Meeting Program

3rd Nano@IAState Meeting - Friday, August 16, 2019 – 8:30 am to 6:00 pm
Iowa State University, Hach Hall Atrium

•Meeting Overview

Nano@IAState is a single day meeting to bring together ISU, Ames Lab and industrial scientists and researchers working on the synthesis and characterization of nanomaterials and applications of nanoscience. The meeting is open to ISU and Ames Lab graduate and undergraduate students, staff and faculty, and members of local industry.

•Sponsors

We are grateful to the following sponsors whose generous contributions have made the meeting possible:

Department of Chemistry, Department of Chemical and Biological Engineering, Department of Materials Science and Engineering, The Ames Laboratory and the Vice President of Research.

•Presentation Information

Contributed Oral Presentations will have a total duration of 15 minutes, including a few minutes for questions from the audience. The boards for Poster Presentations will be 4' x 4'. Please make sure your poster is 4' wide or narrower. Poster boards will be available immediately in the morning. Please bring your posters in the morning so that you can hang them up early and show them at breaks throughout the day.

•Organizing Committee

Aaron Rossini - Chemistry - arossini@iastate.edu
Matthew Panthani - Chemical and Biological Engineering - panthani@iastate.edu
Martin Thuo - Materials Science and Engineering - mthuo@iastate.edu

•Nano@IAState – Friday Aug. 16, 2019 – Conference Program

All events take place in the **Hach Hall Atrium**

Time	Event/Talk Title	Presenter
8:00	Registration/Badge Collection - Coffee, Tea and Light Breakfast Provided	
	Oral Presentations	
8:25	Opening Remarks	
8:30-9:15	Plenary Lecture - Selective Hydrogenation of Aqueous Nitrate to Ammonia over Ni_2P	Javier Vela (Chemistry)
9:15	Nano-scale Surface Templating of Complex Metal Particles	Andrew Martin (MSE)
9:30	Reshaping and Sintering of 3D fcc Metallic Nanocrystals	King Chun Lai (Physics)
9:45 – 10:05	High Entropy Materials for Electrochemical Water Splitting	Sonal Padalkar (ME)
10:05-10:30	Coffee Break – Light Refreshments	
	Oral Presentations	
10:30-11:30	Plenary Lecture - Directing Assembly of Molecular Electronics Inspired by Living Systems	Ying Diao (UIUC, Chem. Eng.)
11:30	Thin, Biobased, Nano Assembled Coatings for UV-Blocking	Emily Olson (MSE)
11:45	Probing the Edge Termination of Exfoliated Hexagonal Boron Nitride Nanosheets	Rick Dorn (Chemistry)
12:00-12:20	Functional Nanoparticles: Basic Concepts and Beyond	Duane Johnson (MSE)
	Lunch	
12:20-12:50	Boxed Lunches Provided	
12:50-1:25	Career Panel Discussion and Lunch	
	Oral Presentations	
1:25-1:45	Highly efficient earth-abundant electrocatalysts for hydrogen generation via water splitting	Shan Hu (ME)
1:45-2:05	Designing Nanotherapeutics Against Resistant Infections	Bryan Bellaire (Vet. Med.)
2:05	In vitro Investigation of the Influence of Nano-cellulose on Food Digestion and Nutrient Absorption	Lingling Liu (Food Science)
2:20	Energy Scaling Relations for Simple Adsorbates in the Presence of a Single Solvent Molecule	Jaeryul Park (CBE)
2:35-2:55	Single Walled Carbon Nanotubes as Spatiotemporal Sensors of Hydrolytic Activity	Nigel Reuel (CBE)
2:55-3:20	Coffee Break – Light Refreshments	
	Oral Presentations	
3:20-3:40	Nanotech Approach for Structuring Food Components to Stabilize, Protect and Efficiently Deliver Functional Components	Nuria Acevedo (Food Sci)
3:40	Catalytic Applications of Metal-Loaded, Bipyridine-Functionalized Covalent Organic Frameworks	Patrick Heintz (Chemistry)
3:55-4:15	Multifunctional Soft Materials for Electronics and Robots	Michael Bartlett (MSE)
4:15 – 5:45	**Poster Session** – Snacks Provided	
5:45	Student Poster and Oral Presentation Prizes Announced	

List of Poster Presenters

Poster Number	Presenter	Poster Title
1	Jonghyun Lee	Solution electrostatic levitator combined with in situ micro Raman and synchrotron X-ray for advanced materials research
2	Jacob Austin	Emergence of Mesoscopic Chirality in Nanoparticle Systems
3	Geet Gupta	Selective Catalytic Conversion of Glycerol to Higher Value Products
4	SHAILJA GOYAL	Synthesis, Characterization of Carborane containing cyanate ester with excellent thermal Stability
5	Paul Gregory	Formation of Micro-scale Graphitic Carbon Tubes via inverted Thermal Degradation (iTD)
6	Chuanshen Du	Conformational Dynamics in charge transport across self-assembled monolayers (SAMs) based molecular tunneling junctions
7	Yunhua Chen	Solid State NMR Characterization of Inorganic Semiconducting Nanoparticles Surfaces
8	Liyang Shen	Block copolymer modified epoxy resins for additive manufacturing
9	Xun Zha	Free energy calculation of superlattices
10	Dr. Daniel Attinger	Dropwise Condensation on Multiscale Bioinspired Metallic Surfaces with Nanofeatures
11	Lingling Liu	In vitro Investigation of the Influence of Nano-cellulose on Food Digestion and Nutrient Absorption
12	DohGyu Hwang	Kirigami-Inspired Materials for Adhesion Control
13	Yifan Li	Morphology Evolution in Seeded Emulsion Polymerization and Coating Applications
14	Lin Wei	Oxyanion Hydrogenation over Binary Metal Phosphides
15	Baker Kuehl	Toughening PLLA with Block-Copolymer Self-Assembly
16	Yiliang Cheng	3D Printing and Characterization of Hydroxypropyl Methylcellulose and Methylcellulose for Biodegradable Support Structures
17	Utkarsh Ramesh	Tuning the Optical Properties of Silicon Nanosheets via Surface Halogenation
18	Warren Straszheim	How to (not) do Poor Microanalysis of Nanomaterials
19	Faez Qahtani	Fabrication of a coatless superhydrophobic on 7075 Aluminum Alloy surface by using Nanosecond Laser Followed by Simple Heat Treatment.
20	Dapeng Jing	Materials Analysis and Research Laboratory: A core material characterization facility at Iowa State University
21	Carena Daniels	Synthesis of Intermetallic Compounds from Heterobimetallic Single-Source Precursors
22	Cicero C. Pola	Laser-induced graphene for foodborne pathogen detection
23	Atefe Hadi	Stability enhancement in layered cesium lead iodide perovskites
24	Tung-ping Wang	Developing a method for isolating hollow-core elastomeric vesicles
25	Xiao Zhang	Reliability Analysis of 3D Surface Measurement Data of Additive Manufactured Parts Based on Optical Metrology

Oral Presentation Abstracts

1. **Selective Hydrogenation of Aqueous Nitrate to Ammonia over Ni2P**

Javier Vela

Abstract: A better understanding of the chemistry of molecular precursors is useful in achieving more predictable and reproducible nanocrystal preparations. Using commercially available organophosphite precursors, we have used a chemical reactivity approach to synthesize nickel and nickel phosphide nanocrystals with high selectivity (Ni, Ni12P5 and Ni2P phases). Some organophosphites, such as P(OMe)3 or P(OiPr)3 transiently form zerovalent, metallic nickel; the latter is persistent with the bulky organophosphite P(O-2,4-tBu2C6H4)3. Along with other first row, transition metal phosphides, Ni2P is a very active catalyst for the hydrogen evolution reaction, as well as for hydrodesulfurization, and other reforming reactions. Based on this information, we hypothesized that Ni2P should be active in the reduction of oxyanions. Indeed, we have recently succeeded in using this material as a catalyst for the near ambient removal of nitrate from water.

2. **Nano-scale Surface Templating of Complex Metal Particles**

Andrew Martin (PI: Martin Thuo)

Abstract: Liquid metal particle interfaces contain abundant inter-esting thermodynamic properties that can dictate bulk behavior, however study of said interfaces has been lim-ited due to its challenging nature. Challenges come from the size of these interfaces and further increased by the reactive attribute of liquid metal itself. However, engi-neering the surface oxide can lead to multitude of unique approaches for different chemical processes. Dif-fusion mechanics heavily governs the formation of me-tallic oxide layers and thus controlling it through ma-nipulating chemical potential gradient and atomic mobility can help tune the formation of surface oxides. This work demonstrates the use of certain thermody-namic parameters to predict and extend thermal treat-ment mechanism that leads into nano-scale texturing and composition inversion of ternary liquid metal alloy.

3. **Reshaping and sintering of 3D fcc metallic nanocrystals: Stochastic atomistic modeling with realistic surface diffusion kinetics**

King Chun Lai (PI: James W. Evans)

Abstract: Controlled synthesis of metallic nanocrystals allows tuning of shapes and thus properties for applications, e.g., to catalysis and plasmonics. However, these shapes are metastable. Far-from-equilibrium evolution back to equilibrium Wulff shapes is mediated by surface diffusion, and is sensitive to the numerous atomistic-level diffusion barriers for diverse local surface configurations. Realistic description of surface diffusion kinetics is thus crucial to predict the stability of non-equilibrium nanocrystal shapes, a prerequisite for functionality in applications. We develop a stochastic lattice-gas model incorporating appropriate barriers for terrace, edge, and interlayer diffusion (contrasting previous generic bond counting prescriptions). Kinetic Monte Carlo (KMC) simulation of this model enables reliable assessment of: the reshaping of Ag nanocubes to Wulff polyhedra; the pinch-off of Ag nanorods; and sintering for orientationally-aligned nanoclusters [Chemical Reviews 119 (2019) 6670]. The time scale for sintering of ~4 nm Au nanoclusters observed in HR-TEM studies was also recovered.

4. **High Entropy Materials for Electrochemical Water Splitting**

Sonal Padalkar (PI:)

Abstract: The increasing demand for energy generation and concerns of global warming, have led to large investments in the renewable energy sector. The research area focusing on the generation of renewable energy from renewable sources has gained much attention. One such energy carrier is hydrogen. Electrolysis of water hydrogen generation will significantly contribute to the long-term, high volume production of hydrogen gas. This talk will focus on the electrolysis of water, carried out by high entropy materials, namely chalcogenides. The talk will include the electrode fabrication using chalcogenides and their characterization. Briefly, the high entropy materials were prepared by ball milling and annealing. The various process parameters in the synthesis were fine tuned to obtain a family of high entropy materials, including MoS2, MoSe2, WS2 and WSe2. The electrode fabrication was performed via high voltage electrophoretic deposition. The talk will also discuss the trends observed within the families of chalcogenide materials.

5. **Directing Assembly of Molecular Electronics Inspired by Living Systems**

Ying Diao (PI:)

Abstract: Molecular assembly, crystallization and controlled phase transition have played a central role in the development of modern electronics and energy materials. Recent years, printed electronics based on semiconducting molecular systems have emerged as a new technology platform that promise to revolutionize the electronics and clean energy industry. In contrast to traditional electronic manufacturing that requires high temperature and high vacuum, these new electronic materials can be solution printed at near ambient conditions to produce flexible, light-weight, biointegrated forms at low-cost and high-throughput. However, it remains a central challenge to control the morphology of semiconducting molecular systems across length scales. The significance of this challenge lies in the order of magnitude modulations in device performance by morphology parameters across all length scales.

This challenge arises from the fact that directed assembly approaches designed for conventional hard materials are far less effective for soft matters that exhibit high conformational complexity and weak, non-specific intermolecular interactions. On the other hand, biological systems have evolved to assemble complex molecular structures highly efficiently. We are eager to transfer the wisdom of living systems to developing printed electronics technologies as to enable next generation electronics for clean energy and healthcare. In this talk, we

6. **Thin, Biobased, Nano Assembled Coatings for UV-Blocking**

Emily Olson (PI: Shan Jiang)

Abstract: A biobased, UV-blocking, and visually transparent coating of ZnO nanoparticles and 2-hydroxyethyl cellulose (HEC) is formulated. The coating is highly effective (< 5% UV and ~ 65% visible transmittance) and film thickness is ~100 times thinner than coatings of similar capacity. The performance of the coating is a result of the formation of fractal aggregates of ZnO within the HEC matrix, visualized via scanning electron microscopy and small angle x-ray scattering. This effect can only be achieved with the HEC binder, and when 2-hydroxyethyl starch (HES) is used, the UV-blocking performance is reduced. HES induces the formation of dense, globular aggregates, which are less effective in providing adequate UV-blocking and visual transparency. This is surprising, as HEC and HES share the same glucose unit in the polymer backbone. The conformational characteristics of the binder must determine the nanoparticle aggregation and resulted performance across visible and ultraviolet wavelengths.

7. **Probing the Edge Termination of Exfoliated Hexagonal Boron Nitride Nanosheets**

Rick W. Dorn (PI: Aaron J. Rossini)

Abstract: Using high-resolution solid-state NMR (SSNMR) spectroscopy and plane-wave DFT calculations, we determined the molecular edge termination of exfoliated hexagonal boron nitride nanosheets (h-BNNS). 1H-11B cross-polarization magic angle spinning (CPMAS) SSNMR experiments of h-BNNS reveal distinct trigonal-planar boron environments with a distribution in the 11B isotropic chemical shift due to hydroxyl/oxygen coordination. A DNP-enhanced 1H-15N CPMAS spectrum recorded at natural abundance showed four distinct nitrogen sites while a 2D 1H{14N} dipolar-HMQC revealed three nitrogen sites, two of which exhibited a large quadrupolar induced shift due to asymmetry near the nitrogen nucleus. Lastly, DFT calculations of h-BNNS provided aid in explain the 14N/15N spectra and allowed us to conclude that both B2N-H armchair and zigzag edge terminations are present, with the armchair edge termination being most prevalent. The structural information acquired and techniques used should provide usefulness to the nanomaterial community by fully understanding the molecular edge termination of atomically-thin layer materials.

8. **Functional Nanoparticles: basic concepts and beyond**

Duane D. Johnson (PI:)

Abstract: Leonardo da Vinci said: “Simplicity is the ultimate sophistication.” In materials science, processing-structure-property-performance paradigm is complex but critical to materials development. We introduce simple concepts on stability and topology of nanoparticles (e.g., core-shell structures) forming the basis of functionality/performance. To assess structure, which controls some properties, we use so-called RCA gas tables, which hide sophisticated chemical and thermodynamic effects, to predict core-shell nanoparticle structure, where machine-learning was unable. A key lesson with simplicity of message: “artificial intelligence” is not a replacement for “real intelligence”. These concepts are then expanded to line-compound nanoparticles (nanoalloys) and molecular adsorption on nanoparticle surfaces, showing how to alter stability and control over surface catalytic properties, especially when particles are encapsulated to control surface-to-volume effects, for example, using “ship-in-a-bottle” synthesis techniques. So, simplicity can yield ultimate sophistication in materials chemistry that appear so complex, but then there is the rest of the story.

9. **Highly efficient earth-abundant electrocatalysts for hydrogen generation via water splitting**

Shan Hu (PI:)

Abstract: Water electrolysis using electricity generated from renewable sources is a CO2-emission free process for hydrogen production. During electrolysis of water, electrical voltage is applied to two electrodes inserted in aqueous electrolyte and two half reactions, i.e. the oxygen evolution reaction (OER) and the hydrogen evolution reaction (HER), occur on the positive and negative electrodes respectively. To reduce the energy consumption of water electrolysis, electrocatalysts are applied to the electrodes to reduce the reaction potential needed to drive each half reaction. Current water electrolysis systems use precious metals, such as platinum iridium, and ruthenium, as catalysts. The high cost and scarcity of these catalysts make it economically inviable to scale up the electrolysis system for large-scale hydrogen production. In this talk, two synthetic routes towards defect-rich transition metal hydroxide will be presented: one being anion-leaching induced surface reconstruction and the other is in-situ etching and hydrolysis of metal organic framework (MOF). The structural characterization and performance evaluation of the TMH as highly efficient OER catalysts will also be presented.

10. **Designing Nanotherapeutics Against Resistant Infections**

Bryan Bellaire (PI:)

Abstract: Innovative technologies are needed to address the challenges infectious diseases posed by antibiotic resistant pathogens. Effective countermeasures need to be developed that are broadly applicable to a wide range of threats from bacterial to parasitic diseases. We examine the benefits of nanotherapeutic delivery of existing drugs as a platform technology to create a next generation nanomedicine countermeasure against difficult to treat and antibiotic resistant infections. Nanoparticles have been developed through tailoring copolymer ratios with molecular characteristics of antibiotics to design nanotherapeutics to a variety of acute and chronic infections including Tuberculosis, Lymphatic Filariasis, Melioidosis and Primary Amoebic Meningioencephalitis.

11. **In vitro Investigation of the Influence of Nano-cellulose on Food Digestion and Nutrient Absorption**

Lingling Liu (PI: Keith Vorst)

Abstract: The influence of three types of NC (nano-fibrillated cellulose (CNF)), TEMPO (2,2,6,6-tetramethylpiperidine-1-oxyl radical) oxidized CNF (TEMPO-CNF) & nano-crystalline cellulose (CNC) on food digestion and nutrient absorption as well as its behavior during gastrointestinal (GI) digestion were investigated by using a simulated in vitro digestion model consisting of salivary, gastric and intestinal phase. NC at high concentrations (0.5~1% CNF, 0.36% TEMPO-CNF and 2~4% CNC) reduced glucose diffusion, delayed lipid digestion and free amino nitrogen diffusion. Moreover, three types of NC showed different behaviors during digestion. In particular, CNF was morphologically stable, while TEMPO-CNF became aggregated and CNC formed hydrogels at the gastric phase. This study indicates that NC is advantageous than cellulose in the GI tract in terms of increasing digesta viscosity, delaying food digestion and nutrient absorption, and has potential to be used in the development of functional foods to control nutrient absorption and promote satiety.

12. **Energy Scaling Relations for Simple Adsorbates in the Presence of a Single Solvent Molecule**

Jaeryul Park (PI: Luke T. Roling)

Abstract: Density functional theory calculations are useful for understanding reaction mechanisms, but calculating the energetics of entire reaction networks can be costly. Linear scaling relations between energies of complex adsorbates and simpler chemical species have been widely used to estimate binding energies of intermediates for reactions at the gas-solid catalytic interface. However, their utility in complex condensed phase environments is unknown. In this study, we identify linear scaling relations in the presence of solvent molecules. Gas-phase linear scaling relations are preserved, but are simply shifted due to preferential interactions between adsorbates and solvents. This trend was observed universally in various functional groups including carbon, oxygen, nitrogen, and sulfur in the presence of a water and methanol molecule. The extent of shift varies depending on the number of solvent molecules and types of solvent and adsorbate. Our approach improves the affordability of computational materials design in the condensed phase.

13. **Single Walled Carbon Nanotubes as Spatiotemporal Sensors of Hydrolytic Activity**

Nigel Reul (PI:)

Abstract: The Reuel group focuses on developing low-cost, untethered, passive (no on-board power) sensors for closed systems. Examples of closed systems include bioreactors, soil environments, bandages, and plastic parts where making internal measurements is inconvenient or impossible with traditional, wired sensors (e.g. electrochemical, potentiometric, amperometric). This talk will primarily focus on one platform: near infrared optical probes. Our group uses single walled carbon nanotubes (SWCNT) as highly-stable, optical reporters for assessing activity of hydrolytic enzymes; these are active protein catalysts present in many natural and synthetic processes. In brief, a non-covalent coating is applied to the nanotube that is affected by the target analyte and causes a spectral shift in the fluorescence of the SWCNT. This talk will mention best practice methods to fabricate these sensors and discuss applications of these in quality control of animal feed, fundamental studies of tumor microenvironments, and in measuring the health of soil.

14. **Nanotech Approach for Structuring Food Components to Stabilize, Protect and Efficiently Deliver Functional Components**

Nuria acevedo (PI:)

Abstract: In recent years, an alternative route to structuring edible oils, termed “oleogelation”, has emerged as a potential strategy to impart the functional properties associated with trans and saturated fats. The goal of this work was to engineering stable and semi-solid lecithin-based oleogels (LOG) and oleogel emulsions (LOGE) and evaluate their potential as a protective environment for probiotics as well as their ability to prevent or delay the progress of lipid oxidation. Nanostructural and functional analysis of the systems indicated that LOG are primarily formed through the entanglement of bundles of SL reverse worm-like micelles. LOGE were structured mainly through SA crystalline network that synergistically with the SL reverse micelle fibers and water droplets to stabilize the three dimensional network. LOG and LOGE can be used as an alternative to hardstock fats particularly when the objective is to achieve semi-solid characteristics while reducing phospholipids oxidation and increasing the survival of probiotics.

15. **Catalytic Applications of Metal-Loaded, Bipyridine-Functionalized Covalent Organic Frameworks**

Patrick Heintz (PI: Dr. Wenyu Huang)

Abstract: Covalent Organic Frameworks (COFs) are a recently discovered class of porous material constructed from organic linkers to form ordered, nanoporous channels. Their high surface areas, exceptional porosities, and readily modulated frameworks make these structures promising heterogeneous materials for practical applications such as catalysis, drug delivery, purification, carbon-dioxide capture, and storage. The ability to functionalize a variety of organic linkers allows for the design of COFs with unique properties and the ability to tune the utility of these structure for a desired use. This talk focuses on the synthesis and application of a robust, recyclable COF containing metal-loaded bipyridine units for use in catalytic transformations. Specifically, a palladium-functionalized COF is an active catalyst of conjugate additions of aryl boronic acids to a variety of enone substrates. In addition, an iridium-loaded COF is an active catalyst for the borylation of aromatic C-H bonds with B2(pin)2.

16. **Multifunctional Soft Materials for Electronics and Robots**

Michael Bartlett (PI:)

Abstract: Multifunctional soft materials create intriguing new opportunities to enhance performance and enable innovative designs. Here, I will present an all-soft matter approach that combines soft elastomers with dispersions of liquid-phase eutectic Ga-In (EGaIn) metal alloy microdroplets. Experimental and theoretical investigations show that liquid metal droplets incorporated into elastomers enables exceptional combinations of soft elasticity and electrical and thermal properties with extreme toughness, autonomously self-healing circuits, and mechanically triggered stiffness tuning. These approaches provide model systems to study fundamental material properties while enabling electronic skins, soft robots, and damage sensing materials for a variety of soft matter systems.

Poster Presentation Abstracts

1. **Solution electrostatic levitator combined with in situ micro Raman and synchrotron X-ray for advanced materials research**

Jonghyun Lee

Abstract: A solution electrostatic levitator (S-ESL) was recently developed at ISU. The S-ESL levitates a liquid droplet (or solid particle) of 2-3 mm in diameter and allows for novel containerless processing. The concentration of a levitated solution droplet increases gradually by evaporation and reaches unprecedentedly deep supersaturation before the solution crystallizes thanks to the absence of preferred nucleation sites (container). An in situ micro-Raman is coupled with the S-ESL to probe the evolution in molecular structure during supersaturation and crystallization. The S-ESL is made portable to be combined with the beamline x-ray at the Advanced Photon Source to investigate atomic structures of levitated materials. The S-ESL is being utilized to understand the nanoscale structural behaviors of supersaturated salt solutions during crystallization and the self-assembly of colloid particles. This talk also intends to inform the ISU research community of successful development of the S-ESL to explore future collaboration opportunities.

2. **Emergence of Mesoscopic Chirality in Nanoparticle Systems**

Jacob Austin (PI:Alex Travesset)

Abstract: Chiral molecules are found ubiquitously in nature, with nearly all occurring in the laevus (L) configuration. Molecular scale chirality has been shown to translate into mesoscopic organizations such as helicoids, twists, etc. In this study we present a detailed analysis of the interaction between two nanoparticles capped with chiral ligands. For this purpose, we use all-atom molecular dynamics to compute the potential of mean force between two gold hexagon plane cores that are functionalized with L-/L-form, D-/D-form, L-/D-form, and a racemic mixture of cysteine. We provide rigorous calculations to verify the chiral potential and identify its origin. We discuss the implications of our results for self-assembly of nanoparticles functionalized with enantiomers. In addition to the enormous potential applications of nanoparticle assemblies, the addition of chirality adds a plethora of potential new possibilities.

3. **Selective Catalytic Conversion of Glycerol to Higher Value Products**

Geet Gupta (PI:Luke Roling)

Abstract: Glycerol, a product of biodiesel processing (about 10% w/w), has the potential to be selectively converted to high value chemicals and stabilize the economics of other bio-derived chemicals. Previous studies have observed the product selectivity of glycerol conversion is related to the catalyst structure and composition; however, a detailed understanding of the reaction mechanism is still limited. Based on density functional theory (DFT) calculations, selective glycerol conversion and the variation in catalytic activity from one transition metal to other can be explored and an optimized, commercially viable metal nanoparticle catalyst can be designed. In our work, we investigate trends in selective oxidation of glycerol by studying structure sensitivity of C-H, O-H, C-C, and C-O bond cleavage on transition metals including Ag, Au, Pt, Pd, Cu, and Rh. Also, we place a special emphasis to ensure that our computational model represents the realistic glycerol reactivity conditions on a given catalytic surface.

4. **Synthesis, Characterization of Carborane containing cyanate ester with excellent thermal Stability**

SHAILJA GOYAL (PI:Dr. Eric Cochran)

Abstract: Cyanate ester (CE) are an important class of materials among high temperature performance thermosets due to their high glass transition temperatures (>220°C), excellent thermal stability, and low flammability. This study aims at synthesizing nanocomposites containing various hydroxy or epoxy functionalized carborane fillers to further improve the thermal stability of the CE. Carboranes are solvent blended at various mass loadings in the resin and cured to study their effect on thermal properties. TGA tests demonstrate that the final char content can be increased from 5% to as high as 75% for about 20% filler concentration.
The development of structure-property relationships will be discussed, as supported by SEM and DMA experiments. In further studies, embedding the carboranes through physical/ionic interactions with the cyanate esters might offer an interesting outlook. Also, incorporation of engineering thermoplastics with carboranes may yield a material with excellent thermal and mechanical properties.

5. **Formation of Micro-scale Graphitic Carbon Tubes via inverted Thermal Degradation (iTD)**

Paul Gregory (PI:Martin Thuo)

Abstract: Low cost paths to the formation of high value materials is an ever-expanding field. One such case is high value carbon in forms such as graphene or carbon nanotubes. The formation of such often requiring significant processing in both steps and time. Building from previous studies in the degradation of cellulosic material after chemi-sorbed surface modification, this work introduces the formation of high value carbon material via a simple, frugal, and quick process. Short cellulose fibers treated with alkyl-silanes create a self-assembled polymer on the surface that acts as a sacrificial thermal barrier. When rapidly degraded via high-temperature pyrolysis, the surface polymer limits degradation to the center of the fiber. This process creates high surface area, tube-like carbon microstructures.

6. **Conformational Dynamics in charge transport across self-assembled monolayers (SAMs) based molecular tunneling junctions**

Chuanshen Du (PI:Martin Thuo)

Abstract: The cyclohexane conformation shows great influence on the physical and chemical properties of cyclohexane, yet there exists very few simple method to determine the conformation. This study reports a method utilizing charge transport across self-assembled monolayers based tunneling junctions to study the conformational structure of certain cyclohexane molecules. By putting a cycloamide group on top of a alkanethiolate molecule, the dipole moment of the terminal group as well as the packing ability of the molecule changed significantly, resulting a major change in the charge tunneling behavior of the SAM formed. We uncovered that, with certain length of carbon chain supporting the cycloamide group, different conformation resulted in difference in charge tunneling ability of the SAM. We hypothesized that the change was partially due to the reduction in degree of freedom caused by the cycloamide group, thus comparative study using amide group in place of cycloamide group was also conducted.

7. **Solid State NMR Characterization of Inorganic Semiconducting Nanoparticles Surfaces**

Yunhua Chen (PI:Aaron Rossini & Javier Vela)

Abstract: Inorganic semiconducting nanoparticles (NPs) have gained much attention over past several decades due to their excellent optoelectronic properties. Since nanoparticles have comparatively higher surface area than bulk materials, surface structure and composition is crucial to their optical and electronic properties. However, it is very challenging to characterize surface structures as conventional structure analysis techniques such as microscopy (SEM, TEM, AFM, etc.), spectroscopy (IR, absorbance, Raman and XPS) and X-ray diffraction provide limited structural information. Here we show that solid-state NMR spectroscopy is ideal for probing surfaces. NMR interactions are sensitive to slight changes in the local environment around nuclei of interest. Here we use we use 13C-1H, 31P-1H, 113Cs-1H and 207Pb-1H 2D correlation NMR experiments to probe interactions of ligands with $CsPbBr_3$ nanoparticles. We also apply DFT calculations to model the structures of ligand-terminated nanoparticles and predict NMR observables such as chemical shifts.

8. **Block copolymer modified epoxy resins for additive manufacturing**

Liyang Shen (PI:Eric Cochran)

Abstract: The main objective of this project is to achieve direct-write 3D printing of epoxy resin. Block copolymer fillers are used as the reinforcing fillers as well as toughenners. The curing agents are determined based on curing kinetics to accommodate both printing and curing conditions. The printability of ink is investigated by rheological tests. The curing condition is verified by the fidelity of a cured part. The mechanical properties of the cured parts are examined by tensile, flexural and impact tests.

9. **Free energy calculation of superlattices**

Xun Zha (PI:Alex Travesset)

Abstract: I present simulations of hydrocarbon-capped monodisperse nanocrystal superlattices. I compute the free energy for both bcc and fcc, including several ligand lengths, as well as the entropy and Gibbs free energy. We find that bcc superlattices with oriented or random nanocrystal cores have slightly different free energy and lattice constant. Consistent with experimental findings, we observe that nanocrystals capped with relatively long ligands form bundles. We also compared our calculated lattice constants to experimental values and predictions for the OTM (Orbifold Topological Model).

10. **Dropwise Condensation on Multiscale Bioinspired Metallic Surfaces with Nanofeatures**

Dr. Daniel Attinger

Abstract: Nonwetting surfaces engineered from intrinsically hydrophilic metallic materials are promising for self-cleaning, anti-icing, or condensation heat transfer applications where the durability of commonly applied hydrophobic coatings is an issue. In this work, we fabricate and study the wetting behavior and the condensation performance on two metallic nonwetting surfaces with varying number and size of roughness tiers without the need for further hydrophobic coating procedure. On one hand, the surface resembling a rose petal exhibits a sticky nonwetting behavior as drops wet the microscopic roughness features with consequent enhanced drop adhesion, which leads to filmwise condensation. On the other hand, the surface resembling a lotus leaf provides super-repellent nonwetting behavior prompting the continuous nucleation, growth, and departure of spherical drops in a dropwise condensation fashion. The two different condensation behaviors reported are well supported by a drop surface energy analysis, which accounts for the different wetting performance and the surface structure underneath the condensing drops. This work offers a novel path for the design and manufacture of noncoated metallic super-repellent surfaces for condensation phase change applications, among others.

11. **In vitro Investigation of the Influence of Nano-cellulose on Food Digestion and Nutrient Absorption**

Lingling Liu (PI:Keith Vorst)

Abstract: The influence of three types of NC (nano-fibrillated cellulose (CNF)), TEMPO (2,2,6,6-tetramethylpiperidine-1-oxyl radical) oxidized CNF (TEMPO-CNF) & nano-crystalline cellulose (CNC) on food digestion and nutrient absorption as well as its behavior during gastrointestinal (GI) digestion were investigated by using a simulated in vitro digestion model consisting of salivary, gastric and intestinal phase. NC at high concentrations (0.5~1% CNF, 0.36% TEMPO-CNF and 2~4% CNC) reduced glucose diffusion, delayed lipid digestion and free amino nitrogen diffusion. Moreover, three types of NC showed different behaviors during digestion. In particular, CNF was morphologically stable, while TEMPO-CNF became aggregated and CNC formed hydrogels at the gastric phase. This study indicates that NC is advantageous than cellulose in the GI tract in terms of increasing digesta viscosity, delaying food digestion and nutrient absorption, and has potential to be used in the development of functional foods to control nutrient absorption and promote satiety.

12. **Kirigami-Inspired Materials for Adhesion Control**

DohGyu Hwang (PI:Michael D Bartlett)

Abstract: We developed reversible adhesives by controlling layouts of elasticity without creating microstructures. The fabrication is performed using the Japanese art of cutting, kirigami, allowing systematic programming of stiffness. This controls the spatial peeling resistance by a factor of ~100. The kirigami-inspired adhesive displays enhanced adhesion over homogeneous systems and strong directional characteristics in peeling by a factor of ~10. This provides strategies to develop high capacity, easy release adhesives for medical and household applications. This advance is important in new adhesion control tools for bio-monitoring bandages for biomedical applications. Medical adhesives removal caused 1.5 million traumatic injuries in the US. Fragile skin of senior citizens, infants and diabetic patients are susceptible to skin tearing. The adhesive we developed controls peeling by spatial distribution of elasticity. This enables development of smart adhesives with high adhesion and easy release capacity that adhere to skin without causing damage when released.

13. **Morphology Evolution in Seeded Emulsion Polymerization and Coating Applications**

Yifan Li (PI:Shan Jiang)

Abstract: Novel morphologies of polymeric nanoparticles can significantly change the fundamental assembly structures and improve industrial applications such as coating materials, construction chemicals and cosmetics. However, controllable and scalable production of the polymer nanoparticles with various morphologies and functionalities remains a significant barrier to their broad applications. In this work, we explored different reaction conditions and developed a synthetic platform based on emulsion polymerization to engineer polymeric nanoparticles with complex morphologies, including the anisotropic dumbbell morphology. With the assistance of computer simulation and theoretical modeling, we further elucidated the mechanisms of the shape evolution and provided novel approaches to produce and control hierarchical polymeric nanoparticle morphologies. Furthermore, we demonstrate the colloidal stratification of amphiphilic Janus nanoparticles and their application as multifunctional coatings.

14. **Oxyanion Hydrogenation over Binary Metal Phosphides**

Lin Wei (PI:Javier Vela)

Abstract: Oxyanion pollution in drinking water is becoming a public health threat due to the growth of human activity. Hydrogenation is one of the most state-of-the-art technologies for oxyanion removal. However, a majority of available catalysts for hydrogenation employ scarce and expensive noble metals (Pd, Pt, Ru), limiting their utility and potential for large-scale deployment. In this study, we investigate a binary metal phosphide catalyst to hydrogenate oxyanion under a continuous H2/Ar flow. We are able to recover and recycle the catalyst multiple times maintaining major activity. Control experiments show there is no reduction without metal phosphide catalyst. Residual activity is observed without H2 when catalyst is present. To study possible intermediates, alternative substrates are also tested.

15. **Toughening PLLA with Block-Copolymer Self-Assembly**

Baker Kuehl (PI:Dr Eric Cochran)

Abstract: Poly(L-lactide) (PLLA) is a biodegradable polymer that demonstrates high strength. However, PLLA is very brittle and unsuitable for high impact strength applications unlike petroleum-based plastics such as ABS (Acrylonitrile Butadiene Styrene). In order to compensate for these undesirable traits, poly(n-butyl acrylate) (PNBA), a rubbery phase, can be blended into the PLLA matrix in order to increase the elongation of PLLA. Generally, polymers are immiscible so a compatibilizer must be used to increase the interfacial adhesion, the adhesion where the interfaces between the phases or components are maintained by intermolecular forces, chain entanglements, or both, across the interfaces, of the rigid matrix with the rubbery dispersed phase. A diblock copolymer of PLLA-b-PNBA can be synthesized to increase the miscibility of the PLLA and PNBA homopolymers by promoting self-assembly inside of the PLLA matrix. Ideally, the PLLA-b-PNBA will microphase separate into cylindrical micelles providing improved impact resistance and elongation.

16. **3D Printing and Characterization of Hydroxypropyl Methylcellulose and Methylcellulose for Biodegradable Support Structures**

Yiliang Cheng (PI:Xiaolei Shi)

Abstract: The currently available support materials used with 3D printing technology have challenges of poor dissolvability in chemical solution and difficulty to be removed from the finished part. Current support materials are usually petroleum based which has a negative impact on the environment. The goal of the project is to identify a suitable biomaterial for support structures that will eliminate the challenges of poor dissolvability and toxic waste generated by the current material. In this study, three biodegradable cellulose derivatives of methylcellulose (MC) and hydroxypropyl methylcellulose (HPMC), with different degree of substitution of hydroxyl group were used. We investigated the effect of concentrations (8, 10, and 12% w/v) of various cellulose derivatives on the rheological properties for understanding their printability. The rheological analysis revealed that all hydrogels exhibit shear-thinning properties with relatively low yield stress. Effects of printing parameters (extrusion rate, nozzle diameter, and printing speed) were optimized to obtain the desired three-dimensional structures.

17. **Tuning the Optical Properties of Silicon Nanosheets via Surface Halogenation**

Utkarsh Ramesh (PI:Matthew Panthani)

Abstract: Silicon nanosheets (Si NSs) have emerged as a promising candidate for next generation optoelectronics due to the prevalence of silicon in present electronics architecture. One method of tuning the optical properties of these sheets has been to vary the surface termination of the sheets. Herein, we present preliminary data towards halogenating the surface of the Si NSs using chemistry contemporary to silicon wafers, with changes in optical properties being monitored via photoluminescence (PL). Fourier transform Infrared spectroscopy (FTIR) and X-Ray photoelectron spectroscopy (XPS) are used to probe the effects of the reactions of the sheets and to determine extent of halogenation. Finally, temperature dependent PL of a brominated sample is shown to study the effects of temperature on PL and to determine if any meaningful trends are observed.

18. **How to (not) do Poor Microanalysis of Nanomaterials**

Warren Straszheim (PI:)

Abstract: With the continuing emphasis on micro- and nano-materials, scanning electron microscopy (SEM) remains a primary tool for characterizing them. However, nano-materials push SEM to its limits. It is no longer enough to use techniques learned in an introductory microscopy course and expect to get good results. Researchers are encouraged to consider what their samples should be expected to look like given their material's properties and the physics. They need to deal with resolution limits, interaction volume, contamination, peak overlaps, statistics and more in order to get decent results. The equipment and experienced staff at MARL is positioned to help with these difficult cases. They have pushed the limits for years as they served researchers looking at progressively smaller materials. Several examples will be given of how to and how not to characterize micro- and nano-materials.

19. **Fabrication of a coatless superhydrophobic on 7075 Aluminum Alloy surface by using Nanosecond Laser Followed by Simple Heat Treatment.**

Faez Qahtani (PI:pranav shrotriya)

Abstract: Creating the superhydrophobic surface on the metal's surface has gotten the researcher attention for over a decade. Issues such as stability and sustainability were the main concerns to fulfill the applicability in sites. It is the time to move towards making alternatives and study the factors that contributed to these issues. This poster is presenting a new method of creating a coatless superhydrophobic surface on Aluminum Alloy. The way begins by using nanosecond laser followed by post-process annealing at low temperature in the presence of the ethanol inside the oven. The water contact angle measurements before and after the heat treatments process recorded. The areas irradiated at higher fluence showed a superhydrophobic behavior after the annealing process. Ten days after the annealing process, the contact angle remained the same for sample 1 and changed at sample 2. The SEM and EDS for topography and chemical composition used for further investigation.

20. **Materials Analysis and Research Laboratory: A core material characterization facility at Iowa State University**

Dapeng Jing (PI:Warren Straszheim)

Abstract: The Materials Analysis and Research Laboratory (MARL) of the Iowa State University Office of Biotechnology is open to faculty and students from the university, other educational institutions, and industry scientists. The laboratory emphasizes materials characterization utilizing scanning electron microscopy (SEM), energy-dispersive x-ray spectroscopy (EDS), x-ray diffraction (XRD), x-ray fluorescence (XRF), x-ray photoelectron spectroscopy (XPS), thermal analysis (SDT, TGA) and light microscopy.

MARL's function is three-fold, namely research and development, teaching, and service. Its facilities are used for chemical and physical characterization of a wide variety of materials to support research and teaching programs within the university. MARL also conducts research on unusual material evaluation problems for outside agencies and undertakes analyses for industry when comparable facilities are not available.

21. **Synthesis of Intermetallic Compounds from Heterobimetallic Single-Source Precursors**

Carena Daniels (PI:Javier Vela)

Abstract: Intermetallics are atomically ordered structures of two or more different transition or main group metals. The unique crystalline structure of these compounds, different from structures of the constituent elements, has enhanced activity for many types of catalysis. Intermetallics have been typically synthesized through high-temperature solid state methods, but recently low temperature soft chemical methods have been developed for better synthetic control. These methods, such as the modified polyol and 'ship-in-a-bottle' methods, have helped advance the study of intermetallics but still face challenges such as phase segregated products and long, multi-step syntheses. Demonstrated here is the use of heterobimetallic complexes as single source precursors to a variety of 10-15 and 11-15 binary intermetallics. This is a highly versatile approach, due to both the coordination environment of the precursor and the reaction temperature having an effect on the intermetallic phase produced. Also shown is the application of a recently developed plasma processing technique to remove graphitic carbon that was observed on the surface of some products. The versatility of this single-source precursor approach makes it an important addition to previously used methods toward the research and development of catalytically active intermetallics.

22. **Laser-induced graphene for foodborne pathogen detection**

Cicero C. Pola (PI:Carmen Gomes)

Abstract: Traditional methods for foodborne pathogen detection are either time-consuming, expensive, or require highly trained technicians. Graphene-based electrochemical biosensors are a promising alternative for point-of-service detection of foodborne pathogens, especially due to graphene's high electrical conductivity, high mechanical strength, and biocompatibility. Laser-induced graphene (LIG) is a direct-write method for electronic devices fabrication where a CO2 laser converts a precursor substrate into graphene by changing the carbon hybridization. Herein, LIG electrodes were developed and evaluated according to their potential for pathogen detection. LIG presented resolution of 95 μm and a highly electroactive surface. Raman spectroscopy suggested the presence of edge plane defects on LIG carbonic structure, which associated to the superficial oxygen groups indicated by XPS increases the sites for antibody immobilization. LIG electrodes were able to sense Salmonella Typhimurium in a range of 10–200 CFU/mL within 18 minutes, confirming its potential as a biosensor for future application in food products.

23. **Stability enhancement in layered cesium lead iodide perovskites**

Atefe Hadi (PI:Matthew Panthani)

Abstract: Lead (Pb) halide perovskites with high efficiency, low cost, and simple processing have gained a lot of attention in photovoltaics. However, their instability upon exposure to operating conditions and presence of toxic solvents in the thin film fabrication process pose challenges to their commercialization. In this work, we addressed the stability by reducing the dimensionality of CsPbI3 perovskites by implementing bulky organic cations, which results in the formation of layered halide perovskites. We showed that the presence of additive solvents with strong complexation to Pb atoms is necessary to improve the crystallinity and monodispersity in thin films. The long term stability of these films and their parallel orientation to the substrate suggest potential utilization in electronic devices such as FETs. To address solvent toxicity, we fabricated MAPbI3 by melting and spreading 2D perovskites, which were then exposed to methylammonium iodide via solid state reactions.

24. **Developing a method for isolating hollow-core elastomeric vesicles**

Tung-ping Wang (PI:Eric W Cochran)

Abstract: Present work developed a method to isolatae hollow-core polymeric vesicles prepared from polymer blend. The poly(isoprene-b-simethylsiloxane) (PI-b-PDMS) di-block copolymer was used as vesicle formation polymer. The PI-b-PDMS was first blending with PDMS homopolymer as matrix, then the PI block was crosslinked by thermal curing. The PDMS matrix in the mixture was separated by dialysis to prepared isolated hollow-core vesicles. TEM and SAXS were used to investigate the morphology of samples at different steps. Dynamic light scattering measurement of as-blended and as-crosslinked samples dispersed in tetrahydrofuran provided the evidence of vesicles were able to be crosslinked by thermal crosslinking. Energy disperse spectroscopy analysis indicate present work successfully removed the PDMS matrix from the core of vesicles. We also mixed isolated hollow-core vesicles as fillers with crosslinkable PDMS matrix to evaluate the possibility of using the method provided from present work for future application on providing porous polymer or other potential applications.

25. **Reliability Analysis of 3D Surface Measurement Data of Additive Manufactured Parts Based on Optical Metrology**

Xiao Zhang (PI:Hantang Qin)

Abstract: Surface topography and surface finish are significant factors when evaluating the quality of products in additive manufacturing (AM). AM parts are fabricated layer by layer, which is quite different from traditional formative or subtractive methods. Despite rapid progress in additive manufacturing and associated optical metrology for quality control and in-situ monitoring, limited research has been conducted to investigate the reliability of 3D surface measurement data. The surface topologies portrayed by multiple optical systems demonstrated significant differences due to varying sampling mechanisms, resolutions, system noises, etc. When extracting data from 3D surface measurements as quality assurance or feedback control parameters, the fundamental question must be answered: are the 3D datasets trustworthy? In this paper, we set up new standards to evaluate reliability 3D surface measurement data and analyze the variation in the topographical profile. In this work, two non-contact optical methods based on Focus Variation Microscopy and Structured Light System were adopted to measure the surface topography of the target components.