



Meeting Program

5th Nano@IAState Meeting – Monday May 13, 2024 – 9:00 am to 4:30 pm
Iowa State University, Memorial Union Great Hall

•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 industry members.

•Sponsors

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

ISU Office of Intellectual Property and Technology Transfer, Department of Chemical and Biological Engineering, Department of Chemistry, Department of Materials Science and Engineering, College of Engineering, Ames National 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
Boyce Chang - Materials Science and Engineering - boyce@iastate.edu

•Nano@IAState – Monday May 13, 2024 – Conference Program

All events take place in the **Memorial Union Great Hall and South Ballroom**

Time	Event/Talk Title	Presenter
8:30 to 9:00	Registration/Badge Collection - Coffee, Tea and Light Breakfast Provided - Memorial Union Great Hall	
	Oral Presentations - Memorial Union Great Hall	
9:00-9:05	Opening Remarks	
9:05-10:00	Plenary Lecture - Block Copolymer Compatibilizer Design for Mechanical Recycling of Polyolefin-containing Mixed Plastic Waste	Chris Ellison (University of Minnesota)
10:00-10:20	Non-precious single-site catalyst for polyolefin hydrogenolysis in micropore	Simin Sun (Chemistry)
10:20-10:50	Invited Talk - Towards a General Framework for Nanomaterials Assembly Prediction	Alex Travesset (Physics/Ames Lab)
10:50-11:05	Coffee Break	
	Oral Presentations	
11:05-11:35	Invited Talk - Synthesis and characterization of graphene-based nanomaterials	Marek Kolmer (Ames Lab)
11:35-12:05	Invited Talk - Mechanistic-Design of Metal-Metal and Metal-Ceramic Nanolaminates	Sid Pathak (MSE)
12:05-1:35	Lunch and Poster Session - Boxed Lunches Provided (Poster Numbers and Titles on Following Page)	
	Oral Presentations - Memorial Union Great Hall	
1:40-2:10	Invited Talk - A polypeptide nanoparticle platform for peptide drug discovery and delivery	Jing Wang (CBE)
2:10-2:30	DNP Enhanced ¹¹³ Cd Solid-State NMR Reveals Trigonal bipyramidal CdSe Nanocrystals are Terminated by {100} Facets.	Anuluxan Santhiran (Chemistry)
2:30-2:50	Statistical Design of Experiments (DoE) Enable Optimized Solid-State Synthesis of Thermoelectric Skutterudites	Thomas Seymour-Cozzini (Chemistry)
2:50-3:10	Coffee Break	
3:10-3:30	Heterogeneous mixed molecular weight polymer brushes as neutral templates for BCP orientation control	Kaitlyn Hillery (MSE)
3:30-3:50	Unraveling the Structure-Sensitive Nature of the Selective Electrocatalytic Hydrogenation of cis,cis-Muconic Acid	Deep Patel (CBE)
3:50-4:20	Invited Talk - Nanomaterial Ink Formulation for Aerosol Jet Printing of Electronics	Ethan Secor (ME)
4:20-4:30	Closing Remarks and Student Awards	

List of Poster Presenters

Poster Number	Presenter	Poster Title
1	Liuqing Wang	Understanding the Role of Chain Stiffness in Conformational Behaviors of Conjugated Polymers
2	Govinda Ghimire	Laser-Induced Graphene (LIG) for Sensing Application
3	Heshani Walgamage	Vat Photopolymerization of Porous Polymer Scaffolds: Effect of the Structure on the Mechanical Performance.
4	Ashleigh Ballard	3D Printing of Porous Hydrogel-Based Scaffolds for Biomedical Applications
5	Sepehr Hejazi	Collagen Immobilized Single-Walled Carbon Nanotube Sensors for High Throughput Screening of ECM Degrading Enzymes
6	Kanika Lalit	Navigating Dilute CO ₂ Reduction: Investigating the Role of Pore Channels and Size in Modified Mesoporous Carbon
7	Nayanathara Hendeniya	The role of crystallization of 3-pentadecylphenol in self-assembly of polystyrene – block – poly (4 – vinyl pyridine)
8	Farshid Noormohammadi	Optimizing Laser-Induced Graphene for Glucose Sensing: A Machine Learning Approach
9	Jacob Mayer	Observing Surface Dynamics in Heterogenous Catalysts Using NMR
10	Shaghayegh Abtahi	Energy-Efficient Synthesis of Organic-Inorganic Hybrids Through Polymer Complexation
11	Andrew Lamkins	Controlling Dispersion of Rhodium from Single-Atoms to Nanoparticles
12	Longji Li	Catalytic Deconstruction of Polyethylene via Hydrogenolysis using Localized Zirconium Oxide Catalyst in Core-Shell Architecture
13	Maharram Jabrayilov	Elucidating the Role of HSQ polymer structure on the Photoluminescent Properties of Silicon Nanocrystals
14	Minghui Niu	Polyethylene Deconstruction by Non-Precious Molybdenum Oxycarbide via Hydrocracking
15	Andrew Tan	2D Materials for the Future of Neuromorphic Computing
16	Zeinab Hajali Fard	Assessing the formation of Lewis and Brønsted sites in the hydrodeoxygenation of lignin derivatives over MoO ₃
17	Lukman Yunusa	Structure Determination of 2D Main Group Semiconductors by Solid-State NMR Spectroscopy

Oral Presentation Abstracts

1. Plenary Lecture - Block Copolymer Compatibilizer Design for Mechanical Recycling of Polyolefin-containing Mixed Plastic Waste

Chris Ellison

Mechanical recycling is presently the dominant recycling technology where plastic waste is sorted, ground, washed, and melt reprocessed into a new form. A major challenge for mechanical recycling is imperfect physical sorting which leads to impure recycle streams that phase-separate as immiscible polymer blends when melt reprocessed. The final products are usually brittle making them unsuitable for most applications because of sharp polymer-polymer domain interfaces a few nanometers wide that are mechanically weak. Copolymer compatibilizers containing molecular components that mechanically anchor in each domain of the blend can help by localizing at the interface to facilitate stress transfer producing tougher blends. In this talk, two examples of compatibilizers for producing tough poly(ethylene terephthalate)/polyethylene blends will be discussed. Importantly, both compatibilizers have proven to be remarkably efficient, toughening blends at loadings as low as 0.5 wt% suggesting they are attractive for mechanical recycling at an industrial scale.

2. Non-precious single-site catalyst for polyolefin hydrogenolysis in micropore

Simin Sun

The rapid and continuous accumulation of plastic waste has brought a serious plastic crisis, while polyolefin accounts for more than half. Hydrogenolysis is a promising method that can convert polyolefin to value-added products under milder conditions. However, the saturated C-C bonds in the backbones of polyolefin make it difficult to be cleaved. The random cleavages will generate a lot of low-value methane and unselective products. Therefore, the control of selectivity in C-C bond cleavages is a major challenge. In this work, we design a microporous system that facilitates silicalite-1 with sub-nano pores to mimic the confinement effect of natural enzymes and thus modulate the configuration of polymer chains. Meanwhile, the involvement of well-defined single sites imitates the precisely located active sites in enzymes, suppressing the formation of methane by inhibiting terminal C-C bond cleavages. Combining all these design concepts together, Co¹@S-1 shows excellent catalytic performance in polyolefin hydrogenolysis and matches the behavior of processive enzymes. The property of processivity helps the catalyst achieve the lowest methane yield of 0.4% and extremely selective liquid products from C₅ to C₁₄ in the hydrogenolysis reactions of polyolefin. Also, the selection of non-precious metals provides a promising avenue in industrial applications.

3. Invited Talk - Towards a General Framework for Nanomaterials Assembly Prediction

Alex Travesset

Materials whose fundamental units are nanocrystals (NC)s, instead of atoms or molecules, are emerging as major candidates to solve many of the technological challenges of our century. In this talk I will present an overview of the methods developed in my group to predict assembly. I will present theory, simulations and a recently introduced mean field model that successfully predicts all the known phenomenology of single component nanoparticle systems obtained by solvent evaporation.

4. Invited Talk - Synthesis and characterization of graphene-based nanomaterials

Marek Kolmer

Atomically precise graphene-based nanomaterials attract great attention due to their highly tunable electronic, optical, magnetic, and transport properties. In the first part, I will discuss epitaxially grown graphene on a SiC(0001) surface. I will present our developed protocol for tunable nanopatterning of epitaxial graphene via control of its buried interface with SiC. I will show that the covalent bonds between the graphene buffer layer and the silicon carbide substrate may be reversibly broken and restored using the polarity of an electric field from the scanning tunneling microscope tip. The manipulation can be applied locally to pattern epitaxial graphene with lateral precision, reaching single unit cells of the interface moiré lattice (~1.8 nm). In the second part of the talk, I will present a bottom-up, on-surface synthesis approach, which relies on rationally designed molecular precursors undergoing preprogrammed chemical reactions. I will focus on our recent efforts in designing strategies for directly synthesizing nanographenes (NGs) on model metal oxide surfaces via activation of C-F bonds. Future work will address ways to control kinetics and increase the length of NGs.

5. Invited Talk - Mechanistic-Design of Metal-Metal and Metal-Ceramic Nanolaminates

Sid Pathak

6. Invited Talk - A polypeptide nanoparticle platform for peptide drug discovery and delivery

Jing Wang

The peptide drug market is experiencing exponential growth, yet it faces challenges such as low stability, suboptimal bioactivity, limited tissue penetration, and rapid clearance in vivo. Nanoparticle delivery systems offer a promising solution to these limitations. Here, we introduce a novel thermo-responsive elastin-like polypeptide nanoparticle designed to revolutionize peptide drug discovery and delivery. Firstly, our approach enables the genetic synthesis of polypeptides with a 100% conjugation ratio to peptide drugs, surpassing the inefficiencies of traditional chemical conjugation methods. Secondly, these polypeptide-peptide drug conjugates self-assemble into 40 nm nanoparticles at body temperature, presenting 40 peptide drugs per nanoparticle surface consistently, regardless of peptide length or hydrophobicity. These distinctive features of elastin-like polypeptide nanoparticles make them an ideal platform for peptide drug discovery and delivery. They facilitate comparative studies among peptide drugs targeting the same protein, streamlining the identification of compounds with the highest bioactivity. Additionally, they enable the analysis of peptide structure-function relationships by allowing for convenient modification of key amino acids within the peptides, facilitating the design of optimized compounds. Moreover, the optimized bioactive peptide drugs delivered via polypeptide nanoparticles are readily deployable for both in vitro and in vivo assessments, promising enhanced efficacy and bioavailability over free short peptides.

7. DNP Enhanced ^{113}Cd Solid-State NMR Reveals Trigonal bipyramidal CdSe Nanocrystals are Terminated by $\{100\}$ Facets

Anuluxan Santhiran

Semiconductor nanocrystals (NCs) offer unique optical and optoelectronic properties arising from quantum confinement effects and which can be tuned by varying the size and composition of the NCs. CdSe NCs with different shapes can be synthesized by varying the temperature and the precursors. Here, we synthesized right trigonal bipyramidal CdSe using two different synthetic methods and studied them using Dynamic Nuclear polarization enhanced (DNP) advanced solid-state NMR (ssNMR) spectroscopy. DNP-enhanced ^{113}Cd and ^{77}Se CP-CPMG and CP-pulse cooling ssNMR spectra helped distinguish the chemical environments of Cd and Se atoms on the surface of CdSe NCs and those below the surface, which have bulk-like environments. ^{113}Cd cross-polarization magic angle turning (CP-MAT) experiment correlates the anisotropic chemical shifts in the direct dimension to the isotropic chemical shifts in the indirect dimension. Based upon the observed ^{113}Cd chemical shifts, we conclude that these NCs are trigonal bipyramidal in shape and composed of six polar $\{100\}$ facets and are terminating with CdSe $_2\text{O}_2$ on the surface. We will also show preliminary results describing the use of DNP-enhanced ^{113}Cd NMR spectroscopy to study colloidal atomic layer deposition.

8. Statistical Design of Experiments (DoE) Enable Optimized Solid-State Synthesis of Thermoelectric Skutterudites

Thomas Seymour-Cozzini

Thermoelectric materials convert temperature gradients into electric potential gradients, enabling the direct interconversion of heat and electricity. Efficient thermoelectric materials are electrically conductive thermal insulators with a high magnitude of induced voltage in response to a temperature gradient, enabling the scavenging of waste heat and compact electrical generators. Antimonide thermoelectric materials often feature complex structures with diverse bonding arrangements, resulting in favorable thermoelectric properties as exhibited by $\text{Yb}_{14}\text{MnSb}_{11}$, Zn_4Sb_3 and Mg_3Sb_2 .¹ High Seebeck coefficients and low electrical resistivities have made antimonide skutterudites the focus of extensive study as thermoelectric materials. The skutterudite crystal structure features a framework of corner-sharing TPn_6 octahedra, T = Group 8-10th transition metal, and Pn = P, As, Sb or Ge. Filling the large icosahedral void in the center of the skutterudite structure with monatomic cations, resulting in the filled skutterudites $\text{AT}_4\text{Pn}_{12}$, lowers their thermal conductivity. For thermoelectric applications, a typical filler atom is A = alkaline earth or rare-earth metals, while the framework is based on T = Fe and Co, and Pn = Sb. Doping and substitution can result in n-type or p-type semiconducting skutterudites with low thermal conductivity,² but ultimately require targeting a specific composition in multicomponent systems, preferably utilizing lower synthesis temperatures. The hydride route has been applied to antimonide synthesis³ before, and results in fine compositional control with lower reaction temperatures and fast kinetics by mitigating diffusion limitations in solid-state synthesis.³ We used the hydride route to synthesize skutterudites, replacing Ba or Sr metal for mixable salt-like BaH_2 or SrH_2 . Leveraging fast reactions kinetics, we applied statistical Design of Experiments (DoE) approaches to optimize synthesis conditions by altering more than one variable per trial, conserving resources when optimizing complex syntheses with mutually dependent synthetic parameters. High-temperature in-situ synchrotron powder X-ray diffraction enabled by fast hydride-route reactions allowed us to observe the formation mechanism of the skutterudite $\text{BaFe}_3\text{NiSb}_{12}$ from BaH_2 , Fe, Ni and Sb. Precise formation temperature from the mechanistic study validated the accuracy of statistical analysis results for $\text{BaFe}_3\text{NiSb}_{12}$ synthesis. Preparation of the new skutterudite $\text{SrFe}_3\text{NiSb}_{12}$ was optimized using statistical design of experiments, showing the utility of DoE in complex solid-state systems. Thermoelectric properties measured from 298 K to 673 K indicate that Sr-filled skutterudites have superior thermoelectric performance than Ba-filled skutterudites of otherwise similar composition. Alteration of the Fe to Ni ratio effectively tunes electronic transport properties without greatly altering thermal properties, resulting in the highest peak zT of 0.54 for $\text{SrFe}_3.28\text{Ni}_0.70\text{Sb}_{12}$.

References: 1. Beretta, D. Caironi, M. *Materials Science & Engineering R*, 138, 210-255, 2019. 2. Rull-Bravo, M. Martin-Gonzalez, M. *RSC Adv.* 5, 52, 41653-41667, 2015. 3. Cox, T., Zaikina, J., *Chem. Mater.* 30, 8707-8715, 2018.

9. Heterogeneous mixed molecular weight polymer brushes as neutral templates for BCP orientation control

Kaitlyn Hillery

10. Unraveling the Structure-Sensitive Nature of the Selective Electrocatalytic Hydrogenation of cis,cis-Muconic Acid

Deep Patel

cis,cis-Muconic acid (ccMA) is readily produced by fermentation of sugars and lignin, with potential to act as a bio-derived platform for the electrosynthesis of adipic acid (monomer unit of nylon-6,6) and other novel diacid monomers. An abundance of wind energy in the Midwestern United States motivates the use of green electricity to drive transformations in distributed applications, if appropriate catalysts for selective transformations can be developed. Given the wide range of products (trans-2-hexenedioic acid (t2HDA), trans-3-hexenedioic acid (t3HDA), adipic acid (AA), and muconolactone) obtained during the electrocatalytic hydrogenation (ECH) of ccMA [1,2], it is extremely important to develop the ability to control the selectivity of ccMA ECH to bio-advantaged molecules like t3HDA or t2HDA, which cannot be readily accessed from petrochemical feedstocks, as well as AA.

In this study, we use density functional theory (DFT) calculations and electrochemical experiments to obtain detailed fundamental information about the effect of catalyst structure on the reaction pathways involved in electro-reduction of ccMA to t3HDA, t2HDA, and AA. We consider the effects of composition (Pt vs. Pd) as well as surface structure (terraces and steps). Based on these atomic-level insights, we identify strategies to manipulate the selectivity of ccMA ECH by modifying the properties of the electrocatalytic interface.

References

1. Dell, Anna, M.N., Laureano, M., Bateni, H. et al. Green Chem. 23, 6456 (2021).
2. Matthiesen, J.E., Carraher, J.M., Vasiliu, M. et al. ACS Sustain. Chem. Eng. 4, 3575 (2016).

11. Invited Talk - Nanomaterial Ink Formulation for Aerosol Jet Printing of Electronics

Ethan Secor

Nanoscale materials offer unique opportunities to pattern functional devices using liquid-phase processing methods. Aerosol jet printing (AJP) is one such method well-suited for electronics fabrication, offering resolution as fine as 10 microns, non-contact deposition, digital control, and broad materials compatibility. This presentation will focus on materials development for AJP, emphasizing the interactions between colloidal ink formulation and printing process physics to drive morphology and functionality of printed components. This will first discuss the development of a graphene ink for AJP, along with the manipulation of ink chemistry to tailor microstructure and printing characteristics. The concept of multimaterial printing will be discussed, with an example of a nanoscale thermite composition mixed in situ during deposition. Finally, the broad opportunities for multimaterial printing in the area of patterning functionally graded materials will be introduced to highlight future work in this area.

Poster Presentation Abstracts

1. Understanding the Role of Chain Stiffness in Conformational Behaviors of Conjugated Polymers Liuqing Wang

Conjugated polymers (CPs), with their strong central chains and flexible side chains, show great potential for use in many advanced optoelectronic devices. This study employs coarse-grained molecular dynamics (CG-MD) simulations to explore the conformational properties of CPs with varying chain stiffness. The investigation considers a wide range of solvent quality parameters χ^s (i.e., from bad to good), temperatures, and backbone lengths to understand their collective impact on CPs conformations. Key structural metrics (i.e., R_{ee} , L_p , R_h , R_g , and $\langle R^2 \rangle$) are assessed to reveal how solubility and chain rigidity of CPs respond to environmental changes. The χ^s solvent condition is pinpointed to understand the balance of polymer-polymer interactions, where the χ^s parameter is determined under varying conditions. Additionally, the effect of backbone length on CPs structural properties is analyzed, shedding light on size-dependent structural effects. Our findings enrich the knowledge of CPs behaviors in dilute solutions, with implications for material design in organic optoelectronics, biosensing, and energy storage.

2. Laser-Induced Graphene (LIG) for Sensing Application Govinda Ghimire

Graphene is characterized by its infinite two-dimensional monolayer of sp² hybridized carbon atoms arranged in a honeycomb structure. Over the past decade, there has been remarkable growth in the utilization of graphene-based materials across various biosensing applications, owing to their exceptional electrical, chemical, mechanical, and optical properties. However, conventional fabrication strategies have several drawbacks, including complex setups and demanding preparation conditions. Direct laser writing on polyimide (PI) sheets offers a convenient and scalable method for producing Laser-induced graphene (LIG). A commonly employed CO₂ laser with a computer-controlled design makes LIG on the PI sheets. During the laser writing process, the localized heat of the laser dissociates the C-N, C-O, C-H, and C=O bonds on PI sheets, and the rearrangement of sp³ carbons into sp² carbon atoms, thus forming graphene. In this work, I will discuss our recent work toward using surface-modified LIG electrodes for the selective and sensitive detection of glucose molecules using the electrochemical and surface-enhanced Raman spectroscopy (SERS) method.

3. Vat Photopolymerization of Porous Polymer Scaffolds: Effect of the Structure on the Mechanical Performance. Heshani Walgamage

Polymer-based materials are preferred for biomedical applications due to their highly tunable properties and processability. In tissue engineering and regenerative medicine, polymer-based scaffolds are used to regenerate or replace damaged or injured tissues. Different structures such as gyroid, strut-based, and honeycomb can be used as porous scaffolds since they can be designed to help facilitate cell growth and are compatible with tissues. Porous scaffold design is one of the most critical aspects, as it governs the scaffold's overall mechanical behavior. Vat photopolymerization 3D printing is a technique that allows the fabrication of scaffolds with complex and customizable, potentially patient-specific designs. Investigating the complexity achievable via Vat photopolymerization and the effect of different lattice structures, porosity, and unit cell size variation on the mechanical properties of these scaffolds is crucial to obtaining functional and optimum scaffolds for biomedical applications.

4. 3D Printing of Porous Hydrogel-Based Scaffolds for Biomedical Applications Ashleigh Ballard

Hydrogels are 3D networks of hydrophilic polymer chains that absorb large volumes of water and swell, making hydrogels one of the softest materials. Hydrogels are an attractive material for biomedical applications as they can effectively mimic a variety of tissue types and extracellular matrices of human tissues. Bioprinting is a field focused on the 3D printing of hydrogel-based materials to create custom products for various biomedical applications. However, due to the soft nature of hydrogels, 3D printing with these materials creates a challenge that may require various reinforcement strategies for successful printing. Some of these reinforcement strategies may include the creation of a semi-interpenetrating network or an additional crosslinking of the hydrogel structure.

5. Collagen Immobilized Single-Walled Carbon Nanotube Sensors for High Throughput Screening of ECM Degrading Enzymes

Sepehr Hejazi

Extracellular matrix (ECM) degrading enzymes have gained attention in various therapeutic research including cancer treatment, wound healing, and tissue repair. SWCNT fluorescent sensors as an optical biosensor can enable rapid and real-time quantification of extracellular matrix degradation upon introduction of the target enzyme. In this study, we have developed different strategies to detect ECM degradation across a range of platforms, including solution-phase detection and gel-based detection (utilizing smart gels). These strategies depend on immobilized collagen-CMC-SWCNT sensors, enabling high-throughput screening of proteolysis activity in real-time.

6. Navigating Dilute CO₂ Reduction: Investigating the Role of Pore Channels and Size in Modified Mesoporous Carbon

Kanika Lalit

Direct electrochemical reduction of low-concentration CO₂ (8-15 vol%) from flue gas presents a promising pathway that eliminates energy-intensive CO₂ capture and purification, thereby reducing the carbon footprint associated with transforming CO₂ into valuable products. In this study, we introduce a modular synthesis approach for single-atom catalysts (SACs) that enables precise control over the mesoporous architecture of the carbon support. This meticulous control enabled us to regulate mass diffusion effectively within the carbon matrix, which enhanced efficiency in reducing low-concentration CO₂. A variety of templates, such as SBA-15, KIT-6, and MCM-48, were used to control the structural characteristics of the Ni-SACs meticulously. The Ni-SACs demonstrated greater than 80% Faradaic Efficiency (FE) across wide potential windows and exhibited high catalyst activity even at 5% CO₂ concentrations. While maintaining similar selectivity at low CO₂ concentrations, Ni-SACs with varying mesopore structures exhibited differences in the partial current density for CO production. This indicates that the engineering of pore channels and pore sizes in Ni-SACs plays a critical role in facilitating mass transfer within the catalyst, significantly enhancing its overall performance.

7. The role of crystallization of 3-pentadecylphenol in self-assembly of polystyrene – block – poly (4 – vinyl pyridine)

Nayanathara Hendeniya

The self-assembly of polystyrene – block – poly (4 – vinyl pyridine) complexed with 3-pentadecylphenol has been studied widely over the years. It is known that the ratio between the block copolymer and the small molecule can be used to control the rate of self-assembly, domain spacing, and grain size. While the behavior of 3-pentadecylphenol in complexed BCP solution is well-known, the crystallization induced by the long alkyl chain and its effect on self-assembly of the supramolecule in thin-film is not studied. Furthermore, there exists a lack of understanding whether the PDP molecules diffuse into polystyrene block when the ration of PDP is greater than 1. This study focuses on understanding the effects of crystallization of 3-PDP on self-assembly of complex supramolecule, PS-*b*-P4VP(PDP). We focus on ratios ranging from $r=0.5$ to $r=2.0$ (0.5, 1.0, 1.7, and 2.0) to investigate the existence of different crystallization regions depending on small molecule loading. Thermal analysis of the phase behavior is done using differential scanning calorimetry in bulk form. When the supramolecular solutions are cast into thin film form, the self-assembly and crystallization are both affected by surface and interface interactions. Therefore, the mechanism of crystallization may be different in thin films. We employ small-angle and wide-angle X-ray scattering techniques to investigate the phase behavior in thin film form. This study will reveal information on the behavior of 3-PDP in amphiphilic block copolymer complexes which are complementary to the understanding of the kinetic pathways of self-assembly of such supramolecules.

8. Optimizing Laser-Induced Graphene for Glucose Sensing: A Machine Learning Approach

Farshid Noormohammadi

Graphene is a promising biocompatible carbon material with potential applications in biosensor development owing to its high electrical conductivity, electroactive surface area, and mechanical strength. Localized heat produced by direct laser writing on polyimide (PI) sheets offers a convenient and scalable method for producing graphene, commonly called Laser-induced graphene (LIG). Different lasering parameters like laser speed, pulse width, wavelength, and power affect the quality of the graphene. Optimizing all these inter-dependent parameters to achieve good quality graphene using conventional methods such as grid search or random selection is very challenging. In our work, we have employed an AI-based machine learning (ML) approach and applied Bayesian model-based optimization to find the optimum lasing parameters. The optimized parameters yielded the LIGs with excellent conductivity and mechanical stability. We will use these optimized LIGs for the selective and sensitive detection of glucose molecules.

9. Observing Surface Dynamics in Heterogeneous Catalysts Using NMR

Jacob Mayer

Much like enzymes, their biological counterpart, understanding how synthetic catalysts work often comes down to structure and dynamics. While considerable work has been done to determine the structure of heterogeneous catalytic active sites using electron microscopy, NMR, and X-ray spectroscopy, molecular motions and their impacts on catalysis are poorly understood. A key factor limiting the study of molecular motions for surface sites is the lack of dynamically-sensitive methods that can be applied to low-abundance surface sites. Common approaches to detect molecular motions include the measurement of anisotropic interactions using NMR spectroscopy. Dipolar couplings are sensitive to molecular reorientations, and thus motions, and are frequently used to resolve motions with atomic resolution. Most methods, however, require expensive isotope enrichment to have the necessary sensitivity for surface characterization. We introduce a new method which combines frequency selection with multiple-quantum excitation to measure intra-CH₂ dipolar coupling that can be used as sensitive dynamics probes, without the need of isotopic labeling. We demonstrate the applicability of the method on the study of motions in silica-supported metallocene complexes.

10. Energy-Efficient Synthesis of Organic-Inorganic Hybrids Through Polymer Complexation

Shaghayegh Abtahi

Vapor phase infiltration (VPI) processing is an emerging gas-phase method for producing organic-inorganic hybrid materials. This method involves the diffusion of vapor phase metalorganic precursors into organic polymers, leading to their transformation into versatile organic-inorganic hybrids. These materials have a broad range of applications ranging from lithography patterning to foam and textile manufacturing. Nonetheless, a notable challenge in this method is the requirement for highly pyrophoric and cost-effective precursors such as trimethylaluminum (TMA) to diffuse into the polymer chains and the bulk of material. These constraints necessitate a transition towards more environmentally friendly and economically viable alternatives for VPI precursors. Addressing these limitations, we introduce a novel approach to depositing metalorganics into polymer films. By using elements of periodic table with accessible d-blocks such as Silicon, capable of readily forming dative bonds with electron donor polymers such as poly(4-vinylpyridine) (P4VP) we can effectively infiltrate metalorganic precursors into the polymer chains to create organic-inorganic hybrid complexes at ambient room temperature, while minimizing the use of toxic gases.

11. Probing the Hard Carbon Anode Materials for Sodium-Ion Batteries

Isuru Gusthignawadu

Hard carbon also known non graphitizable carbon is a promising anode material for alkaline ion batteries such as Sodium ion and Lithium ion batteries. The ion storage in this material is still not well understood due to the complex structure of this material. Characterization of this material unveils a structure consisting of both sp² and sp³ hybridized bonding. Thus the microstructure consists of curved and randomly oriented graphene layers giving rise to crystallites and nanovoids between them. It is a well known fact that Li ions can be intercalated inside graphite such that graphite anodes show a high reversible capacity in Li ion batteries around 372 mAhg⁻¹. But graphite performs poorly (35 mAhg⁻¹) in sodium ion batteries compared to hard carbon (300 - 335 mAhg⁻¹). Optimizing hard carbon for better capacity and better capacity retention requires better understanding of its structure. This study investigates the structural evolution of Hard carbon from different carbonaceous precursors and under different carbonizing conditions.

12. Controlling Dispersion of Rhodium from Single-Atoms to Nanoparticles

Andrew Lamkins

The development of single-atom catalysts has been an increasingly popular subject in heterogeneous catalysis research. The ability to ensure every atom of high-value metals can participate effectively in a reaction will lead to lower costs as less metal is needed to achieve the same output. We have developed a method of dispersing single rhodium atoms onto the surface of SBA-15 using simple impregnation. A high amount of Cl⁻ present during reduction leads to atomic isolation of the metals by preventing nanoparticle formation. Additionally, this method can be used to control the dispersion, ranging from single atoms to nanoparticles. We applied these catalysts to the hydroformylation reaction at low temperatures and demonstrated excellent activity towards the formation of aldehyde products. CO-DRIFTS and XAS studies were conducted to characterize the single-atom dispersion of the rhodium atoms.

13. Catalytic Deconstruction of Polyethylene via Hydrogenolysis using Localized Zirconium Oxide Catalyst in Core-Shell Architecture

Longji Li

The accumulation of plastic waste and the consequent pollution of the environment is becoming a threat to our society. As the most produced plastic, polyethylene is well known for its mechanical and chemical stability. In this work, we have used the Earth-abundant, non-reducible zirconium oxide catalyst and localized it in the core-shell architecture and show its application in the hydrogenolysis of low-density polyethylene (LDPE). Spectroscopic studies confirmed the active sites, zirconium oxide, are located on the silica nanoparticles and confined at the bottom of the mesoporous silica shells. The structural design allows polymer chains to diffuse and interact with the zirconia nanoparticles, and the chain gets continuously cleaved into smaller hydrocarbon fragments. The zirconia catalyst demonstrated a 57% conversion of the LDPE within 10 h and a narrow product selectivity of C₂₆-centered paraffin with potential applications in lubricant oil. The presence of a mesoporous silica shell greatly enhanced the activity and selectivity, and the comparison of catalytic performance with the open-ended L-ZrO₂@mSiO₂ catalyst indicated that the closed-ended local environment results in a liquid product with a higher carbon number.

14. Elucidating the Role of HSQ polymer structure on the Photoluminescent Properties of Silicon Nanocrystals

Maharram Jabrayilov

The synthesis of silicon nanocrystals (Si NCs) via various routes has garnered significant interest due to their unique photophysical properties and potential applications. Among these methods, colloidal synthesis from high-temperature pyrolysis of commercial hydrogen silsesquioxane (HSQ) precursors has emerged as a facile approach for achieving size-controllable Si NCs with distinct photoluminescent characteristics. However, challenges such as limited shelf life, high cost, and restricted availability of commercial HSQ necessitate exploration of alternative precursors. Recent studies have investigated the use of sol-gel polymer precursors derived from silanes, offering a cost-effective and tunable option for Si NC synthesis. The structure and composition of these HSQ polymer precursors significantly influence the photoluminescent properties of Si NCs. Understanding the role of HSQ polymer structure is crucial for optimizing Si NC synthesis and enhancing their photoluminescent performance. This abstract elucidates the influence of HSQ polymer structure on the photoluminescent properties of Si NCs, highlighting the importance of precursors selection, synthesis parameters in tailoring Si NC characteristics for diverse applications.

15. Polyethylene Deconstruction by Non-Precious Molybdenum Oxycarbide via Hydrocracking

Minghui Niu

Effective catalytic strategies for upcycling polyethylene and other polymer wastes into valuable hydrocarbon products are highly desirable from both environmental and economic perspectives. Herein, we report new MoO_xC_y nanosheet catalysts that exhibit excellent activity and 81.54 % selectivity for hydrocracking low-density polyethylene into liquid hydrocarbon fuels in the C₈-C₂₅ range, narrowly centered around C₁₂-C₁₃ hydrocarbons. The MoO_xC_y nanosheets were synthesized via a two-step process involving first the growth of MoO_{3-x} nanosheets, followed by carburization and controlled surface oxidation. This treatment generates a bifunctional nanostructure containing metallic Mo₂C sites interspersed with acidic MoO_x sites. The optimized MoO_xC_y-4 catalyst displayed a high rate of polyethylene hydrocracking to liquid hydrocarbons at relatively mild conditions of 300 °C and 200 psi H₂. Characterization data suggests a cooperative mechanism where the Mo₂C metallic sites activate H₂ and initiate hydrogenation steps, while the MoO_x acidic sites promote C-C cleavage via carbonium ion intermediates, resulting in a high degree of isomerization and branching. This nanosheet architecture provides a promising new approach to designing highly active, low-cost catalysts for effectively upcycling polyethylene and other polymer wastes into valuable liquid fuels and chemicals through hydrocracking processes.

16. 2D Materials for the Future of Neuromorphic Computing

Andrew Tan

With the widespread and diverse use of computing systems, it's easy to see why so many are interested in improving our computing hardware. In the past decades, this has mostly been achieved through miniaturization of the transistor nodes which allows more computing power to be packed into smaller chip areas, but this approach can only go so far. With transistor sizes now reaching the single nanometer ranges, physical limitations make it difficult to go farther. With this in mind, it makes sense that we might want to explore other potential computing paradigms that could handle some of the issues that arise from current architectures. One of the largest fundamental flaws of modern computing is the separation of memory and processing units known as Von Neumann architecture. Although this paradigm allows for a high degree of flexibility and modularity in the system, it also requires a lot of energy due to data transmission and storage for the memory and CPU. One solution to this issue is neuromorphic computing. Neuromorphic computing tries to mimic the way brains process information by utilizing units called memristors which can both hold data and perform computations. In my poster I will present my work on a proof of concept ion-intercalation based MoS₂ memristor. I will discuss previous literature in the area, the theorized mechanism, and future work and ideas relating to the project.

17. Assessing the formation of Lewis and Brønsted sites in the hydrodeoxygenation of lignin derivatives over MoO₃

Zeinab Hajali Fard

Molybdenum oxide (MoO₃)-based catalysts are promising for deoxygenating lignin-derived biomass, offering efficient oxygen removal without excessive hydrogen consumption or aromatic ring saturation. However, MoO₃ tends to undesirably convert aliphatic molecules into lower-value alkanes during this process, limiting its economic viability. To enhance catalytic performance, it is crucial to comprehend the surface structure and the roles of Lewis and Brønsted acid sites in the hydrodeoxygenation (HDO) process. This study employs density functional theory (DFT) calculations to investigate the formation of different adsorption sites on the MoO₃ (010) facet and the variation in binding energies for various functional groups adsorbed on Lewis and Brønsted acid sites. Brønsted site creation is most energetically favored at the asymmetric oxygen site, whereas terminal oxygen is the most probable site for Lewis acid site formation. Ketones emerged as the most stable compounds on this surface, with Lewis acid sites being the primary adsorption sites for most of the studied adsorbates, although Brønsted acid site is formed at a lower energy cost. Ongoing work combines experimental methods with activation energy (nudged elastic band) calculations to elucidate the HDO reaction mechanism over this complex surface.

18. Structure Determination of 2D Semiconductor Materials by Solid-State NMR Spectroscopy

Lukman Yunusa

19. Exploring Photoluminescence Dynamics of Silicon-Based Nanosheets For Optoelectronic Devices

Abhishek Chaudhari

This study explores the photoluminescence dynamics of silicon-based nanosheets and their implications for optoelectronic device applications. Silicon nanosheets, with their unique two-dimensional structure, exhibit distinctive photoluminescence properties that are crucial for the development of advanced optoelectronic components. Our investigation centers on how these properties evolve under various excitation conditions. Through comprehensive spectroscopic analysis, we assess the impact of nanostructure and environmental variables on the emission characteristics of the nanosheets. Notably, we demonstrate that modifications in the electronic structure due to different fabrication techniques significantly alter the photoluminescence dynamics, affecting both the intensity and decay patterns of emitted light. Our findings highlight the potential of silicon-based nanosheets in enhancing the efficiency and functionality of optoelectronic devices, including photodetectors and light-emitting diodes.