) complexes and a Zn(II) analog
25	Robert Suber, U. Rochester	Functionalizing cyclometalated N-heterocyclic carbenes on nickel complexes
26	Seamus O'Rourke, SUNY Buffalo	Design, synthesis and photophysical characterization of ternary heterostructures of carboxyferrocene, CdS Quantum Dots, and a zinc(II) porphyrin complex
27	Shamitri Bandyopadhyay, U. Rochester	Investigation of cobalt bis(pyridylmonoimine) catalysts for electrochemical nitrite reduction
28	Thomas Arnold, Cornell U.	Influences of the two Type 1 copper centers in an archaeal multicopper oxidase
29	Thomas Kolpack, SUNY Buffalo	Oxidation and deprotonation in the transformation of α-VOOH to VO2 (P)

30	Vartika Jaiswal, U. Rochester	Oriented porous framework films as microenvironment for electrocatalysts
31	Vivienne Mathias, U. Rochester	Understanding the mechanistic consequences of ligand variation on H_2 evolution catalyzed by molecular thiomolybdate clusters
32	Walker Anfield & Yifei Guo, U. Rochester	Synthesis of thiocines through a ruthenium catalyzed 2,3-sigmatropic rearrangement of thiophenes
33	Zhou Lu, U. Rochester	Proton-coupled electron transfer at Keggin-type polyoxotungstates
34	Qishen (Luke) Lyu	Harnessing electrochemistry for direct recovery of metallic iron from low-concentration sources

PARKING INFORMATION

We are excited to host you at the University of Rochester on August 4th, 2023. Please see the following information about parking on campus.

Parking permits are required at the University of Rochester Campus from 7 am to 7 pm on weekdays.

Parking permits may be purchased for $6/day at the information booth on Wilson Blvd.

Meter parking is available along Wilson Blvd.

Alternative parking is available across the Genesee River at Genesee River Valley Park.

Please be advised to never leave valuables in your car, University of Rochester is not liable for theft or damage to vehicles or contents.