



Meeting Program

Nano@IAState 2017 - Thursday, July 27, 2017
Iowa State University, Memorial Union

•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:

The Startup Factory, Iowa State University Research Park, The Ames Laboratory, ISU VP Economic Development, The College of Engineering, The College of Liberal Arts and Sciences, The Department of Materials Science and Engineering, The Department of Chemistry, The Department of Chemical and Biological Engineering.

•Presentation Information

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 after the first coffee break in the MU Sun Room. Please bring your posters in the morning so that you can hang them up early.

•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

•Meeting Venue

The meeting will take place on the **second floor of the Memorial Union (MU)**. Paid parking is available in the MU parking facility. Alternatively, complimentary ISU visitor parking passes valid for gold lots on campus can be obtained at:

<https://apps-parking.sws.iastate.edu/visitor-permits/>

- Conference badges will be available for pickup in the West Lobby outside of the MU South Ballroom. Light breakfast will be provided from 7:45 to 8:10 in the MU South Ballroom.
- All Oral presentations will take place in the MU Southern Ballroom.
- Lunch will take place in the Oak Room and Durham Great Hall.
- The cocktail hour/poster session will take place in the Sun Room.



•Conference Program and Speaker List

All oral presentations will take place in the MU South Ballroom.

Time	Event/Talk Title	Presenter
7:45	Registration/Badge Collection - Light Breakfast Provided (MU West Lobby/South Ballroom)	
	Oral Presentations (MU South Ballroom)	
8:10	Opening Remarks	
8:15	Plenary Lecture 1: Self-assembly and Stability of Metallic Nanoclusters	Prof. James Evans
8:45	Plenary Lecture 2: Nanotechnology for Gene/Vaccine Delivery and for Biomineralization	Prof. Surya Mallapragada
9:15	Deformation Processed Al/Ca Nano-filamentary Composite Conductors After Conversion to Intermetallic Phase	Charlie Czahor
9:30	Modular Hydrolytic Enzyme Activity Sensor with Substrate-Wrapped Single Walled Carbon Nanotubes	Nathaniel Kallmyer
9:45	Flow Instability Model of Porous Anodic Oxide Formation	Pratyush Mishra
10:00	Role of Nanoparticle Interactions in Supercrystal Self-Assembly	Nathan Horst
10:15 - 10:45	Coffee Break – Light Refreshments - (South Ballroom) Poster boards available (Sun Room)	
	Oral Presentations (MU South Ballroom)	
10:45	Unusual infrared absorption increases in photo-degraded organic films	Satvik Shah
11:00	Silicon Nanocrystal Surfaces Characterized by Multidimensional Solid-State NMR Spectroscopy	Michael Hanrahan
11:15	Nano-optical studies of exciton polaritons in MoSe ₂ waveguides	Fengrui Hu
11:30	Development of Germanium–Tin/Cadmium Sulfide Core/Shell Nanocrystals with Enhanced Near-Infrared Photoluminescence	Brett Boote
11:45	Characterization of Catalytic Materials by Conventional and DNP-Enhanced Solid-State NMR Methods	Zhuoran Wang
12:00	State-of-the-Art Atomic Resolution Characterization Capabilities at the Sensitive Instruments Facility	Lin Zhou
12:15 - 1:15	Lunch – Boxed Lunches (Durham Great Hall and Oak Room)	

	Oral Presentations (MU South Ballroom)	
1:15	Synthesis and Fabrication of Janus Nanoparticles	Kyle Miller
1:30	Solution Phase Synthesis of Filled Tetrahedral Semiconductors: Polytypism, Coloring, and New Opportunities for Enhanced Thermoelectrics	M. Arthur White
1:45	Heat-free processing and low-power additive manufacturing of metallic products through Metastable Material states	Andrew Martin
2:00	Acoustophoretic Platform for High-Throughput Self-Assembly	Meghana Akella
2:15	Creating porous thin films using nanoscale grains	Xinchun Tian
2:30	Thermal Reffusivity of Materials: 0 K-limit and uncovered structure domain size	Bowen Zhu
2:45 - 3:05	Coffee Break (MU South Ballroom)	
	Oral Presentations (MU South Ballroom)	
3:05	Molecular Dynamics Simulations of Diffusion of Chloride Ions in Nano-Pores of Hydrated Cement Paste	Shahin Hajilar
3:20	Theoretical study of water effect on carbinolamine formation with mesoporous silica nanoparticle	Yu Lim Kim
3:35	Dual Delivery Nanoscale Device for miR-345 and Gemcitabine Co-Delivery to Treat Pancreatic Cancer	Metin Uz
3:50	ex vivo Study of Telluride Nanowires in Minigut for Defending Against Photothermal Irradiation	Yijun Qi
4:05	Fabrication and Evaluation of Poly (lactic acid)/Chitosan/Tricalcium Phosphate Biocomposites for Guided Bone Regeneration	Srikanthan Ramesh
4:20	Special Presentation: Connecting Researchers and Companies	Steve Carter (President ISU Research Park)
4:35 – 6:30	Poster Session and Cocktail Hour – Complimentary Drink Tickets and Food Provided (MU Sun Room)	

A complete list of abstracts is provided on the subsequent pages.

•Poster Presentations

Posters will be presented from 4:35 to 6:30 pm in the MU Sun Room.

Poster Number	Poster Title	Presenter
1	In-Field, Disposable Soil Sensor for Monitoring Pesticide Levels via Laser Annealed Graphene Electrodes	John Hondred
2	Imaging the localized plasmon resonance modes in graphene nanoribbons	Yilong Luan
3	Thermolysis of Heterobimetallic Single-Source Precursors: A Springboard to the Synthesis of Binary Intermetallics	Carena Daniels
4	Melt Processing of Hybrid Organic-Inorganic Metal Halide Perovskite Thin Films for Photovoltaic Devices	Matthew I. Milot
5	Germanium–Tin/Cadmium Sulfide Core/Shell Nanocrystals with Enhanced Near-Infrared Photoluminescence	Himashi Andaraarachchi
6	USING DIP-PROCESSING TO PROMOTE CATION EXCHANGE IN MELT-PROCESSED LEAD AND TIN BASED PEROVSKITES	Madeleine Wilsey
7	Experiments for the Purpose of Synthesizing a Silicon, Germanium, and Tin Chemical Alloy	Bevan Whitehead
8	Solvated-Electron Initiated Rapid Polymerization at Ambient-Temperature: A case of Monomer Solubility	Boyce Chang
9	The effect of smoothing electrodes on tunneling behaviors across large area molecular junctions	Jiahao Chen
10	Tuning surface morphology of liquid metal particles via thermal treatment	Joel Cutinho
11	Pd/CeO ₂ Inside Silica Mesopores: Synthesis, Characterization & Catalytic Activity	Pranjali Naik
12	Synthesis of meso-porous oxides from In based Coordination Polymers	Paul Karanja
13	Nitrogen-doped ordered mesoporous carbon(N-OMC): Synthesis, Characterization and Catalysis	Bosky Parikh
14	Size controlled intermetallic compounds for electrocatalysis	Zhiyuan Qi
15	Lead-Free Germanium Perovskites: Synthesis, Size Control and Manganese Doping	Long Men
16	Characterization of LiZnP Nanoparticles by Advanced Solid-State NMR Spectroscopy	Amrit Venkatesh
17	Yield and fluorescence behavior of noncovalently functionalized single-walled carbon nanotubes	Nathaniel Kallmyer

18	Recent progress in thermoelectric nanocomposites based on solution-synthesized nanoheterostructures	Wei Zheng
19	Heterogeneous catalysis by metal nanocluster encapsulated in Metal-Organic Framework	Jason Goh
20	Pair Interactions of Hydrocarbon-capped Nanoparticles: Effect of Chain Conformations	Curt Waltmann
21	Role of Many Body Effects in Self Assembly of Hydrocarbon Capped Nanoparticles	Tommy Waltmann
22	Synthesis and surface functionalization of Group IV Quantum Dots	Yujie Wang
23	Materials Analysis and Research Laboratory: A core material characterization facility at Iowa State University	Dapeng Jing
24	A Theoretical Investigation of Gas phase X-Au-X (X = S, Cl, CH ₃ S, SiH ₃ S) Complexes and Complexes on Au(111) Surface	Jiyoung Lee
25	Synthesis of Polymeric Janus Nanoparticles Using Emulsion Polymerization	Serkan Demirci
26	Process engineering of pure phase quasi-2D layered CsPbI ₃ perovskite thin film for solar cell application	Atefe Hadi
27	Solution-Based Synthesis of Cesium Bismuth Iodide Nanocrystals	Rainie Nelson
28	Refractive Index/Intensity Based Optical Gaseous/Aqueous Sensors	Shawana Tabassum
29	Photoluminescence enhancement of quantum dots in solution coupled to plasmonic gold nanocup arrays	Akshit Peer
30	Vibration-Driven Assembly of Polymer-Nanopowder Composites	Soheila Shabaniverki
31	Assembling gold nanoparticles in polymer gels	Srikanth Nayak
32	Control and Quantification of Local Polarity in Nano-confined Systems	Dilini Singappuli-Arachchige
33	Synthesis and Characterization of Bismuth Halide Perovskite Thin-Films	Umar Hamdeh

A complete list of abstracts is provided on the subsequent pages.

Abstracts for Oral Presentations

Self-assembly and Stability of Metallic Nanoclusters

Jim Evans, Physics/Chemistry/Ames Laboratory

Abstract: Self-assembly of nanoclusters from mobile precursors, either on smooth surfaces or in the solution-phase, provides an efficient route to synthesis of functional nanostructures for applications to catalysis, plasmonics, etc.. An extraordinary diversity of shapes, composition profiles, and structures (leading to broad tunability of properties) reflects the feature that these processes often occur far-from-equilibrium. However, control of these structures depends on understanding the fine details of relaxation of mobile precursors once they are in the aggregated state. Integrated experimental and modeling studies have the potential to provide this understanding. A separate issue is that nature dislikes nano in that nanoclusters are intrinsically unstable. Thus, assessment of metastable lifetimes is also important for functionality.

Nanotechnology for Gene/Vaccine Delivery and for Biomineralization

Surya Mallapragada, Chemical and Biological Engineering

Abstract: We have synthesized a family of self-assembling pH and temperature sensitive multiblock cationic and anionic copolymers with a variety of nanoarchitectures. The copolymers exhibit pH sensitivity and thermoreversible gelation at physiological temperatures and self assemble across multiple length scales from the nanoscale to the macroscale. The cationic multiblock copolymers exhibit complexation with oligonucleotides and serve as excellent delivery vectors for cancer therapies. In addition, these polymer gels can serve as adjuvants for protein-based subunit vaccines and enhance the immune response. The anionic multiblock copolymers and their micelles also serve as templates for biomineralization. These hierarchically self-assembling copolymers, in conjunction with mineralization proteins/peptides, form bioinspired self-assembled nanocomposites. These injectable insitu-forming nanocomposites show mechanical properties similar to that of native cartilage, and are being investigated for cartilage rescue to prevent post-traumatic osteo-arthritis.

Deformation Processed Al/Ca Nano-filamentary Composite Conductors After Conversion to Intermetallic Phase

Charlie Czahor, PI: Iver Anderson, Ames Lab

Abstract: Efficient long-distance power transmission is necessary as the world integrates renewable energy sources that are often cited in remote areas. Conventional aluminum-conductor steel-reinforced (ACSR) cables are not well suited for high-voltage direct current (HVDC) transmission, the preferred technology for long distances. Deformation processed Al/Ca composite conductors are lighter, stronger, and more conductive than ACSR with potential to reduce electrical losses, lower costs, and enhance grid reliability. Atomized aluminum and calcium powders were mixed, die compacted, and indirectly extruded at elevated temperature, then wire drawn giving calcium nano-filamentary reinforcement. Preliminary results show Al/Ca conductors offer superior strength without a heavy and highly resistive steel core. Further experiments will be reported that prove the effectiveness of converting the nano-filamentary material to Al₂Ca intermetallic by annealing. Microstructure, strength, and conductivity will be analyzed with the expectation that high temperature performance will be improved. Work funded by USDOE-OE program through Ames Lab contract DE-AC02-07CH11358.

Modular Hydrolytic Enzyme Activity Sensor with Substrate-Wrapped Single Walled Carbon Nanotubes

Nathaniel Kallmyer, PI: Nigel F Reuel, Chemical and Biological Engineering

Abstract: Hydrolytic enzymes are a topic of continual study and improvement due to their industrial impact and medical implications; however, the measurement of their activity is limited to an established few enzymes and often involves measurement of secondary byproducts or design of a complex degradation probe. Herein we detail a modular single walled carbon nanotube (SWNT) sensor that is straightforward to produce and measure. The enzyme substrate is used to wrap and solubilize the hydrophobic nanotubes. When the hydrolytic enzyme encounters the wrapped substrate, the wrapping is degraded and their fluorescence is quenched. Thus, the change in fluorescence can be used to quantitatively measure hydrolytic enzyme activity. We have demonstrated functionality with protein, polysaccharide, and oligosaccharide substrates. We use an established trypsin assay to correlate these rates with standard techniques. Furthermore, we measure the effect of freeze-thaw cycles and elevated temperature on cellulase activity. Finally, we show how hydrolytic activity of cellulase could be rapidly optimized by generating a response surface of cellulase activity.

Flow Instability Model of Porous Anodic Oxide Formation

Pratyush Mishra, PI: Kurt Hebert, Chemical and Biological Engineering

Abstract: Porous anodic oxide (PAO) films are formed by the electrochemical oxidation of reactive metals. For certain applied voltages and solutions, anodizing produces films with spontaneously ordered arrangements of cylindrical pores, which have been explored extensively as functional materials. Experimental studies have suggested that oxide flow plays an important role in the growth of porous anodic oxide films on reactive metals. Here a mathematical model for anodic oxide formation is presented that includes viscous flow of oxide, coupled with electrical migration of metal and oxygen ions and interfacial reactions. Linear stability analysis of the model shows that pattern formation at the solution interface occurs near the critical value of a parameter expressing competition between stabilizing electrochemical oxide formation and destabilizing flow. The parameter value is quantitatively consistent with experiment. The scaling ratio of pore separation to voltage, as characteristically of anodic films, is predicted by the wavelength at the critical point.

Role of Nanoparticle Interactions in Supercrystal Self-Assembly

Nathan Horst, PI: Alex Travesset, Materials Science and Engineering

Abstract: Many successful strategies are available for the programmable self-assembly of nanoparticle superlattices, where inorganic nanocrystallites are “functionalized” with organic chains, whose properties drive the self-assembly process. The phase diagram of these systems has long been rationalized by borrowing results from hard-sphere packing models, as a clear correlation exists between the maximum of the packing fraction of hard spheres and experimentally discovered superlattice equilibrium phases. However, the organic components of these systems are flexible, which leads to clear deviations from the sphere packing model. We have developed theoretical and computational models that address these systems, and have incorporated them into a comprehensive software package by which we can quickly investigate features of these systems. Using the results of our models, we present our investigation on interactions of functionalized nanoparticles, where we show that we are able to rationalize the entirety of the experimental phase diagram.

Unusual infrared absorption increases in photo-degraded organic films

Satvik Shah, PI: Vikram L Dalal, Microelectronics Research Center

Abstract: Degradation is among the most pressing problems facing organic materials, occurring through ingress of moisture and oxygen, and light exposure. We determine the nanoscale pathways underlying degradation by light-soaking organic films in an environmental chamber, and performing infrared spectroscopy, to identify atomic bonding changes. We utilize as a prototype the low band gap PTB7-PCBM blend. Films light-soaked in the presence of oxygen show unusual increased absorption at 1727 cm^{-1} attributable to increased C[double bond, length as m-dash]O modes, and a broad increase at 3240 cm^{-1} attributable to hydroxyl (O–H) groups bonded within the organic matrix. Films exposed to oxygen in the dark, or light-soaked in an inert atmosphere, do not exhibit significant absorption changes, suggesting simultaneous exposure of oxygen and light that creates singlet excited oxygen is the detrimental factor. Our ab initio electronic structure simulations interpret these by oxidation at the α -C site of the alkyl chains in PTB7, with an irreversible rupture of the alkyl chain and formation of new C[double bond, length as m-dash]O and C–O–H conformations at the α -C. Infrared spectroscopy coupled with ab initio simulation can provide a powerful tool for quantifying photo-structural atomic bonding changes. Understanding nanoscale light-induced structural changes will open avenues to designing more stable organic materials for organic electronics.

Molecular Structure of Silicon Nanocrystal Surfaces Characterized by Multidimensional Solid-State NMR Spectroscopy

Michael Hanrahan, PI: Aaron Rossini, Chemistry

Abstract: The chemical and photophysical properties of silicon nanocrystals (Si NCs) are strongly dependent on the chemistry and structure of their surfaces. Here we use fast magic angle spinning (MAS) and proton detection to enable the rapid acquisition of dipolar and scalar 2D 1H - 29Si heteronuclear correlation (HETCOR) solid-state NMR spectra and determine the structure of hydride-terminated and alkyl-functionalized Si NC surfaces. We show that proton-detected scalar 1H - 29Si refocused INEPT experiments can be used to unambiguously differentiate signals from different surface hydrides allowing populations of the different surface hydrides to be quantified. This analysis confirms that monohydride species are the predominant surface species on the as-synthesized, plasma-grown Si NCs. A reduction in the populations of the di- and trihydrides is observed upon functionalization with alkyl groups, consistent with previous hypothesis that the trihydride (silyl) group is primarily responsible for initiating surface functionalization reactions.

Nano-optical studies of exciton polaritons in MoSe₂ waveguides

Fengrui Hu, PI: Zhe Fei, Physics & Astronomy

Abstract: We performed systematic nano-optical studies of exciton-polaritons in MoSe₂ planar waveguides by scattering-type scanning near-field optical microscope (s-SNOM). By imaging and analyzing the polariton interference fringes, we found that these polariton modes could travel over tens of microns with a wavelength down to a few hundred nanometers. Furthermore, we were able to map the entire dispersion of polaritons that shows a back-bending behavior close to the exciton energy. All above observations are consistent with our mode calculations and modeling. (References: F. Hu et al. "Imaging exciton-polariton transport in MoSe₂ waveguides". Nature Photonics (2017))

Development of Germanium–Tin/Cadmium Sulfide Core/Shell Nanocrystals with Enhanced Near-Infrared Photoluminescence

Brett Boote, PI: Emily Smith, Chemistry

Abstract: Ge_{1-x}Sn_x alloy and Ge_{1-x}Sn_x/CdS core/shell nanocrystals (6 to 13 nm) were prepared via solution-phase synthesis and their size, composition, and optical properties were characterized. Raman spectroscopy is a useful characterization technique for inorganic nanocrystals as the effects of alloy composition and interfacial strain can be quantified. Using Raman spectroscopy and other techniques such as X-ray diffraction, electron microscopy, FT-IR, and X-ray photoelectron spectroscopy, the nanocrystal synthesis was optimized and the prepared Ge_{1-x}Sn_x/CdS nanocrystals exhibit up to 15x photoluminescence enhancement over Ge/CdS nanocrystals with a pure Ge core. This is most likely due to more effective surface passivation by the CdS shell as a result of improved epitaxy (smaller lattice mismatch). With enhanced photoluminescence in the near-infrared, Ge_{1-x}Sn_x/CdS core/shell nanocrystals might be useful alternatives to other materials for energy capture and conversion applications and as imaging probes.

Characterization of Catalytic Materials by Conventional and DNP-Enhanced Solid-State NMR Methods

Zhuoran Wang, PI: Marek Pruski, Chemistry Department / Ames Lab

Abstract: Characterization of atomic-scale structures of heterogeneous catalysts is the key step toward understanding the catalytic mechanisms and rational design of improved catalysts. Solid-state (SS)NMR is recognized as one of the most powerful tools for this task, however, the technique is inherently insensitive due to low natural abundance, low gyromagnetic ratio and low concentration of nuclei of interest. Various advances have been recently made to boost NMR's sensitivity, including indirect detection under fast magic angle spinning (MAS) and dynamic nuclear polarization (DNP). By developing and applying these techniques, we derived important structural information about a variety of supported catalysts. We will show examples of multinuclear SSNMR studies of several catalytic systems prepared in the Ames Laboratory Catalysis Program.

State-of-the-Art Atomic Resolution Characterization Capabilities at the Sensitive Instruments Facility

Lin Zhou, PI: Matt Kramer, Ames Laboratory

Abstract: The Sensitive Instruments Facility (SIF) was completed in 2016 and is now fully functional. The facility houses four state of the art electron beam instruments that bring a plethora of new characterization capabilities to Iowa State University. These include scanning and transmission electron microscopy techniques that will enable atomic-level quantification of chemistry, crystallography, defects, electric and magnetic field imaging, as well as a wide range of in situ and in operando studies. This talk will briefly introduce a number of techniques and their applications. Topics will include atomic resolution imaging, energy dispersive and electron energy loss spectroscopy, Lorentz imaging, tomography etc.. Specialized stages allow for applying a range of external fields to samples while acquiring images or chemistry simultaneously. The specialized holders include cooling, heating, liquid cell and strain and electric biasing on a variety of samples.

Synthesis and Fabrication of Janus Nanoparticles

Kyle Miller, PI: Shan Jiang, Materials Science and Engineering

Abstract: Janus particles have shown interesting assembly behaviors and great potential in applications. However, it remains challenging to synthesize and fabricate Janus particles in nanometer size range. In our lab, we have developed both top down and bottom up strategies of obtaining Janus particles with desired morphology and material chemistry. Details of Janus particle formation and areas of future opportunity will be discussed.

Solution Phase Synthesis of Filled Tetrahedral Semiconductors: Polytypism, Coloring, and New Opportunities for Enhanced Thermoelectrics

M. Arthur White, PI: Javier Vela, Chemistry

Abstract: Ternary filled tetrahedral semiconductors comprised of group I, XII, and V elements have attracted considerable attention as energy materials and viable replacements for cadmium containing semiconductors. We report the first solution phase synthesis of these ternaries using the model compound LiZnP. The synthesis is quite flexible with various Li, Zn, and P precursors able to be used successfully. Furthermore, this method was extended to the interesting thermoelectric compound LiZnSb. LiZnSb samples prepared in solution display cubic symmetry despite prior literature only reporting the hexagonal polytype. Along with rationalization for the observed polytypism, transport property calculations find LiZnSb to be an extremely promising thermoelectric material with a zT value of > 1.5. The samples reported have been characterized with a wide range of techniques including X-ray diffraction, optical absorption, transmission electron microscopy, X-ray photoelectron spectroscopy, and nuclear magnetic resonance to confirm their identity and probe their mechanism of formation.

Heat-free processing and low-power additive manufacturing of metallic products through Metastable Material states

Andrew Martin, PI: Martin Thuo, Materials Science and Engineering

Abstract: Metals have led to significant technological advances, hence processing technologies are well developed. Recent advances in soft and composite platforms calls for non-traditional metal processing and manufacturing methods. Frustrating thermodynamic relaxation can, potentially, be used to overcome high energy demands and, hence, incompatibility in mixed material processing. We recently demonstrated high yield synthesis of undercooled metal particles by using core-shell architecture to frustrate solidification. Herein, we demonstrate application of this frustrate metal state as a pathway to low-energy processing and manufacturing. The solvent-free metal particles were formed using powder processing techniques, dry pressing, mechanical rolling, and low-laser power additive manufacturing. Using suspended undercooled metal particles; direct-write, screen printing, ink-jet printing, and chemical sintering were used to form 2D and 3D structures. This demonstrates that metastability in materials can be used to mitigate high energy demands in processing.

Acoustophoretic Platform for High-Throughput Self-Assembly

Meghana Akella, PI: Jaime Juarez, Mechanical Engineering

Abstract: This talk presents the continuous, high-throughput assembly of colloidal crystals in an acoustofluidic device fabricated with off-the-shelf components. Our technique does not require clean room access and costs approximately \$20 per device. Optical video microscopy shows that hydrodynamics and acoustic compression both play a role in tuning crystal microstructure. Highly ordered crystals are assembled at a rate of more than 100 particles per second. We observe grain-boundary defects arise from hydrodynamically formed slip planes. Cross-channel density distributions of particle illustrate the effect that acoustic compression has on crystal formation. Hexagonal close-packing is experimentally quantified and compared to a model for hexagonally close-packed spheres. Micro-particle image velocimetry data is used to quantify the effect of fluid flow and acoustic trapping on the ensemble. Future work will focus on the viability of this approach for nanomanufacturing of colloid-based materials for photonics, sub-diffraction limited imaging and battery templates.

Creating porous thin films using nanoscale grains

Xinchun Tian, PI: Dr. Ludovico Cademartiri, Materials Science and Engineering

Abstract: Random packing of grains, such as in soils and biological tissues, represents one of the mostly adopted strategies by nature to create porous structures. In this project, we use the same idea to make mesoporous thin films with HfO₂ nanorods (<20 nm) as building blocks. Preparation of mesoporous HfO₂ is still challenging. Here, colloidal HfO₂ nanorods capped with organic ligands are synthesized with well-controlled size, shape, and high crystallinity. These units are spin-coated onto desired substrates forming disordered, uniform thin films. Room temperature plasma is chosen to remove ligands and leave a clean surface without sintering. Ion beam analysis, Ellipsometry, and X-ray reflectometry confirmed ~50% porosity of the processed thin films. The equivalent pore diameter is ~5 nm as determined by absorption/desorption isotherm. The specific surface area is estimated to be 149 m²/g. The simplicity of this approach makes it attractive for manufacturing of ultralow-k dielectrics, battery electrodes, and sensors.

Thermal Reffusivity of Materials: 0 K-limit and uncovered structure domain size

Bowen Zhu, PI: Xinwei Wang, Mechanical Engineering

Abstract: This talk will introduce a new concept: thermal reffusivity, which is the inverse of thermal diffusivity, and present the studies we have conducted for various materials from micron down to nanoscales from room temperature down to 10 K. Direct measurement of thermal reffusivity is made possible using the transient electro-thermal (TET) technique, which was first developed in our lab to provide one of the most reliable measurements of thermal transport properties of micro/nanosize materials. The variation of the thermal reffusivity against temperature, in comparison with that of bulk counter part, directly uncovers the contribution of defects. The 0 K-limit of the thermal reffusivity, termed residual thermal reffusivity, is directly used to determine the structure domain size uncovered by low-momentum phonon scattering. This size is very close to that determined by x-ray diffraction. Materials including metals, dielectrics, and organic and bio-materials have been studied to uncover their structure domain size.

Molecular Dynamics Simulations of Diffusion of Chloride Ions in Nano-Pores of Hydrated Cement Paste

Shahin Hajilar, PI: Behrouz Shafei, Department of Civil, Construction, and Environmental Engineering

Abstract: The long-term durability of cementitious composite materials is adversely affected by the ingress of chloride ions into their intrinsic nano-pore spaces. The chloride ions can be originated from a variety of sources, including seawater, deicing salts spread on the roads, or soils with saline environments. In concrete structures exposed to chloride contamination, chloride ions diffuse towards reinforcing steel bars embedded in the concrete matrix and initiate the destructive corrosive reactions. Despite growing concerns about corrosion-induced degradations, there is a major gap in the literature to understand the origin of chloride diffusion mechanisms at the molecular level and characterize how water molecules and chloride ions interact with the hydrated cement paste. This research gap is addressed in this study by conducting a set of Molecular Dynamics simulations supported by experimental tests to provide qualitative and quantitative measures of chloride diffusion, particularly at the interfaces of hydrated cement paste.

Theoretical study of water effect on carbinolamine formation with mesoporous silica nanoparticle

Yu Lim Kim, PI: Mark Gordon, Chemistry

Abstract: The carbinolamine formation in the aldol reaction is catalyzed by water and silanol which is from amine-substituted mesoporous silica nanoparticle (amine-MSN). Water catalyzes the carbinolamine formation in three different ways by a silanol group of amine-MSN. The computational result shows that water is involved in covalent bond rearrangement and the number of water molecules affects the catalytic capability on the reaction. Therefore, the energy barrier is remarkably reduced since water and silanol stabilize the transition state of the carbinolamine formation. In the future, the fragment molecular orbital (FMO) method will be used to investigate the reaction mechanism on amine-MSN. In addition, this research will be completed for studying the water catalytic effect with large number of water molecules on amine-MSN surface.

Dual Delivery Nanoscale Device for miR-345 and Gemcitabine Co-Delivery to Treat Pancreatic Cancer

Metin Uz, PI: Surya Mallapragada, Chemical and Biological Engineering

Abstract: Pancreatic cancer (PC) has extremely poor prognosis with five-year survival rate of less than 7%. Currently applied standard therapy for PC, involving surgical cytoreduction followed by systemic gemcitabine (GEM) based chemotherapy, has not provided desired outcomes. Alternatively, microRNA-345(miR-345)-based therapy has been proposed. However, co-delivery of miR-345 and GEM is challenging due to varying physicochemical properties. Therefore, we propose temperature and pH responsive, cationic, amphiphilic and biocompatible pentablock copolymer based dual delivery nanoscale device (DDND) for in vitro and in vivo combined delivery of miR-345 and GEM for PC treatment. This novel DDND facilitates cellular uptake due to amphiphilic character, endosomal escape due to protonatable tertiary amine groups, and provides simultaneous miR-345 and GEM release in cytoplasm through temperature responsive micellization. We found that miR-345 restoration through DDND treatment results in down regulation of sonic hedgehog (shh) signaling pathway and inhibition of desmoplasia, and tumor growth and metastasis.

ex vivo Study of Telluride Nanowires in Minigut for Defending Against Photothermal Irradiation

Yijun Qi, PI: Qun Wang, Chemical Engineering Department

Abstract: Telluride nanowires have many potential applications owing to their unique electronic, optical, and thermal properties. However, their use in biomedical applications is seldom explored, mainly due to the unclearness of their nanotoxicity. In this study, we demonstrated a case study on Bi₂Te₃ nanowires. Through live/dead cell viability testing, bright-light image analysis, and surface area calculations, we showed that 50 µg/mL Bi₂Te₃ exerts minimum influence on shrinking crypts and disrupting lumen structure, which causes unhealthy growth. In addition, under infrared exposure, nanowires stimulated cell growth and prevented cell death. Within this optimal concentration, Bi₂Te₃ nanowires can stay as a stable and non-toxic material inside the intestine, as potential candidate for the construction of a tight junction-like structure to prevent cell shedding and can provide a solution for curing inflammatory bowel diseases.

Fabrication and Evaluation of Poly (lactic acid)/Chitosan/Tricalcium Phosphate Biocomposites for Guided Bone Regeneration

Srikanthan Ramesh, PI: Iris Rivero, Industrial and Manufacturing Systems Engineering

Abstract: This study validates an approach for preparing biodegradable polymer-bioactive ceramic composites and evaluates their suitability for Guided Bone Regeneration (GBR), a dental surgical procedure that uses barrier membranes to direct and delineate regions of osteogenesis. Biomaterials were pre-processed using cryomilling, since it generates particles with improved surface area-to-volume ratio and mechanochemical properties that enhance biological activity.

X-Ray diffractometry and differential scanning calorimetry were used to characterize the molecular structure and glass transition temperature of the cryomilled composites. Scanning electron microscopy was used to study the morphology of the electrospun membranes, and Raman spectroscopy was used to confirm their material homogeneity. In vitro studies with MG-63 cells quantified the blend's ability to encourage cell proliferation. Coherent Anti-Stokes Raman Scattering and fluorescence microscopies were employed to analyze cell proliferation. CellTiter-Blue® cell viability assay revealed that cells maintain viability and metabolic activity after seeding, indicating the suitability of the biocomposites for GBR.

Connecting Researchers and Companies

Steve Carter (President ISU Research Park/Director Pappajohn Center for Entrepreneurship)

Abstract: This presentation will provide an overview of the eco system available to help connect researchers with companies and vice versa. He will highlight large company partners at ISU Research Park as well as talk about the opportunity ISU Startup Factory represents for both businesses, entrepreneurs and researchers.

Poster Abstracts

#1, In-Field, Disposable Soil Sensor for Monitoring Pesticide Levels via Laser Annealed Graphene Electrodes

John Hondred, PI: Jonathan Claussen, Mechanical Engineering

Abstract: While the use of pesticides (organophosphates) is critically important to meet current and future food demands, their overuse has shown long-term detrimental impacts. Current pesticide measurement methods are costly, require trained technicians, and take days; thus, farmers are taking an “over-application approach” which is polluting the environment and waterways. A disposable, in-field soil sensor would provide farmers the opportunity of precisely regulating the application of pesticides. Electrochemical biosensors provide the unique ability to quickly detect analytes with disposable sensors; however, the detection limit and sensitivity of these biosensors are inadequate for current applications. Three approaches are simultaneously performed to address this issue: 1) Increasing the enzymatic efficiency by strategically functionalizing to nanomaterials. 2) Improving the electroactive transduction material of the biosensor 3) Performing enhanced electrochemical measurement techniques by use of complex geometries. This work demonstrates the manufacturing of a simple, low-cost electrochemical biosensor suitable for rapid in-field detection of organophosphates.

#2, Imaging the localized plasmon resonance modes in graphene nanoribbons

Yilong Luan, PI: Zhe Fei, Physics

Abstract: We performed a real-space nano-infrared study of the localized surface plasmon resonance modes of graphene nanoribbons (GNRs) by combining near-field optical microscopy and finite-element plasmonic simulations. From the imaging data, we found symmetric plasmonic interference fringes when excitation laser beam is parallel to GNRs and asymmetric ones in the case of perpendicular excitation. Our analysis and modeling indicate that the observed asymmetric fringes are formed due to the interference between the localized surface plasmon resonance modes and the propagative surface plasmon polariton mode. Reference: F. Hu, Y. Luan et al. Imaging the localized plasmon resonance modes in graphene nanoribbons. Submitted.

#3, Thermolysis of Heterobimetallic Single-Source Precursors: A Springboard to the Synthesis of Binary Intermetallics

Carena Daniels, PI: Javier Vela, Chemistry

Abstract: Intermetallic compounds have important applications in the areas of catalysis, energy storage, and materials chemistry. These compounds are most commonly made by high-temperature solid state reactions by mixing stoichiometric ratios of desired elements in a flux solution. This synthesis method is often impractical due to the use of high-temperatures and phase segregation in the resulting products. In order to work around this, heterobimetallic “lantern” complexes have been used as single-source precursors in the synthesis of different intermetallic compounds. These air-stable heterobimetallic lantern complexes contain two different metals bonded together, along with a phosphine ligand scaffold, and were originally studied for energy storage applications and the unusual bonding properties of the metals. Decomposition of single-source precursors is an ideal synthesis method due to the already existing metal-metal bond, lower decomposition temperatures than solid state flux synthesis, and the diversity of precursors available. During this study, 8 different precursors have successfully been used to synthesize intermetallic products such as NiSb, NiAs, PtSb, PdSb, and Au₂Bi. Other important intermetallic products may also be easily synthesized just by changing the metals in the heterobimetallic precursor template.

#4, Melt Processing of Hybrid Organic-Inorganic Metal Halide Perovskite Thin Films for Photovoltaic Devices

Matthew I. Milot, PI: Matthew G. Panthani, Department of Chemical and Biological Engineering

Abstract: Recent advancements in the area of Perovskite-based photovoltaics have resulted in high efficiencies for electronic devices, of which solar cells are an important case. With the potential to eventually rival silicon based solar cells, hybrid organic-inorganic metal halide Perovskites have shown the most promising results as a basis for device fabrication, with solar cell efficiencies reaching almost 22% (methylammonium lead iodide). Despite this, certain drawbacks arise when the more common methods of film preparation, one being solution processing via spin coating, are applied. The issue of recycling the solvent, which requires expensive equipment and is generally not practical, leads to a large loss of capital in the form of evaporated waste. As a consequence, it has become more advantageous to apply cheaper methods to allow for the large-scale manufacture of Perovskite thin films. Currently, the more typical industrial approach is to use vapor processing, which requires the use of a vacuum and, although expensive to utilize in the laboratory, is less costly than solution processing at larger scales. In this study, we demonstrate the results of experimentation using the method of melt-processing for the production of lead and tin-based Perovskite thin films to be used in photovoltaic devices.

#5, Germanium–Tin/Cadmium Sulfide Core/Shell Nanocrystals with Enhanced Near-Infrared Photoluminescence

Himashi Andaraarachchi, PI: Javier Vela, Chemistry

Abstract: Elemental germanium (Ge) is a group IV semiconductor that has a small indirect band gap (0.661 eV) and a large Bohr radius (24 nm). These attributes provide for a wide range of tunable emission energies through size tunable quantum confinement. Near IR active Ge nanocrystals can be used in variety of applications such as photovoltaics, sensors, telecommunication, and bioimaging. However, indirect energy band gap makes it difficult to achieve efficient light harvesting and emission. Prior literature indicates that doping germanium with tin (up to 6%) may result in a direct band gap material. We synthesized Ge_{1-x}Sn_x alloy nanocrystals and coated them with CdS monolayers. While Sn inclusion alone does not enhance photoluminescence intensity, Ge_{1-x}Sn_x/CdS core-shell structure exhibits enhanced photoluminescence, which might result from more effective surface passivation and decrease of surface oxidation by the CdS shell.

#6, USING DIP-PROCESSING TO PROMOTE CATION EXCHANGE IN MELT-PROCESSED LEAD AND TIN BASED PEROVSKITES

Madeleine Wilsey, PI: Matthew Panthani, Chemical and Biological Engineering

Abstract: By reaching power conversion efficiencies of 22%, lead and tin based Perovskites, like methylammonium lead/tin iodide, have generated interest in the area of photovoltaics. However, the processes it takes to make these films, such as solution processing and vapor-phase deposition, both pose challenges when scaling up for industry. Solution processing involves solvents which are difficult to separate from the evaporated waste and harmful to the environment. Likewise the process of vapor-deposition uses vacuums, which can become costly. Melt-processing has been developed as a cheap alternative to these processes. Despite that, the melting temperatures of many of these hybrid perovskites are at or near their decomposition temperatures, posing an obstacle in the use of this method. The thermal properties of methylammonium lead/tin iodide can be changed by substituting phenethylammonium for methylammonium, which reduces the melting point well below the decomposition temperature. Phenethylammonium lead/tin iodide however, does not have nearly the same power converting capabilities in comparison to methylammonium lead/tin iodide. Consequently, dip-processing in isopropanol is used to promote cation exchange and replace the phenethylammonium with the methylammonium, in order for the melt-

#7, Experiments for the Purpose of Synthesizing a Silicon, Germanium, and Tin Chemical Alloy

Bevan Whitehead, PI: Matthew Panthani, Chemical Engineering

Abstract: The goal of this project is to chemically alloy the elements of Silicon, Germanium, and Tin to create a more efficient solar panel. Silicon is widely used in electronics, but lacks the absorbance properties to make it efficient for solar panels. Germanium and Tin possess better absorbance properties. Our experiments have focused on alloying two of the three elements together. One line of experiments is combining triethoxysilane (TES) with tin or germanium halides in water and hydrochloric acid. A second line of experiments is the annealing of metallic powders with group one elements and then combining these alloys with Silicon nano crystals in an organic solvent such as toluene. We have also performed UV/Vis spectrophotometry for these alloyed powders. We have been able to alloy silicon and germanium using TES and germanium iodide. We have been able to show that compounds made with silicon, germanium and potassium have photoluminescence.

#8, Solvated-Electron Initiated Rapid Polymerization at Ambient-Temperature: A case of Monomer Solubility

Boyce Chang, PI: Martin Thuo, Materials Science and Engineering

Abstract: In efforts of expanding our library of methods for polymer synthesis, very few have been applied in industries due to their complexity and stringent requirements. We demonstrate the application of solvated electrons, which can be prepared at room temperature, in rapid and selective polymerization of commercially available monomers. The molecular weight distribution of the resulting polymer was found to be closely related to its solubility in the solvent used, whereby a departure from the expected normal distribution was observed in poor solutes. Furthermore, although monomers with negative inductive effects proved to be a requirement, our observations do not fully agree with purely anionic mechanism, leading to the proposal of a bi-mechanistic radical anion polymerization. This method is then further employed as a straightforward approach for producing block copolymers.

#9, The effect of smoothening electrodes on tunneling behaviors across large area molecular junctions

Jiahao Chen, PI: Martin Thuo, Materials Science and Engineering

Abstract: Large area self-assembled monolayers (SAMs) based tunneling junctions have recently received great attentions, in part due to its simple fabrication, high yield of working device, and reproducibility. One of these challenges is the effect of electrode (top and bottom) morphologies on the tunneling behavior of the junctions. To address these challenges, we fabricated super-flat Au and Ag surfaces as bottom electrodes. The fabrication method entails interface stress-driven surface reconstruction coupled with template-stripping. To improve the top electrode, and thereby the nature of the contact, we polished the EGaln top-electrode by a chemical polishing method that entails selective thinning of the tip-oxide and gravity driven settling with concomitant regeneration of the passivating oxide to give a smooth stretched surface. We observe that with these modifications the distribution in repeated measurements of current density as significantly narrow. This allows us to better delineate molecular level disparities in the SAM.

#10, Tuning surface morphology of liquid metal particles via thermal treatment

Joel Cutinho, PI: Martin Thuo, Materials Science and Engineering

Abstract: Over the past decade, liquid metals have been exploited due to their easy moldability, flow properties, conductivity and zero modulus. Most approaches used to fabricate functional liquid metal particles result in smooth surfaces thus, limiting their applications in surface science. We demonstrate that by utilizing the ultra-thin metastable native oxide on eutectic gallium indium (EGaln) particles, surface texture and morphology can be engineered by varying temperature. SEM images depict particles characterized by crumples, patches and either one or two-tiered roughness with temperature. By using XRD, XPS and Auger spectroscopy, we validate that the new surface consists of mixed crystalline gallium and indium oxides of varying composition. Our results suggest that this material can be used in applications demanding surface roughness, most notably, catalysis and drug delivery.

#11, Pd/CeO₂ Inside Silica Mesopores: Synthesis, Characterization & Catalytic Activity

Pranjali Naik, PI: Igor Slowing, Chemistry/ISU

Abstract: The unique property of cerium oxide (ceria, CeO₂) to undergo reversible oxygenation/ deoxygenation cycles without disruption of its fluorite lattice has resulted its application in several important technologies including three-way catalysts, solid oxide fuel cells, photo catalysts, and antioxidants. The redox chemistry of ceria is strongly dependent on particle size and morphology, therefore significant research has been devoted to produce ceria nanoparticles with controlled shapes and sizes. Importantly, ceria nanoparticles have poor thermal stability and undergo crystallite growth (sintering) when treated at high temperatures especially under reducing conditions, resulting in decreased catalytic activity due to loss of surface area. To prevent or minimize sintering of ceria and develop multifunctional catalysts, we prepared hierarchical architectures containing ceria inside the pores of mesoporous silica nanoparticles (MSN). Confining ceria into the pores of MSN allowed controlling its particle size and preventing its agglomeration. The detailed characterization of the CeO₂@MSN materials was performed using low and wide angle X-ray diffraction, nitrogen adsorption-desorption analysis, and TEM imaging. As an active metal for catalysis, palladium was introduced into the composite via incipient wetness impregnation and the interaction between palladium and ceria was studied using temperature-programmed reduction (TPR) and energy dispersive x-ray spectroscopy (EDS) mapping. It was found that because of the metal-support interaction Pd was able to get in contact with ceria rather than remaining adsorbed to silica in the composite. We explored the performance of the composite as a catalyst for phenol hydrogenation in water to produce high cyclohexanone yields under mild reaction conditions (1 atm H₂, 35 °C).

#12, Synthesis of meso-porous oxides from In based Coordination Polymers

Paul Karanja, PI: Martin Thuo, Materials Science and Engineering

Abstract: Porous metal oxides with molecular sized periodic structures have attracted a lot of attention due to their range of application in storage and transformation of small molecules.

We produce porous oxides by forming metal organic coordination polymers using an acid and metal. The coordination polymer formed is heat treated through which organic content is eliminated to form a porous material. We demonstrate that the surface area and morphology of the material can be tuned by varying temperature. X-ray diffraction was also employed to ascertain the changes in atomic structure.

#13, Nitrogen-doped ordered mesoporous carbon(N-OMC): Synthesis, Characterization and Catalysis

Bosky Parikh, PI: Igor Slowing, Chemistry

Abstract: We have synthesized palladium supported on ordered mesoporous carbon(OMC) and nitrogen-doped ordered mesoporous carbon (N-OMC) via two-step process and the effect of nitrogen doping on the properties of mesoporous carbon was then studied using nitrobenzene hydrogenation as a test reaction. The OMC materials were synthesized first using Pluronic F127 as the structure directing agent (SDA), and resorcinol and 3-aminophenol as carbon and carbon-nitrogen source for OMC and N-OMC respectively. To control the rate of polycondensation, formaldehyde was generated in situ via hydrolysis of hexamethylenetetramine. The SDA was removed via pyrolysis under nitrogen flow, conditions that also led to the carbonization of the precursors. The detailed characterization of the materials was performed using low and wide angle X-ray diffraction, Diffuse Reflectance Infrared Fourier Transform Spectroscopy (DRIFT), CHN elemental analysis and nitrogen physisorption analysis. After successful characterization, palladium nitrate dihydrate was impregnated on the supports and was then reduced using sodium borohydride/ethanol solution and nitrobenzene hydrogenation was performed.

#14, Size controlled intermetallic compounds for electrocatalysis

Zhiyuan Qi, PI: Wenyu Huang, Chemistry

Abstract: Pt based alloy and intermetallic have been intensively studied as electro-catalysts over the last two decades. Adding another metal can effectively reduce the amount of Pt cost, tune the availability and activity of surface active sites and alter the binding strength of reactants, intermediates, products, and thus tune the catalytic activity. However, the insufficient utilization of Pt due to the aggregation of particles under synthesis conditions will hamper the catalytic performance. Intermetallic compounds have higher free energies of formation than alloys, which usually requires high temperature annealing (e.g. 600 °C for Pt₃Zn) treatment. Therefore, the aggregation of nanoparticles is unavoidable, leading to the lack of size control. Moreover, the larger particles limit catalytic activity due to their low surface to volume ratio, and thus hamper the effective utilization of precious metals. We encapsulated nanoparticles with thermally stable inorganic shell that could prevent the aggregation of particles at high temperature annealing.

#15, Lead-Free Germanium Perovskites: Synthesis, Size Control and Manganese Doping

Long Men, PI: Javier Vela, Chemistry

Abstract: Organometal halide perovskites, as promising photovoltaic and optoelectronic materials, have drawn enormous interest recently for their unique and remarkable properties; however, lead is a heavy metal element and its potential toxicity raises concerns for environmental compatibility. To address this problem, we have developed a synthesis route to bulk cesium germanium triiodide (CsGeI₃) and their nanocrystals. With a bandgap of 1.6 eV and a corner-sharing octahedral network crystal structure, which are comparable to CH₃NH₃PbI₃, CsGeI₃ is potentially promising for photovoltaic applications. Transmission electron microscopy (TEM), X-ray diffraction (XRD) and diffuse reflectance corroborate the structural and optical properties of this material. We have also doped high-spin, divalent manganese ions into the octahedral Ge sites of CsGeI₃. Electron paramagnetic resonance (EPR) helps us better understand the local ion environment and composition of CsGeI₃ and its doped analogues. Our results may help expand the lead-free halide perovskite family and broaden their application beyond photovoltaics into spintronics and magnetic data storage.

#16, Characterization of LiZnP Nanoparticles by Advanced Solid-State NMR Spectroscopy

Amrit Venkatesh, PI: Aaron J. Rossini, Department of Chemistry

Abstract: Lithium Zinc Phosphide (LiZnP) is a promising material for thermoelectric and photovoltaic devices due to its favorable optical and electrical properties. New synthetic strategies have enabled the synthesis of LiZnP nanoparticles and the properties of the material can be altered by controlling the particle size. Here we apply solid-state NMR spectroscopy to probe the structure of LiZnP nanoparticles (NPs). The application of state of the art fast-magic angle spinning (MAS) and dynamic nuclear polarization (DNP) techniques allows us to enhance the sensitivity and resolution of solid-state NMR experiments. We show how it is possible to detect and differentiate ³¹P NMR signals arising from nuclei in the inorganic core and the ligand passivated oxidized surface. The solid-state NMR experiments suggest LiZnP NPs can be described by an oxidized core-inorganic shell structural model and unambiguously show the presence of secondary phosphines (R₂PH) species in both the surface and core of the NPs.

#17, Yield and fluorescence behavior of noncovalently functionalized single-walled carbon nanotubes

Nathaniel Kallmyer, PI: Nigel Reuel, Chemical and Biological Engineering

Abstract: As nanomaterial technology has improved nanoscale biosensors have become an increasingly relevant area of research. One such nanomaterial is the single-walled carbon nanotube (SWNT), which fluoresces in the near-infrared window of biological material, making it ideal for in vivo applications. SWNT may be suspended in water if wrapped with an amphiphilic polymer and modified to function as a sensor. This is typically achieved by sonication. While application-focused research has been performed, little has been done to understand factors affecting SWNT-biosensor synthesis. We have explored effects of sonication power and duration on an array of potential wrappings including proteins, DNA, oligosaccharides, polysaccharides, synthetic polymers, and surfactant solutions. Trends between polymer length and nanotube yield suggest fragmentation of the wrapping to play a large role in SWNT functionalization. Although apparent yield increases with sonication power and time, quality of the nanotubes begins to deteriorate with increased power. These trends may be used to predict promising SWNT wrappings and design processes for large-scale production of SWNT-based nanosensors.

#18, Recent progress in thermoelectric nanocomposites based on solution-synthesized nanoheterostructures

Wei Zheng, PI: Yue Wu, Chemical & Biological Engineering

Abstract: Thermoelectric materials, which can convert waste heat into electricity, have received increasing research interest in recent years. This paper describes the recent progress in thermoelectric nanocomposites based on solution-synthesized nanoheterostructures. We start our discussion with the strategies of improving the power factor of a given material by using nanoheterostructures. Then we discuss the methods of decreasing thermal conductivity. Finally, we highlight a way of decoupling power factor and thermal conductivity, namely, incorporating phase-transition materials into a nanowire heterostructure. We have explored the lead telluride–copper telluride thermoelectric nanowire heterostructure in this work. Future possible ways to improve the figure of merit are discussed at the end of this paper.

#19, Heterogeneous catalysis by metal nanocluster encapsulated in Metal-Organic Framework

Jason Goh, PI: Wenyu Huang, Chemistry

Abstract: Heterogeneous catalysis plays an essential role for the development of efficient, economical, and sustainable chemical and energy industries. Selective catalysts ensure the progress of a reaction to the desired products, which can minimize the amount of by-products/waste produced during chemical reactions and achieve atomic efficiency, one of the focuses of green chemistry. MOFs, as crystalline porous materials, possess identical cavities of atomic-level defined structures. Using MOFs as templating materials to synthesize NC catalysts confined in their cavities has many advantages. The uniform cavities of MOFs provide the opportunity to synthesize cavity-matched NCs with extremely narrow size-distribution. The large structure and composition tunability of MOFs greatly broaden the possibility to design MOF-confined NC catalysts with desired catalytic properties. The research goals of this project are to synthesize monodisperse NCs using metal-organic frameworks (MOFs) as templates, as well as to apply these NC catalysts in selective chemical conversion processes.

#20, Pair Interactions of Hydrocarbon-capped Nanoparticles: Effect of Chain Conformations

Curt Waltmann, PI: Alex Travesset, Materials Science and Engineering

Abstract: Hydrocarbon capped nanocrystallites arranged in periodic order constitute an emerging class of materials with a rich phase diagram. However, while these systems are now experimentally realized, they are not well-described by theoretical models. We have developed theoretical and computational models that address these systems, and have incorporated them into a comprehensive software package, which allows us to quickly and reliably investigate problems that supplement theoretical understanding of these systems. To this end, we investigate the interaction between two particles with varying core sizes and chain lengths, including the case where the ligand is much longer than the core radius, where no theoretical model currently exists. This is done by calculating effective pair potentials, along with the internal energy and entropy, via the Weighted Histogram Analysis Method. Then we examine configurational characteristics of the ligand shell, to elucidate the mechanisms that drive this interaction.

#21, Role of Many Body Effects in Self Assembly of Hydrocarbon Capped Nanoparticles

Tommy Waltmann, PI: Alex Travasset, Ames Laboratory

Abstract: In this poster, I investigate the properties of nanoparticles consisting of 201 gold atoms with Sulfur atoms used to attach the hydrocarbon chains to the rigid nanoparticle body. I ran computer simulations of small, planar systems with a central particle and a varying number of particles spaced equally in a circle around a central nanoparticle via the HOODLT and HOOMD software packages. From output data, I could calculate the free energy of the system and the many body effects in the system. I found that the free energy of these systems, many-body effects, and equilibrium separations all increase with increasing coordination of the central particle. In addition, I found that the central particle only exhibits neutral lines for the 2 and 3 coordinated systems.

#22, Synthesis and surface functionalization of Group IV Quantum Dots

Yujie Wang, PI: Matthew Panthani, Chemical and Biological Engineering Department

Abstract: Quantum dots (QDs) have been the focus of research for several decades due to their size-tunable properties and potential application in many areas including photovoltaic, LEDs, photodetector, computing and biological labeling. Group IV QDs are particularly interesting. Si, the cornerstone of modern electronics, has an indirect bandgap and therefore doesn't emit or absorb light efficiently. This problem can be solved by making Si QDs. In addition, Group IV QDs can be tuned to emit and absorb light in relevant telecommunication bands by controlling size and/or composition. The synthesis of Group IV QDs with controlled size and composition has been challenging for many reasons, including a need for high temperature to crystallize Group IV elements and poor understanding over factors that govern precursor decomposition and crystallite nucleation.

#23, Materials Analysis and Research Laboratory: A core material characterization facility at Iowa State University

Dapeng Jing, PI: Warren Straszheim, Materials Analysis and Research Laboratory

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. MARL major Equipment: FEI Quanta 250 FEG Scanning Electron Microscope (SEM), TA Instruments Discovery Thermal Gravimetric Analyzer (TGA), TA Instruments 2960 Simultaneous DTA/TGA (SDT), Oxford Aztec Energy-Dispersive Spectrometer (EDS), Siemens D500 X-ray Diffractometer (XRD), PANalytical PW2404 X-ray Fluorescence (XRF) spectrometer.

#24, A Theoretical Investigation of Gas phase X-Au-X (X = S, Cl, CH₃S, SiH₃S) Complexes and Complexes on Au(111) Surface

Jiyoung Lee, PI: Theresa Windus, Chemistry

Abstract: Experimental results show that linear AuX₂ complexes are observed on the Au(111) surface with X = CH₃S, sometimes observed with X = Cl, but not X = S. To address the observations, stabilities of AuX₂ on surface are studied using density functional theory (DFT). Au(CH₃S)₂ and Au(SiH₃S)₂ are more stable than individually chemisorbed CH₃S and SiH₃S on surface whereas adsorbed AuS₂ are found less stable than S. AuCl₂ complexes show different stability depending on the used functionals. Gas phase AuX₂ is also studied using DFT and the coupled cluster (CC) method. Bond strengths of X-Au-X are found to be similar regardless of X, which implies the bond strength of the ligand to the surface affects more to the stabilities of adsorbed complexes. These explains the reasons why Au(CH₃S)₂ complexes can be found on Au surface but not AuS₂.

#25, Synthesis of Polymeric Janus Nanoparticles Using Emulsion Polymerization Serkan Demirci, PI: Shan Jiang, Materials Science and Engineering

Abstract: Janus particles (JNPs) are special types of nanoparticles that have two sides with different chemistry. In this study, anisotropic dumbbell-shaped poly(styrene)/poly(styrene-co-t-butyl acrylate) (PS/PS-tBA) nanoparticles were synthesized by seeded emulsion polymerization. The results showed that smooth JNPs can be prepared by controlling the crosslinker amount, reaction temperature and stages of the reaction. Besides Janus geometry, many other morphologies, including dimple and multi-lobe, were observed in the experiment.

#26, Process engineering of pure phase quasi-2D layered CsPbI₃ perovskite thin film for solar cell application

Atefe Hadi, PI: Matthew Panthani, Chemical and Biological Engineering

Abstract: Lead-based organic-inorganic hybrid perovskites have been of interest due to its high power conversion efficiencies, but exhibit structural degradation on exposure to humidity and temperature thus preventing its large scale commercialization. Recent use of inorganic perovskite such as CsPbI₃ has showed enhanced stability under moisture and temperature thus providing an alternative to hybrid perovskite. Nevertheless, these materials have large bandgap in ambient conditions, making them inefficient for solar cell application. Herein, we have synthesized quasi-2D ($n > 1$) structures of CsPbI₃ by incorporating large organic cation, PEA⁺ (C₈H₉NH₃⁺) resulting in stable low energy band gap perovskite thin film absorber. We studied crystallization of layered 2D PEA₂CsPb₂I₇ ($n=2$) films in order to obtain 2D ($n=2$) pure phase thin films for solar cell application. Our preliminary results shows that rapid crystallization of spin coated film prepared from precursor solution in DMSO leads to pure $n=2$ phase having large grain and dense morphology

#27, Solution-Based Synthesis of Cesium Bismuth Iodide Nanocrystals

Rainie Nelson, PI: Matthew Panthani, Chemical and Biological Engineering

Abstract: Methylammonium lead iodide and other lead halide perovskite materials have been investigated for a variety of optoelectronic applications. However, these perovskites are unstable when exposed to atmospheric operating conditions. Much perovskite research therefore seeks to improve their stability. Bismuth halide perovskites are relatively unexplored, but have promising initial performance and are predicted to have similar properties to lead-based perovskites.

This work reports on the use of solution-based methods to synthesize cesium bismuth iodide nanocrystals. Improved phase-stability is observed in the Bi-perovskite nanocrystals as compared to CsPbI₃ perovskite nanocrystals. Transmission electron microscopy and X-ray diffraction were used to characterize nanoparticle morphology and crystal structure. These Bi-based perovskite nanocrystals have potential for high performance, stable, and non-toxic solution-processable optoelectronics.

#28, Refractive Index/Intensity Based Optical Gaseous/Aqueous Sensors

Shawana Tabassum, PI: Ratnesh Kumar, Electrical and Computer Engineering

Abstract: Optical refractive index or transmission/reflection intensity offer high sensitivity to analytes. For agricultural application, plant released gaseous compounds were sensed from refractive index changes on a nanopatterned optical fiber tip supporting guided-mode resonance to determine plant health under biotic/abiotic stresses. In a medical application, cancer biomarkers were sensed using nanopatterned surface supporting plasmonic resonance, causing optical resonance wavelength to change in the presence of biomarkers.

#29, Photoluminescence enhancement of quantum dots in solution coupled to plasmonic gold nanocup arrays

Akshit Peer, PI: Rana Biswas, Ames Laboratory and ECpE

Abstract: We have fabricated a metasurface with an array of gold-coated nano-cups with a pitch of 750 nm. We demonstrate strong plasmonic enhancement of photoluminescence (PL) decay rate in quantum dots (QDs) coupled to arrays of gold-coated nanocup. CuInS₂ QDs that emit at a wavelength that overlaps with the extraordinary optical transmission (EOT) of the gold nanocup arrays are placed in the cups as solutions. Time-resolved PL reveals that the decay rate of the QDs in the plasmonically coupled system can be enhanced by more than an order of magnitude. Using finite-difference time-domain (FDTD) simulations, we further show that this enhancement in PL decay rate results from an enhancement factor of ~100 in field intensity provided by the plasmonic mode of the nanocup array, which is also responsible for the EOT. The simulated Purcell factor approaches 86 at the bottom of the nanocup. This opens new possibilities for biosensing and bioimaging.

#30, Vibration-Driven Assembly of Polymer-Nanopowder Composites

Soheila Shabaniverki, PI: Jaime Juarez, Mechanical Engineering

Abstract: Externally-driven assembly of nanoparticles directs the formation of complex patterns that enable the fabrication of electrically conductive networks for bioelectronics. A variety of approaches are available for assembling nanoparticles (e.g., microfluidics, magnetic fields, electric fields). However, many of these approaches offer only low-volume production. This talk presents a large-scale approach to assembly of nanoscale particles by relying on vibration to generate an acoustic radiation force that drives complex pattern assembly. A fluid dispersion of nominal 50-100 nm iron oxide nanopowder is introduced to a vibrating glass petri-dish stage. The patterns formed during assembly are highly sensitive to frequency, with the nanopowder assembling at vibrational nodes. A photocurable polymer is added to the dispersion and exposed to a UV light, immobilizing the nanostructures. The resulting polymer gel is robust and can be held by hand. Future work focuses on quantifying the magnetic and electrically conductive properties of the assembled nanopowder structures.

#31, Assembling gold nanoparticles in polymer gels

Srikanth Nayak, PI: Surya Mallapragada, Chemical and Biological Engineering

Abstract: Ordered arrays of metallic nanoparticles forming super-lattices have several potential applications including plasmonic metamaterials and photonic bandgap materials. Traditional top-down methods are typically limited to the fabrication of meta-surfaces and are expensive. Hence self-assembly processes at the nanoscale are being actively pursued towards the fabrication of bulk metamaterials and plasmonic structures. Self-assembly of polymers into microphase separated domains such as gyroid and lamellar can be utilized for ordering metallic units in such super-lattices. One of the main approaches for obtaining such ordered polymer – nanoparticle composites is the in situ synthesis method, wherein the nanoparticles are grown selectively in a particular phase of the block copolymer. Here we discuss some results we have obtained with synthesizing and assembling gold nanoparticles in aqueous gels of Pluronic block copolymers. Pluronic block copolymers act as a reducing and stabilizing agent in the formation of nanoparticles under basic pH.

#32, Control and Quantification of Local Polarity in Nano-confined Systems

Dilini Singappuli-Arachchige, PI: Igor Slowing, Chemistry

Abstract: Surface functionalization affects local environments and induces solvent-like effects at liquid-solid interfaces. We explored structure–property relationships between functional groups on the pore surface of MCM-41 type mesoporous silica nanoparticles and Stokes shifts of adsorbed solvatochromic dye Prodan. We produced a local polarity scale for functionalized pores by correlating the shifts of the dye inside the pores with its shifts in solvents of known polarities. The scale was validated by studying the effects of pore polarity on quenching of Nile Red fluorescence and on the vibronic band structure of Pyrene. Then, we explored the effect of local polarity on the catalytic activity of TEMPO for the aerobic oxidation of primary alcohols to aldehydes. We found an inverse relationship between pore polarity and catalytic activity of pore-residing TEMPO. Our findings suggest that the activity of nano-confined catalysts can be adjusted by controlling the local polarity around an active site.

#33, Synthesis and Characterization of Bismuth Halide Perovskite Thin-Films

Umar Hamdeh, PI: Matthew Panthani, Chemical and Biological Engineering

Abstract: Lead-based halide perovskite materials have generated broad interest for applications in optoelectronic devices; however, there are major issues concerning stability and toxicity. Therefore, Pb-free halide perovskites are being explored as stable and non-toxic alternatives. Bi-based halide perovskites have the potential to replace Pb-based halide perovskites because they have similar electronic structures, and are non-toxic and have superior stability to Pb-based halide perovskites. Proof-of-concept devices demonstrate the potential for Bi-based halide perovskites for photovoltaic application. We demonstrate that thin-film morphology of Bi-halide thin-films can be greatly improved by annealing in solvent vapor. Bi-halide thin-films can then be further processed using a two-step deposition procedure to synthesize Bi-based halide perovskite thin-films. We compare the material chemistry of bismuth halide perovskite thin-films fabricated using a one-step and two-step deposition process.