ORCAS 2020

International Conference on Energy Conversion & Storage

September 10–11, 2020

CLEAN ENERGY INSTITUTE
UNIVERSITY of WASHINGTON

Agenda

Day 1: Thursday, September 10 (PST)

8:30 - 8:45 am	Welcome remarks – Alexandra Velian and Chun-Long Chen, ORCA chairs
8:45 - 9:00 am	The Clean Energy Institute and Energy Research at UW – **David Ginger, CEI Chief Scientist**

Designer Materials for Energy Storage and Conversion

9:00 - 9:45 am	Solar Electricity from Metal Halides? Who would have thought…: Incredible Perovskites **– Mercouri Kanatzidis (**Northwestern University) *Moderators: Daniel Gamelin & Michael de Sienna (Gamelin)*
9:45 - 10:30 am	Molecular Metal Oxide Charge Carriers for Electrochemical Energy Storage **– Ellen Matson (**University of Rochester) *Moderators: Jon Kephart (Velian) & Ben Mitchell (Velian)*
10:30 - 11:15 pm	*Electrically Conductive Metal-Organic Frameworks for Applications in Electrical Energy Conversion and Storage* **– Mircea Dincă (**Massachusetts Institute of Technology) *Moderators: Dianne Xiao & Jack Geary (Xiao)*
	(15 minute break)
11:30 am - 12:50 pm	Poster Session 1
	(10 minute break)
1:00 - 2:00 pm	**Keynote Talk:** Materials by Design Principles in Artificial Photosynthesis: Discovery and Synergistic Integration of Light Absorbers, Electrocatalysts and Membranes for a Complete, Stable, Efficient, and Safe Solar Fuels Generator **– Nathan Lewis (**California Institute of Technology) *Moderators: Alexandra Velian, Ricardo Rivera (Cossairt) & Kendahl Walz (Velian)*

2:00 - 3:00 pm	**Career Panel:** **Mercouri Kanatzidis**, **Ellen Matson**, **Mircea Dincă** and **Nathan Lewis** *Moderators: Alexandra Velian & Dianne Xiao*

Career Development Session

3:00 – 3:30 pm	My career path: From biochemistry major to science writer **– Linda Wang (**Senior Correspondent at Chemical & Engineering News) *Moderator:* ***Holly Shelton (UW)***
3:30 – 4:00 pm	**Writing Workshop:** Creating a research space: From an elevator pitch to the introduction paragraph of your PhD thesis (see abstract for details) **– Holly Shelton (Department of English, UW**)
4:00 - 5:00 pm	**Happy hour & breakout rooms for meetings**

Day 2: Friday, September 11 (PST)

8:45 - 9:00 am	Day 2 welcome remarks – Alexandra Velian and Chun-Long Chen, ORCA chairs

Frontiers in the Science, Engineering and Commercialization of Batteries

9:00 - 9:45 am	Scientific and Engineering Challenges and Opportunities to Enable Net Zero Emissions Energy Systems **– Nathan Lewis (**California Institute of Technology) *Moderators: David Ginger*
9:45 - 10:30 am	Materials and chemistry of novel redox flow batteries **– Wei Wang (**Pacific Northwest National Lab) *Moderators: Vincent Holmberg & Elena Pandres (Holmberg)*
10:30 - 11:15 am	**– Yang Shao-Horn (**Massachusetts Institute of Technology) *Moderators: Lilo Pozzo & Caitlyn Wolf* *(15 minute break)*

11:30 am - 12:50 pm	**Poster Session 2**
	(10 minute break)
1:00 – 1:45 pm	From Molecules to Megawatts – A Journey from Lab Discovery to Bankable Products of a New Generation Vanadium Redox Flow Battery **– Gary Yang (Chief Strategy Officer,** UniEnergy Technologies) *Moderators: Emma Cave (Schlenker) & Sarah Pristash (Schlenker)*
1:45 – 2:30 pm	Towards High-Voltage Non-Aqueous Organic Flow Batteries **– Tom Sisto (Co-founder and Chief Executive Officer,** XL Batteries) *Moderators: Emma Cave (Schlenker) & Sarah Pristash (Schlenker)* *(5 minute break)*
2:35 – 3:30 pm	**UW/PNNL Panel** with: **Jim DeYoreo (**Pacific Northwest National Lab) **David Ginger (**University of Washington) **Wendy Shaw (**Pacific Northwest National Lab) **Wei Wang (**Pacific Northwest National Lab) *Moderator: Chun-Long Chen*
3:30 – 4:30 pm	Event Conclusion with **Daniel Schwartz (Clean Energy Institute Director)** Poster Awards Presentation & Happy Hour

Speaker Abstracts

Solar Electricity from Metal Halides? Who would have thought…: Incredible Perovskites

Mercouri Kanatzidis
Northwestern University

Suggested Readings:
DOI: 10.1038/nature18306
DOI: 10.1021/acs.accounts.5b00229
DOI: 10.1021/jacs.8b10851

Molecular Metal Oxide Charge Carriers for Electrochemical Energy Storage

Ellen Matson
University of Rochester

The worldwide push to generate electricity from renewable sources has created a critical need to develop improved energy storage and fuel-production strategies. Recent advances in the conversion of solar and wind energy have been increasingly economical, yet without effective methods for storage, it is impossible to integrate these resources into the electrical grid without compromising reliability. Research in the Matson Group focuses on the development of earth-abundant, metal-oxide clusters to serve as electrolytes for redox-flow batteries. Redox-flow batteries are among the most promising technologies for grid-scale energy storage. While traditional battery cells rely on internal solid electrodes for energy storage, redox flow batteries use the circulation of two soluble redox couples as electrolytes, rendering these energy storage systems highly modular and functional. In order to make redox flow batteries commercially viable, inexpensive electrolytes that provide dense electrical output must be developed. Our approach to electrolyte design capitalizes on the stability, solubility, and rich redox chemistry of the transition metal-functionalized polyoxovanadate-alkoxide clusters discovered in our laboratory. These heterometallic complexes are generated via single-step, self-assembly pathways from inexpensive, commercial starting materials and undergo multiple reversible redox events, making them promising candidates for flow-battery applications.

Suggested Reading:
DOI: https://doi.org/10.1080/02603594.2019.1587612

Electrically Conductive Metal-Organic Frameworks for Applications in Electrical Energy Conversion and Storage

Mircea Dinca
Massachusetts Institute of Technology

Traditional applications of metal-organic frameworks (MOFs) are focused on gas storage and separation, which take advantage of the inherent porosity and high surface area of these materials. The MOFs' use in technologies that require charge transport have lagged behind, however, because MOFs are poor conductors of electricity. We show that design principles honed from decades of previous research in molecular conductors can be employed to produce MOFs with remarkable charge mobility and conductivity values that rival or surpass those of common organic semiconductors and even graphite, some even showing metallic character. We further show that these, ordered, and crystalline conductors can be used for a variety of applications in energy storage, electrocatalysis, electrochromics, and selective chemiresistive sensing. This presentation will focus primarily on the design and applications of electrically conductive MOFs for energy storage and conversion.

Suggested Readings:
DOI: 10.1038/s41557-019-0372-0 and Doi: 10.1038/nmat4766

Materials by Design Principles in Artificial Photosynthesis: Discovery and Synergistic Integration of Light Absorbers, Electrocatalysts and Membranes for a Complete, Stable, Efficient, and Safe Solar Fuels Generator

Nathan Lewis
California Institute of Technology

We are developing an artificial photosynthetic system that will utilize sunlight and water as the inputs and produce hydrogen and oxygen as the outputs. We are taking a modular, parallel development approach in which three distinct primary components-the photoanode, the photocathode, and the product-separating but ion-conducting membrane-are fabricated and optimized separately before assembly into a complete water-splitting system. The design principles incorporate two separate, photosensitive semiconductor/liquid junctions that will collectively generate the 1.7-1.9 V at open circuit necessary to support both the oxidation of H2O (or OH-) and the reduction of H+ (or H2O). The photoanode and photocathode will consist of rod-like semiconductor components, with attached heterogeneous multi-electron transfer catalysts, which are needed to drive the oxidation or reduction reactions at low overpotentials. The high aspect-ratio semiconductor rod electrode architecture allows for the use of low cost, earth abundant materials without sacrificing energy conversion efficiency due to the orthogonalization of light absorption and charge-carrier collection. Additionally, the high surface-area design of the rod-based semiconductor array electrode inherently lowers the flux of charge carriers over the rod array surface relative to the projected geometric surface of the photoelectrode, thus lowering the photocurrent density at the solid/liquid junction and thereby relaxing the demands on the activity (and cost) of any electrocatalysts. A flexible composite polymer film will allow for electron and ion conduction between the photoanode and photocathode while simultaneously preventing mixing of the gaseous products. Separate polymeric materials will be used to make electrical contact between the anode and cathode, and also to provide structural support. Interspersed patches of an ion conducting polymer will maintain charge balance between the two half-cells

Suggested Reading:
DOI: 10.1038/NNANO.2016.194

Writing Workshop:
Creating a research space: From an elevator pitch to the introduction paragraph of your PhD thesis

Holly Shelton
University of Washington

How can you introduce your research for general and specific audiences to understand what it is, how it's situated, and what it contributes? This session will focus on the genre-based Create a Research Space (CARS) model for crafting a research study introduction paragraph. The session facilitator will briefly preview typical writing moves of intro paragraphs and what role each of these moves play. Participants will then adapt these moves for their own current or prospective projects and draft an intro paragraph of their own. This will be a very practical, focused writing session.

Scientific and Engineering Challenges and Opportunities to Enable Net Zero Emissions Energy Systems

Nathan Lewis
California Institute of Technology

A successful transition to a future net-zero emissions energy system is likely to depend on vast amounts of inexpensive, emissions-free electricity; mechanisms to quickly and cheaply balance large and uncertain time-varying differences between demand and electricity generation; electrified substitutes for most fuel-using devices; alternative materials and manufacturing processes for structural materials; and carbon-neutral fuels for the parts of the economy that are not easily electrified. Recycling and removal of carbon from the atmosphere (carbon management) is also likely to be an important activity of any net-zero emissions energy system. The specific technologies that will be favored in future marketplaces are largely uncertain, but only a finite number of technology choices exist today for each functional role. To take appropriate actions in the near term, it is imperative to clearly identify desired end points. To achieve a robust, reliable, and affordable net-zero emissions energy system later this century, efforts to research, develop, demonstrate, and deploy candidate technologies must start now.

Suggested Readings:
DOI: 10.1039/c8ee90070a
DOI: 10.1126/science.aas9793

Materials and chemistry of novel redox flow batteries

Wei Wang
Pacific Northwest National Lab

Redox flow battery technologies are leading candidates for stationary energy storage, which provide a potentially cost-effective approach that would be beneficial for renewable energy integration, balancing the mismatch between supply and demand, as well as improving the overall reliability and efficiency of the grid, etc. Until very recently, most research in this area has focused on transition-metal redox species, with not only limit energy density due to solubility issue, but also in some cases increase cost. Materials selection and chemistry development are therefore of critical importance to expand the chemical space for the flow battery technology for future flow battery technologies. This presentation will discuss materials and chemistry development for redox flow battery technologies PNNL, including electrolyte solvation chemistry study, electrode materials development, and flow battery stack systems etc.

TBA

Yang Shao-Horn
Massachusetts Institute of Technology

From Molecules to Megawatts – A Journey from Lab Discovery to Bankable Products of a New Generation Vanadium Redox Flow Battery

Gary Yang
UniEnergy Technologies

Technology innovation drives economic growth and social progress. Inventions in history—such as the steam engine, electricity, or the Internet—have radically changed the world. Meanwhile, there have been plenty of untold stories of inventions that never saw the light of day. Many potentially breakthrough ideas fall into the so-called technology "valley of death", between academic achievements and industrial commercialization.

From lab research to bankable products is a long journey that goes through multiple technology readiness levels (TRLs), across concept development, technology validation, prototyping, product validation in the fields to design optimization. The long march to mature a technology is well exemplified in the development and advancement of a new generation vanadium flow battery (VFB). The new VFB chemistry was first conceived and developed at DOE' Pacific Northwest National Laboratory in late 2010's. Its excellent electrochemical properties were subsequently validated at the lab scale. In 2012 UniEnergy Technologies (UET) was founded to commercialize the VRFB technology, with a mission to turn it into a rugged energy storage product for commercial, industrial and utility applications.

Scaling up the novel and compelling flow battery technology was challenging, requiring a highly specialized combination of electrochemical, chemical, mechanical, electric and controls engineering. Nonetheless, after over seven years of engineering optimization, productization, field demonstrations and design validation, UET has advanced the new generation VFB to deliver a safe, reliable and commercially competitive product for kW to MW scale applications.

This seminar will discuss the new generation VFB and share the experience and learnings of the journey from molecules to megawatts in advancing the new technology from lab discovery to a bankable product.

Towards High-Voltage Non-Aqueous Organic Flow Batteries

Tom Sisto
XL Batteries

This talk will detail the use of synthesis to address challenges towards high-voltage, long-lifetime flow batteries. Currently, battery capacity in America can store a mere 0.005% of our daily electricity use. With 60% of all new power installations predicted to be backup-requiring intermittent power sources such as solar and wind, there will be a demand for inexpensive, safe, and simple to manufacture batteries. Flow batteries, a unique architecture where power and capacity are decoupled, provide an ideal platform for both grid-scale and consumer level stationary energy storage. This talk will showcase the use of synthetic chemistry to build both the charge storage compounds as well as the physical components for long-lifetime, high-voltage organic flow batteries using non-aqueous solvents.

Additionally, this talk will touch on aspects of spinning out a company from academia.

Poster Abstracts

Band-Edge Engineering in Aliovalently Doped Metal-Oxide Nanocrystals

Jose Araujo

Degenerately doped metal-oxide nanocrystals (NCs) are attractive for optoelectronic applications because their localized surface plasmon resonances (LSPRs) are tunable via their tunable excess charge-carrier densities. The addition of delocalized conduction band (CB) electrons can be achieved through aliovalent doping or by post-synthetic techniques such as photodoping. Here, we examine the role of charge-compensating cations on the redox properties of excess electrons in colloidal degenerately doped oxide NCs both experimentally and through modeling. Taking Sn4+:In2O3 (ITO) NCs as a model system, we use spectroelectrochemical techniques to illustrate a key difference between aliovalent doping and photochemical doping. Whereas photodoping introduces excess CB electrons by raising the Fermi level relative to the CB, aliovalent impurity substitution introduces excess CB electrons by stabilizing the CB relative to the Fermi level. A significant difference is thus observed electrochemically between delocalized CB electrons compensated by aliovalent dopants and those compensated by surface cations (protons). Spectroelectrochemical titrations allow the band-edge stabilization as a function of Sn4+ doping to be quantified. Theoretical modeling illustrates the very different potentials that arise from charge compensation via aliovalent substitution and surface charge compensation, both in the total stabilization and in its spatial distribution. These results highlight the role of charge compensation in determining the chemical and physical properties of degenerately doped semiconductor NCs.

Interfacial Ion Dynamics in Electrochemical Energy Storage

Emma Cave

Understanding processes that occur at the electrode/electrolyte interface within a rechargeable battery is one of the most important and difficult challenges facing the field of energy storage. The presented work aims to better understand how the interfacial ion dynamics affect the charge transfer kinetics at such interfaces. We hypothesize that ion solvation and association play a critical, if not rate-limiting, role in the charge/discharge kinetics of electrochemical energy storage devices. One model system that we will discuss is a titanium dioxide (TiO2) electrode immersed in an electrolyte of perchlorate salt dissolved in IR-active acetonitrile. To study this system, we used in situ vibrational spectroelectrochemistry. Fourier transform infrared (FTIR) spectroscopy was coupled with potentiostatic measurements which allowed us to correlate the chemical phenomena with the electrochemical response at the electrode/electrolyte interface. Using this technique, we were able to correlate the spectral response of the free carrier absorption within the TiO2 electrode and the chronoamperometry current signal. Interestingly, by applying global target analysis, we also observe kinetic correlations with vibrational signatures associated with ion solvation and ion paring as a function of electrical charge storage.

Modular Polymers for Nanocrystal Composites with Enhanced Processability and Luminescence

Theodore Cohen

Inorganic lead-halide perovskite nanocrystals (NCs) are an exciting class of luminescent materials with high defect tolerance and broad spectral tunability, but such NCs are vulnerable to degradation under ambient conditions. Here, we report a class of modular zwitterion-functionalized polymers designed to stabilize a wide variety of perovskite NCs of different compositions, while also enabling processing in green solvents. Specifically, we report polymers in which the zwitterion spacing is tuned to accommodate the different lattice parameters of CsPb(Cl1-xBrx)3 and CsPbI3 NCs, and we report partially fluorinated polymers prepared to accommodate the needs of infrared-emitting NCs. We show that as-synthesized CsPbBr3, CsPbI3, and Yb3+:CsPbCl3 NCs are easily transferred into these zwitterionic polymers via a simple ligand-exchange procedure. These NC/polymer composites were then cast into thin films that showed substantially improved photoluminescence (PL) and stability compared with more conventional NC/polymer films. Specifically, CsPbBr3 and CsPbI3 NCs in films of their appropriately designed polymers had PL quantum yields of ~90% and ~80%, respectively. PL quantum yields decreased under continuous illumination, but self-healed completely after dark storage. We also found that all the NC compositions studied here maintain their PL quantum yields in NC/polymer composite films even after 9 months of ambient storage. These encouraging results demonstrate the utility of such modular zwitterion-functionalized polymers for hosting specific perovskite NCs, potentially opening avenues for robust new photonic applications of this important class of NCs.

Computational study of the kinetics of the Menshutkin reaction using explicit and implicit solvent representations

Nida Janulaitis

Many of the solvents currently used in the chemical industry are hazardous to human health and detrimental to the environment [1]. Replacing toxic solvents frequently used to carry out organic chemistry reactions with less toxic, “green” alternatives could improve the sustainability of chemical production and reduce the energy required to work with and dispose of hazardous solvents. In order to evaluate the role of solvent models on kinetics, we have used string search and eigenvector following with density functional theory (DFT) to find minimum energy pathways (MEPs) for the ground-state, well-studied [2], [3] Menshutkin reaction. We investigated the reaction in gas and liquid phase, with both an entirely implicit and a mixed implicit-explicit description of the aqueous solvent. The MEPs, combined with classical transition state theory, were used to calculate the reaction rate constants. Comparison between our results and previous work validates our methods and provides insight regarding the construction of an initial data set for guiding the prediction of reaction rate constants in solvents.

Hierarchical nanomaterials built from superatomic clusters

Jonathan Kephart

Tuning the properties of atomic crystals in the two-dimensional (2D) limit is synthetically challenging, but critical to unlocking their potential in fundamental research and nanotechnology alike. 2D crystals assembled using superatomic blocks could provide a route to encrypt desirable functionality, yet strategies to link the inorganic blocks together in predetermined dimensionality or symmetry are scarce. Here, we describe the synthesis of anisotropic 2D crystalline frameworks using the designer superatomic nanocluster Co3(py)3Co6Se8L6 (py = pyridine, L = Ph2PN(Tol)), and ditopic 4-pyridyl-based linkers. Post-synthetically, the 3D layered crystals can be mechanically exfoliated into ultrathin flakes (8 to 60 nm) or intercalated with the redox-active guest tetracyanoethylene in a single-crystal-to-single-crystal transformation. The nanocluster's high-spin Co(II) edges, and its rich redox profile make the nanosheets both magnetically and electrochemically active, as revealed by solid state magnetic and cyclic voltammetry studies. Preliminary results show that self-assembly of the related nanoblock, Mn3(THF)3Co6Se8L6, with 4,4’-bpy affords a unique porous 3D framework. Within this system, structural templating for 2D assembly is overcome due to increased affinity of the Mn edge sites for the pyridyl linker. These results demonstrate how dynamic edge-support interactions within the M3Co6Se8 nanoblock have long-ranging influence over their performance as designer building blocks. With these findings we introduce a deterministic and versatile synthetic method to achieve programmable functionality and symmetry in both 2D and 3D superatomic crystals.

Screening the Structure of Gold Nanoparticles Formed in Presence of Amphiphilic Solid Binding peptides

Kacper Lachowski

Energy conversion applications, such as plasmonic photocatalysis and plasmonic-enhanced solar cells, make use of localized surface plasmon resonance (LSPR) induced in metallic nanoparticles (MNP) by light. Composition, shape, and arrangement of MNP's are some of the many knobs that can be dialed to design and utilize the LSPR response. Although the synthesis of spherical and monodisperse MNP's is now well understood, the multifactorial problem of connecting experimental conditions to non-spherical morphologies and novel particle assemblies still has many open challenges. In general, the number of samples required for statistical significance scales with the number of variables being explored. Hence, we have directed our focus towards increasing throughput in our study of how peptide sequences and their state of assembly affect gold particle growth in a wide range of experimental conditions. We show how higher (UV-VIS) and lower (TEM, SAXS) throughput characterization techniques can be used in complementary ways to map the structure of gold nanoparticles to sample composition for three gold binding peptides and their fatty acid conjugates (e.g. myristic acid C14). Finally, we summarize both the successes and challenges faced in increasing the throughput of sample creation, characterization, and data analysis.

Atomically Defined Nanoclusters as Functional Models for the Electronic Metal-Support Interaction and High Catalytic Activity for Carbodiimide Formation

Ben Mitchell

Currently, catalytic process account for a quarter of the global energy usage however, traditional heterogeneous catalysts lack efficiency due to poorly defined active sites. Single Atom Catalysts (SACs) have recently emerged as potential candidates to bridge the gap to a more efficient, and sustainable, future. SACs are a class of heterogenous catalysts, important for stability and recyclability, however in contrast to other systems, they feature well defined active "edge" sites in direct contact with the "support" material. Well defined active sites improve catalytic efficiency and increase metal atom utilization, an important trait especially when using expensive noble metals (Pd, Pt, Ru, etc.). Despite these advantages, the rational synthesis of SACs remains a challenge, primarily due to the difficulty in studying the complex interactions that occur between the "edge" and the "support" during catalysis. Our group has recently developed an atomically precise metal-chalcogenide cluster framework in which surface "edge" metals are in direct contact the cluster "support". This system allows for the in-depth study of the physical properties of the cluster and therefore elucidating in impact of the metal-support interaction during catalytic transformations. Two clusters were studied: one with three catalytically active Fe edge sites, Fe3Co6Se8L6, and one with a single catalytically active Fe edge site, FeCo6Se8(PEt3)4L2. The coupling reaction between tosyl azide (TsN3) and ¬tert-butyl isocyanide (CNtBu) to form the asymmetric cabodiimide, TsN=C=NtBu, was explored. Herein we report extensive single-crystal X-ray data, NMR studies, electrochemical analysis, DFT calculations, and in-depth reactivity analysis.

Morphological and Interfacial Engineering of Nanostructured Alloying Electrodes for Battery Applications

Elena Pandres, Kevin Lee, Yao Yu

Alloying electrode materials – like silicon and germanium – are particularly attractive for batteries due to their large Li-ion capacity, and antimony's rate capability is especially intriguing for high-power-density battery applications. Although each of these materials has a much larger theoretical capacity than graphite, they all undergo significant volume change upon cycling, which can result in strain, fracture, and capacity fade. Nanostructuring these electrode materials has been shown to reduce strain, improving capacity retention and cycle life. Still, there are many aspects of nanostructured alloying electrode materials that affect capacity retention and rate capability, including morphology, composition, and surface chemistry.

Here, we discuss the electrochemical cycling of germanium-nanowire-based composite electrodes and observe that controlled electrode surface modification, when paired with certain binders, significantly improves the cycling retention and lifetime of germanium-nanowire-based electrodes in the absence of fluorinated reductive decomposition products. We also present recent developments of a supercritical-fluid-based synthesis to produce compositionally tunable, alloyed silicon-germanium nanostructures for targeted capacity and rate capability.

In addition, we developed a morphologically tunable, supercritical-fluid-based synthesis for nanostructured antimony and demonstrate how morphological selectivity can be used to evaluate how structural anisotropy affects sodiation and desodiation as well as how oxidation and temperature influence the electrochemical alloying process. Understanding the transformations that take place during the high-rate electrochemical alloying of nanostructured antimony will enable the structural optimization of high-rate-capability, antimony-based alloying electrodes. Investigations of high throughput, microstructured electrode fabrication processes are also underway.

Examining the effect of surface stoichiometry on the photoluminescence properties of InP/ZnSe quantum dots

Nayon Park

TBD

Develop of an Efficient Electrochemical Engineering Modeling for Lithium Sulfur Batteries

Caitlin Parke

As the energy requirements for electric transport outgrow lithium ion batteries, research on Lithium-Sulfur batteries has increased dramatically in recent years due to the high theoretical energy density of 2500 Wh/kg. Despite their promise, Lithium-Sulfur batteries suffer from several challenges, ranging from the cycling stability of lithium metal to the insulating nature of the sulfur cathode, which limit power capabilities. Electrochemical modeling can give insight into the underlying mechanisms that contribute to degradation and poor performance through modeling internal states. We have developed a model that bridges the gap between efficient lumped models and descriptive 1D physics-based models that can be used in efforts for parameter estimation and optimization. The Tanks-in-Series model (Tank model) was developed through volume-averaging the 1D model and includes a fitting parameter delta, that describes the extent gradients occur in each of the battery's regions. The implications of the approximations are explored through a small parametric study. The Tank model, even under relatively aggressive conditions, predicts voltage and internal states well compared to the 1D model, with a 5-10 fold increase in speed. This suggests significant potential for real-time applications such as optimal charging, cell-balancing, and estimation, and represents a step forward in efforts to incorporate detailed electrochemical models in advanced Battery Management Systems for Lithium-Sulfur batteries.

Heavy-atom-free Photon Upconversion Using Thionated Organic Sensitizers

Sarah Pristash

Photon upconversion through triplet–triplet annihilation is of interest for diverse applications, notably as a potential means of exceeding the Shockley–Queisser limits in solar cells. We demonstrate a heavy-atom-free triplet sensitizer based on a thionated squaraine. Using this all-organic sensitizer, we demonstrate upconversion through triplet sensitization of several organic annihilator molecules. Thionated squaraines provide an exciting new platform for developing heavy-atom-free upconversion systems.

Laboratory-based X-ray Absorption Fine Structure and X-ray Emission Spectroscopy for Electrical Energy Storage Materials and Systems

Gerald Siedler

Advanced x-ray spectroscopies such as x-ray absorption fine structure (XAFS) play an important role in decoding the atomic-scale state and evolution of battery materials. Ongoing work in the Seidler group at the UW [1] has shown that metal-oxide electrode laminates can be quickly characterized [1] and that many studies of XAFS and x-ray emission spectroscopy (XES) for battery materials can be performed in the laboratory, avoiding the access limitations of synchrotron facilities. In this poster we summarize this effort, including rapid characterization of ex situ metal-oxide battery laminates, fast charging studies of NMC pouch cell batteries [2] and valence-level electronic structure investigation of vanadyl phosphate materials.[3] This new technology holds the promise of accelerating discovery of battery materials and also developing new directions for quality control and failure analysis for industrial applications.

Covalent Functionalization of Black Phosphorus with Metal Carbonyl Complexes

Kendahl Walz Mitra

Electronic metal-support interactions are an important method of controlling the properties of metal catalytic sites in single-site heterogeneous catalysts. Black phosphorus, an elemental 2D-material composed of phosphorus atoms, is a particularly promising support as the lone pairs on each P atom are available to interact with metal centers. While black phosphorus functionalization with metal nanoparticles has previously been explored for catalysis, there is little work focusing on functionalization with mononuclear molecular complexes. However, demonstrating successful functionalization of black phosphorus is not trivial: previous reports of black phosphorus functionalization suffer from low yields of exfoliated nanosheets, low signal-to-noise ratios, and minimal changes in characteristic black phosphorus features upon functionalization. This work will address the covalent functionalization of black phosphorus with catalytically-relevant metal carbonyl complexes to form heterogeneous catalysts. The resulting materials are characterized with infrared, Raman, and X-ray photoelectron spectroscopies.

Improved Non-Bonded Parameters for P3HT Molecular Dynamics Force Fields

Caitlyn Wolf

A better understanding of the relationship between molecular morphology and charge transport behavior in conjugated polymers is important for developing improved materials and devices, e.g. organic photovoltaics (OPVs). This relationship can be difficult to probe with experiments alone, and so researchers employ simulations to gather valuable in-silico information. In past work, we provided a critical assessment of three molecular dynamics (MD) force fields (FFs), or modeling parameters, proposed in the literature for a well-studied conjugated polymer, poly(3-hexyl thiophene) (P3HT). Partial charges and backbone torsion potentials were modified from the classical systems to account for the effect of conjugation, but we found these parameter changes to result in different inter- and intra-chain conformations and dynamics across all modeled systems. Moreover, the FFs failed to capture characteristic backbone dynamics displayed in quasi-elastic neutron scattering (QENS) results. This is significant as the choice of FF would directly affect any additional analyses of charge transport behavior in these systems. In this work, we re-evaluate these models from an intermolecular perspective. Lennard-Jones (LJ) parameters for P3HT are frequently borrowed from small molecules of benzene and thiophene, but would not account for the increased polarizability of these long, conjugated molecules. Here, we re-parameterize these LJ parameters for improved P3HT FFs using a combined density functional theory and MD approach, and find that the interaction strength is currently underestimated in existing models. MD simulations using these updated values (ongoing work) will be used to understand how these LJ parameters then affect molecular morphology of the modeled system.

Peptoid-Controlled Crystallization of Silver Nanoparticles

Wenchao Yang

Under light illumination, various significant reactions concerning energy conversion and storage have been driven and/or enhanced by plasmonic nanomaterials under facile conditions, which make it important to tune the size and shape-dependent optical property of plasmonic nanomaterials by controlling their crystallization. In this work, peptoids were used to develop biomimetic approaches for controlling the size, shape and spatial arrangement of silver nanoparticles, the common utilized plasmonic nanomaterials. Silver nanocubes were obtained by using an amphiphilic peptoids consisting of carboxyl and aromatic side chains as a growth modifier. Additionally, the same peptoid sequence could also template the nucleation of silver nanoparticles resulting in the formation of nanoribbons. Because peptoids are easy to synthesize and have unique advantage of tuning intermolecular and molecule-surface interactions, we expect peptoid-based biomimetic approaches offer great potentials for achieving predictive synthesis of silver plasmonic nanomaterials for energy-related applications.

Direct visualization of hematite mesocrystal growth through near interface nucleation and oriented attachment

Guomin Zhu

A diverse class of materials exhibit characteristics of mesocrystals: single crystals constituting distinct nano-sized domains that are atomically aligned. The formation of such structures is often attributed to crystallization through oriented attachment. However, many questions about the fundamental drivers and dynamic progression of this phenomenon remain. And the process become more complexed when coupled with phase transformation. Here we focus on the crystallization of hematite (hm, Fe2O3) mesocrystals from ferrihydrite (fh) nanoparticles. In the oxalate-free solution, the resulting hm crystals are well faceted rhombohedron, while in the presence of oxalate, hm forms nanoporous spindle-shaped mesocrystals. We applied in situ liquid phase TEM with heating temperatures of 80 °C to investigate the formation. We directly observed both the dissolution of fh and the nucleation of new hm particles, which formed within close proximity (~ 1 nm) of the hm/solution interface. Immediately after nucleation, the hm particles attached to the nearby seed to form a hm mesocrystal. Post analyses using EDX mapping and electron diffraction after disassembling the liquid cell confirmed the growth of spindle-shaped hematite during the liquid phase TEM experiments. In addition, we utilized a quasi in situ approach of using indexed TEM grids to cycle samples between the growth reactor and the TEM in order to track the pathway of crystallization. The results were consistent with those of the in situ experiments and confirmed that the fh serves as a buffer and the Hm grow by creation of new particles in the solution near the hm interface. Based on ATR FTIR measurements, ion chromatography and classic DFT calculation we propose that oxalate plays the role of inhibiting classical monomer-by-monomer growth of the hematite particles while promoting the nucleation of new hm particles at the hm/solution interface by modifying the interfacial energy of hm close to the hm/solution interface. In this way, the oxalate ligands bias the growth process away from classical mechanisms and towards oriented attachment.