AMES Historical Projects Opportunities

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Artificial Intelligence (AI) - Research in One or More Problem Domains

Project Name: DataScience

Title: Data Science for Materials Science **PI:** Long Qi

Description:
Data science has drastically changed and advanced how chemical research is conducted. We would like to introduce new methodologies of data science (artificial intelligence) and robotic high throughput instruments to materials chemistry for catalysis and separation, which is the key in the chemical and mining industries.

In this project, new methods, including 3D printing and artificial intelligence, will be developed and implemented to increase the instrument efficiency and understand more of the experimental data. Workflow with robotic high throughput instruments will be developed for different case studies.

Chemistry

Project Name: AI-driven automated separation **PI:** Lun An

Title: The development of automated separation processes enhanced by artificial intelligence for the efficient and selective recovery of critical materials.

Description:
Accelerating the research, development, and deployment (RD&D) of sustainable manufacturing processes for rare-earth elements (REEs) as critical materials requires both scalable synthesis of extractive ligands and rapid evaluation of extraction conditions. In this project, we will develop an integrated RD&D methodology that combines agile ligand synthesis with automated, high-throughput solvent extraction studies. The use of Rxn Rover automation software enables artificial intelligence (AI)-guided supervision to reduce experimental complexity and significantly shorten process optimization timelines. This work demonstrates the value of coupling automated synthesis with application-driven performance testing to accelerate the discovery of functional extractive ligands. The outcomes of this project will support the development of closed-loop, AI-controlled platforms for intelligent, autonomous manufacturing of critical materials.

Project Name: Single atom catalysts

Title: Novel hybrid materials for single atom catalysts **PI:** Damien Culver

Description:
Heterogeneous catalysts are utilized in industry to produce most of the chemicals utilized in every product in society. Many of these catalysts require significant quantities of precious metals to perform the reactions effectively but much of the metal does not participate in the reactions which is an inefficient utilization of critical resources. Complex organic molecules are capable of stabilizing single atoms of precious and abundant transition metals to the surface of oxides for catalytic reactions with most (if not every) metal atom active. However, stabilization of low valent transition metals necessary for many important catalytic reactions is still very challenging. In this project, we are designing and synthesizing simple organic molecules in the surface of oxides to stabilize important, low-valent transition metals for catalytic reactions relevant to society. This project will provide a SULI intern the opportunity to gain hands-on experience in the handling of air sensitive materials within a glovebox, performing catalytic reactions, and obtaining and analyzing spectroscopic data.

Project Name: Unusual Bonds

Title: Unusual bonding in unusual molecules **PI:** Mark Gordon

Description:
Experimental chemists are extremely clever at synthesizing and characterizing novel and unusual molecules. It is then up to theorists to develop a sound interpretation of the experimental observations. Our quasi-atomic orbital analysis is ubiquitous in this regard having successfully intercepted such unusual molecules as infinitenetetrahedrane and RhB. This project will allow a SULI student to develop a fundamental understanding of recently discovered molecules.

Project Name: Upcycling of Plastics

Title: Chemical Upcycling of Waste Plastics **PI:** Wenyu Huang

Description:
Polymers are irreplaceable in the global economy, with myriad uses in packaging, construction, transportation, electronics, and healthcare industries. However, their massive-scale manufacture, single-use function, long lifetimes, slow decomposition rates, and disruption of sensitive ecosystems have created a plastic waste crisis. Unfortunately, conventional mechanical recycling methods are limited by considerable technological and economic challenges. Chemical upcycling, an emerging alternative to the classical recycling approach, would use plastic waste as a feedstock to synthesize value-added chemicals and materials. This project will focus on developing advanced catalysts and novel catalytic processes that can achieve efficient and selective upcycling of waste plastics to high-value chemicals. In particular, we want to (1) develop catalysts based on cheap and more abundant metal elements, (2) increase the activity and selectivity of the catalytic conversion, and (3) enlarge the scale of the conversion process.

Project Name: Intermetallic Catalysis

Title: Ordered Intermetallic Compounds for Heterogeneous Catalysis **PI:** Wenyu Huang

Description:
Precious metals and metal alloys are important heterogeneous catalysts for renewable energies and materials. However, both of them have their limitations. Precious metals have low natural abundance and are expensive. Metal alloys have unstable surfaces due to surface segregation under reaction conditions, which renders the identification of active sites and the understanding of reaction mechanisms difficult. My research group will address these limitations by developing new intermetallic NP catalysts. Intermetallic compounds, which consist of two or more metallic elements, adopt
specific crystal structures as well as electronic structures different from the constituent

elements. The modified electronic structures of intermetallic compounds make them unique catalytic materials. It has been proposed that such compounds should be treated as new "elements", considering their potential in catalysis. The inherent properties of intermetallic compounds, stable and exhibit a large variety of structures, will help us to discover catalysts with stable surfaces, consisting of more abundant metals, to replace unstable alloy and precious metal catalysts.

Project Name: Flow chemistry

Title: Catalytic CH activation of hydrocarbons enhanced by heterogeneous flow reactions
PI: Yuting Li

Description:
Gas/liquid/solid multiphase reaction plays an important role in chemical reaction engineering. The heterogenous flow reactor for multiphase reactions are wildly applied in petroleum industry, biochemical, fine chemical and pharmaceutical industries, because of their flexibility, simplicity of operation and high throughput. The batch conversion of hydrocarbon into value-added chemicals through C-H activation/functionalization limit the total turnovers and the selectivity of ideal products due to the deactivation of catalysts and side reactions. Therefore, my project is to establish the desired multi-phase reactor and employ it to heterogeneous catalysis including CH borylation or CH activation of hydrocarbons resulting in the better selectivity and accumulated turnovers.

Project Name: 17O-NMR-Shifts

Title: Probing Catalyst Electrophilicity Using 17O NMR **PI:** Fred Perras

Description:
Heterogeneous catalysts are used in the production of about 90% of all goods. These are typically produced via the immobilization of a metal species onto a chemically inert support material; typically, an oxide such as silica or alumina. The activity of a metal center in catalysis is highly dependent on its electronic state. For instance, early transition metals and rare earths are largely Lewis acid sites and catalyze hydrocarbon functionalization or polymerization reactions. They thus tend to have increased activity when they are more electropositive (electron deficient). The metal's electronic state depends on structural factors, such as the bonding motifs to the support material and the ligands coordinating to the site, which enables a certain level of tunability in the activity of the site.

While it is possible to study electronic structure in silico using quantum chemical calculations, this requires knowledge about the exact structure of the species, which requires experimentation. Secondary dative interactions are further difficult to detect, adding ambiguity into the structure that needs to be used to evaluate electronic state using

calculations. Ideally, one would want to decouple estimations of electronic state from the ambiguities in chemical structure and instead measure electronic structure directly.

Ames National Laboratory has world-leading dynamic nuclear polarization (DNP) instrumentation that enables for difficult NMR experiments to be performed on surface sites. Orbital analysis further suggests that the 17O chemical shift from the support-O-M site is highly sensitive to metal electrophilicity. These sites can be investigated directly using DNP potentially enabling the direct investigation of metal electrophilicity.

The SULI student joining this project would perform high-level density functional theory (DFT) calculations of 17O chemical shifts as a function of chemical structure and bonding strength to identify the exact orbital pathways that control the shift and tie it to electronic state. We would also synthesize a variety of group 4 supported metal complexes to measure metal-induced 17O chemical shifts using DNP-enhanced solid-state NMR spectroscopy at two magnetic fields (9.4 T and 14.1 T). We would chiefly vary the electron withdrawing potential of the ligands in a systematic way to control the electrophilicity of the metal. We anticipate the results from this project to lead to a new versatile method for directly probing metal electrophilicity and would have a direct immediate impact on the AMES Catalysis Research Program.

Project Name: Supported catalysts

Title: Supported Catalysts **PI:** Long Qi

Description:
Supported metal complexes are promising heterogeneous catalysts for the selective activation of strong covalent bonds (such as C-O and C-H) in renewable feedstocks. In this project, the project participant will work in diverse interdisciplinary areas, including organic synthesis, electrocatalysis, and materials chemistry alongside lab scientists and postdoctoral researchers. The detailed workflow of the project is described as below; 1) synthesize a series of organic macrocyclic - metal complexes; 2) characterize these molecular complexes using Nuclear magnetic resonance (NMR), mass spectrometry (MS), ultraviolet–visible spectroscopy (UV/Vis), X-ray crystallography, elemental analysis (EA), and cyclic voltammetry (CV) techniques; 3) learn to graft these complexes onto the inorganic material surface; 4) perform catalytic performance evaluation by setting up different reactions.

Project Name: Fragments

Title: Studying Effect of Basis Set Superposition Error on Molecular Properties
PI: Ryan Richard

Description:
In quantum chemistry we necessarily use incomplete basis sets to simulate atomistic systems. If a property is computed using a series of calculations, and those calculations use basis sets of different completeness, then an imbalance occurs. This imbalance is known as basis set superposition error (BSSE). Correcting for BSSE is as "simple" as ensuring that all calculations use basis sets of the same completeness. In practice, needing to BSSE correct a calculation adds a significant amount of computational time. At the same time it is known that some properties are more susceptible to BSEE than others. The goal of this study is to systematically consider how BSSE affects a range of properties including: molecular geometry, molecular orbitals, and multipole moments.

Project Name: Plastic Upcycling

Title: Catalytic Upcycling of Polyolefins **PI:** Aaron Sadow

Description:
The large amount of plastic waste that is produced each year ends up in landfills and in the ocean, as a result of limited end-of-life opportunities. We are discovering new catalytic reactions, synthesizing new catalysts, and developing new catalytic processes for the conversion of these discarded materials into 'upcycled' products. The project will entail catalyst synthesis, reactor construction and modification, catalytic conversion, and product analysis. The student will use gas chromatography and nuclear magnetic resonance spectroscopy, and possibly size exclusion chromatography to characterize polymers and products, from reactions with hydrogen in the presence of a catalyst.

Project Name: Organometallic Catalysis

Title: Organometallic Catalyst Synthesis and Catalytic Reactions **PI:** Aaron Sadow

Description:
We are synthesizing new organometallic compounds for catalysis. This involves organic chemistry, to create the ligand, and then coordination chemistry to make organometallic complexes. Then, the complexes are characterized by advanced spectroscopic methods, such as NMR, IR, and crystallography. Then, we study catalytic transformations. We are particularly interested in main group and lanthanide metal complexes for CH bond activations, to convert hydrocarbons into more valuable products.

Computational Sciences

Project Name: Autonomous Laboratory Software

Title: Autonomous Laboratory Software Development for Critical Minerals and Materials
PI: Theresa Windus

Description:
The United States faces a critical minerals and materials (CMM) shortage that requires rapid research, development, and deployment workflows to utilize untapped domestic feedstocks. At Ames National Laboratory, Rxn Rover - a modular, open-source reactor automation platform - combines reactor hardware, sensors, and artificial intelligence/machine learning (AI/ML) to enable standard CMM processes like autonomous synthesis, separation, and extraction. Self-driving, or autonomous, laboratories enabled by Rxn Rover and similar technologies can save hundreds of person-hours per month and improve data reproducibility and laboratory safety. This project will help develop technologies to address national supply chain issues by expanding Rxn Rover's plugin architecture and AI/ML capabilities. Additionally, this project offers opportunities for interdisciplinary collaboration with experimental researchers as developed technologies are integrated into the laboratory.

Project Name: Lanthanides-peptide binding

Title: Lanthanides-peptide interactionsBenchmarking Computational Methods for Lanthanide–Biomolecule Interactions **PI:** Peng Xu

Description:
Lanthanide elements are critical materials with essential roles in energy technologies, advanced magnets, lighting, nuclear applications, and chemical separations. Understanding how lanthanide ions interact with biomolecular ligands is important both for fundamental coordination chemistry and for the development of bio-inspired ligands for selective binding and separation of f-block elements. This project will focus on the computational characterization of lanthanide–ligand and lanthanide–amino acid interactions, with an emphasis on how different model core potentials (MCPs), effective core potentials (ECPs), and basis sets influence predicted structures and binding energetics. The work will provide a systematic assessment of how computational approximations affect the description of highly charged, strongly polarizing lanthanide ions in aqueous and biomolecular environments.

The student will perform a tiered benchmarking study using density functional theory (DFT) as the primary production method, supplemented by higher-level wavefunction-based methods for small reference systems. Small lanthanide–ligand complexes (e.g., water,

acetate, and imidazole) will be used as benchmark systems for comparing different MCPs, ECPs, and basis set combinations at the DFT and second-order Møller–Plesset perturbation theory (MP2) levels, with coupled-cluster calculations applied where feasible to non-f-block analogs. The best-performing computational protocols will then be applied to more realistic lanthanide–amino acid and short peptide complexes in solution. Through this project, the student will gain hands-on experience in high-performance computing, electronic structure theory, and quantitative data analysis while addressing a problem directly connected to DOE interests in critical materials and molecular-level separations science.

Condensed Matter Physics

Project Name: NMR study on quantum materials

Title: Nuclear magnetic resonance study on quantum materials **PI:** Qing-Ping Ding

Description:
Quantum materials, including unconventional superconductors and quantum spin liquids, hold significant potential for the future of quantum computing. We intend to investigate the physical properties of these materials under extreme conditions—such as ultra-low temperatures, high magnetic fields, and high pressures—using nuclear magnetic resonance (NMR). NMR studies on quantum materials leverage spin dynamics to probe exotic states. This approach provides critical insights into electronic structures, fractionalized excitations, and quantum phase transitions, all of which are essential for understanding superconductivity and developing quantum computation technologies. By detecting the spin textures, NMR allows us to characterize quantum magnets, frustrated magnets, and field-induced quantum phases. These measurements reveal vital details about spin liquids and their fractionalized excitations. These NMR measurements offer non-invasive access to the microscopic world of quantum materials. By uncovering fundamental properties, this research aims to pave the way for new quantum technologies and discoveries.

Project Name: Magnetic Interaction in Quantum

Title: Spiral Spin Liquids **PI:** David Vaknin

Description:
This project involves computational simulations of frustrated magnetic systems, with the goal of inferring exchange interactions from elastic and inelastic neutron scattering data for honeycomb-like magnetic materials such as $CaMn_2P_2$ and $SrMn_2P_2$. The student will learn fundamental concepts in solid-state physics, including diffraction, inelastic scattering, and magnetism, and will apply these principles to simulate novel materials that exhibit exotic magnetic structures and unusual spin dynamics. Simulations will be performed using

established computational packages. Prior experience with Python and/or Julia is preferred but not required, as these skills can be developed during the internship.

Project Name: Magnetization of thin films

Title: Magnetic measurements of ultra-thin films and interfaces **PI:** Ruslan Prozorov

Description:
Magnetic susceptibility of ultrathin superconducting films from tunnel-diode resonator measurements. Magnetic susceptibility is one of the most information-rich thermodynamic and electrodynamic probes of superconductivity. High-precision susceptibility measurements provide direct access to the London penetration depth, l, linked to the superfluid density, rs. Analysis of rs allows making conclusions about the superconducting gap structure. In ultrathin films and two-dimensional (2D) superconductors, such measurements are hindered by extreme demagnetizing effects, and the only technique used was mutual inductance, which has significant limitations. We developed a unique frequency-domain tunnel-diode resonator (TDR) capable of detecting signals from atomic superconducting monolayers. We have also developed a robust protocol to calibrate the results and extract l(T). The physics of 2D superconductors is one of the most vibrant areas of research in condensed matter physics. Not only it is linked to unique effects, such as Berezinskii-Kosterlitz-Thouless (BKT) topological phase transitions, it is used in developing superconducting qubits (transmons) for quantum computing applications. The TDR method combines exceptional sensitivity with contactless measurement in very small AC magnetic fields, enabling quantitative extraction of the London penetration depth (and hence superfluid density) from thin-film data. For the first time in our laboratory, we can obtain a quantitative estimate of the absolute London penetration depth in ultrathin films and track its temperature dependence with high resolution. This provides a direct route to determine the superconducting gap structure and the symmetry of the order parameter (fully gapped vs nodal behavior, single-gap vs multi-gap), and it can constrain microscopic pairing mechanisms. In this SULI project we will focus on modern 2D superconductors and thin-film platforms of broad current interest: (i) interfacial superconductivity between otherwise non-superconducting constituents (e.g., CrTe2/FeTe), (ii) infinite-layer nickelate films believed to be analogs of high-Tc cuprates, (iii) Nb and Ta films used in superconducting quantum circuits (transmon devices), and (iv) additional ultrathin superconducting films where signatures of a BKT transition may be present. In this project, you will perform precision susceptibility measurements on ultrathin superconducting films using our TDR frequency-domain spectrometer and analyze the data to determine the London penetration depth and superfluid density. You will work with a graduate student, a postdoctoral researcher and a senior staff scientist (of Ames National Laboratory), and you will contribute to an active research direction with clear publication potential. This is not a toy project but part of our active research. A specific system to study will be selected based on the availability of samples at the time of the student's internship.

Project Name: QCP by strain

Title: Using linear strain to study quantum phase transitions in superconductors
PI: Ruslan Prozorov

Description:
Research Background Information: Quantum phase transitions (QPT) have been the major topic in condensed matter physics (CMP) research for the last three decades. Conventional phase transitions, such as ice-water-vapor or ferro-para-magnetism, are driven by thermal fluctuations. In contrast, quantum phase transitions occur at T = 0 and are driven by quantum fluctuations. Because these transitions occur at T=0, to navigate through them on the phase diagram, non-thermal parameters must be employed. They include magnetic field, pressure, or material composition. The most interesting questions are in the systems where two quantum phases coexist, such as the electronic density wave and superconductivity. It is believed that fluctuations in the electronic phase may be responsible for superconductivity. This field of physics is a very active area of research at Ames National Laboratory. QPTs occur in many exotic electronic and magnetic phases and quantum materials, particularly in high-temperature and unconventional superconductors, which hold great potential importance for energy-related technologies.

One interesting material studied in our group is $(Ca_{1-x}Sr_x)_3Rh_4Sn_{13}$, which is known to have a charge density wave (CDW) that terminates at the quantum critical point (QCP) inside a superconducting phase. By changing the composition, x, the transition temperature decreases to lower and lower values, vanishing at a QCP as $T \rightarrow 0$. So far, we have demonstrated this physics using the composition, x, and non-magnetic disorder as non-thermal tuning parameters. However, in both cases, we can apply only a discrete set of tuning values – a finite number of compositions and a finite number of electron irradiation fluences due to the nature of their realization. In addition, disorder results in an irreversible change – once the sample is disordered, it cannot be returned to its original state.

In this SULI project, we will explore using tensile and compressive linear strains to drive the system (reversibly) through the QPT. The CDW is coupled with structural distortion, which transforms the crystal lattice from a cubic to a lower symmetry structure. We know the direction of the CDW lattice distortion, and by applying strain along that direction, we aim to tune the crystal towards a QCP. The control experiment will involve applying strain in other directions, where it should not have that effect or have it reduced.

Electrical Engineering

Project Name: AIM-CMM

Title: AI-Accelerated Design of Reduced-Critical-Material Permanent Magnet Motors
PI: Ajay P. Singh

Description:
The growing supply-chain risk of Nd–Fe–B permanent magnets—critical to electric vehicles, wind energy, and defense applications—has intensified the need for less-critical magnet alternatives. However, evaluating substitute materials in permanent-magnet (PM) motors is hindered by the high computational cost of iterative finite-element analysis (FEA)-based design workflows. To address this challenge, this project introduces a novel AI-driven framework that dramatically accelerates PM motor design and performance evaluation. This work assesses the feasibility of using CMI-developed less-critical magnets as substitutes for Nd–Fe–B in e-bike motor applications. The approach combines advanced optimization with high-fidelity FEA to generate a diverse motor design dataset spanning geometry, materials, and operating conditions. This dataset is used to train a deep-learning model capable of rapidly predicting motor performance and proposing feasible designs in near real time. The results demonstrate that AI-enabled modeling can significantly reduce design time while enabling efficient exploration of reduced-critical-material motor solutions.

Materials Science

Project Name: Soft Magnets

Title: Advanced Soft Magnetic Alloys for Next-Generation Electromagnetic Devices
PI: Andrew Kustas

Description:

Conventional soft magnetic alloys exhibit favorable functional properties for electromagnetic devices such as motors, transformers, and switches, including high permeability, high saturation induction, low coercivity, and low core loss. However, many alloys are limited in mechanical strength, ductility, and electrical resistivity, resulting in undesirable and often inversely correlated property tradeoffs that constrain electromagnetic device design and performance. The goal of this project is to develop soft-magnetic alloys with reduced property tradeoffs by leveraging advanced processing and

alloy design strategies to tailor structure-property relationships. Experimental efforts will focus on establishing links between processing, microstructure and properties. We seek a student to contribute to these experimental activities, which may include, but are not limited to: (1) processing of alloys using advanced solidification and powder metallurgy techniques, (2) metallographic preparation with corresponding structural and compositional characterization, and (3) evaluation of mechanical and magnetic properties.

Project Name: Vanadium Powder

Title: Characterization of Vanadium Powders for Nuclear Fusion Applications
PI: Jordan Tiarks

Description:
This project will characterize gas-atomized vanadium powders—focusing on low-activation V–Cr–Ti compositions—being developed as candidate fusion first-wall materials. Developing novel, radiation-tolerant, low-activation materials is essential for the reliability and maintainability of future fusion systems, enabling components that can withstand intense neutron flux, high temperatures, and corrosive plasmas while minimizing long-lived waste. The goal of this project will map process–structure–property relationships by correlating atomization inputs with particle size distribution, morphology, and surface chemistry. Hands-on tasks may include powder size analysis (laser diffraction, image-based PSD from SEM micrographs, complementary sieve/tap density), metallographic sample preparation and microstructural and chemical analysis to understand interstitial pickup and segregation within the powder samples.

Project Name: iRAG for In-Service Ductility

Title: Fine-Tuning RAG Models for Refractory Alloy In-Service Ductility Prediction
PI: Prashant Singh

Description:
This project aims to create a fine-tuned RAG-based model for predicting ductility and strength degradation in structural alloys during service, with a specific focus on refractory multi-principal element alloys (MPEAs) used in extreme environments. While prior work such as DuctGPT focuses on computational and experimental descriptors for designing new alloys, this effort targets in-service performance by integrating physics-based features (composition, grain size, phase fractions), environmental exposure data, irradiation or thermal history, and textual inspection records. A vector-based retriever will be trained to surface relevant historical cases particularly those involving Nb-, Ta-, Mo-, and W-based refractory alloys, and a GPT-style reader will be fine-tuned to output quantitative property predictions with uncertainty estimates. The student will evaluate the impacts of retrieval quality, feature selection, and domain drift, producing a compact model and workflow that

can support future human-AI co-analysis tools for materials reliability assessment in nuclear fusion systems, aerospace propulsion components, high-temperature reactors, and other extreme-environment applications where refractory alloys are critical.

Project Name: AI/ML for Magnet Design

Title: Uncovering Hidden Families in Permanent Magnets via Machine Learning
PI: Prashant Singh

Description:
Understanding intrinsic similarities among permanent magnet materials is essential for accelerating discovery and enhancing magnetic performance. This project develops an integrated machine-learning framework that combines unsupervised clustering and supervised modeling to uncover latent families and predict key properties including saturation magnetization and energy product in rare-earth, transition-metal, and multi-principal-element magnets. Leveraging physics-based feature engineering, we aim to elucidate structure-property relationships and identify pathways to optimize saturation and energy product. This approach provides interpretable guidance for targeted alloy design, microstructural tuning, and the discovery of high-performance magnets.

Project Name: Novel Nanostructures

Title: Novel nanostructures- making each atom count **PI:** Rana Biswas

Description:
The Ames National Laboratory solid-state nuclear magnetic resonance (ss-NMR) project is engaged in the synthesis and characterization of novel nanostructures/nanomaterials including two-dimensional semiconductors (semiconductor nanosheets, borophanes, MXenes), semiconductor quantum dots (including CdSe/CdS), metal-organic frameworks, and inorganic perovskite nanoparticles. Their properties depend critically on the surfaces of these nanostructures including surface functionalization. NMR spectroscopy provides fascinating information on the local environments of atoms on the surface, that are not possible with other probes. This project will computationally model these nanostructures with density functional calculations, utilizing relativistic effects for heavy atoms, to determine the chemical shifts of atoms on surfaces and how these depend on the precise geometry and nanostructure. The modelling tools include the Materials Studio software and Amsterdm Density functional packages. The project is expected to uncover how individual atoms or molecular groups in these nanostructures can explain many puzzling features of ongoing experiments. Past SULI students have published research papers as an outcome. This computational project will be jointly performed with members of the ss-NMR group at Ames National Laboratory, through active discussions and group meetings.

Project Name: REE Data Language Project

Title: REE Data Language Project: Developing Cross-Disciplinary Ontologies for Rare Earth Separations **PI:** Tanya Prozorov

Description:
We are surrounded by vast amounts of scientific data, but much of it is isolated within different fields, each using its own terms and ideas. Mining, extraction, and separation of rare earth elements (REEs) is a prime example of a technologically important area facing this challenge. To make sense of this data and help both scientists and machines connect the dots across disciplines, we need a shared language. Different experimental techniques come with their own terminology, units, and measurement methods. This project focuses on building cross-disciplinary ontologies — structured frameworks that define key terms and relationships — so scientists from diverse fields can more easily understand and collaborate. You will explore and describe important scientific techniques such as X-ray Diffraction (XRD), X-ray Photoelectron Spectroscopy (XPS), Electron Microscopy (including SEM, STEM, and Cryo-EM), Energy-Dispersive X-ray Spectroscopy (EDS), Electron Energy-Loss Spectroscopy (EELS), Infrared and Raman Spectroscopy, X-ray Scattering (SAXS, WAXS), Synchrotron-based X-ray Absorption methods (XAS, EXAFS, XANES), and chemical separation methods. This project will explore ways to create controlled vocabularies and maps that link scientific techniques to their measurements, units, and sample types, as a means to reduce confusion caused by synonyms and varied naming styles. Doing so will promote clear, consistent communication by gathering related terms under a preferred name and distinguishing between words with multiple meanings. By building these vocabularies and mapping how techniques relate to their data, you will make it easier to analyze and compare complex scientific information across disciplines. You will learn how developing common frameworks can accelerate breakthroughs in rare earth element separations. This work provides a strong foundation for organizing scientific data and demonstrates how a shared language enhances collaboration and speeds up discovery.

Project Name: Nanocrystal NMR

Title: Characterization of Semiconductor Nanocrystal Surfaces by Solid-State NMR Spectroscopy **PI:** Aaron Rossini

Description:
The photophysical properties of nanocrystals are strongly influenced by the structure of atoms on their surfaces. Our team develops and applies solid-state nuclear magnetic resonance (NMR) spectroscopy experiments to determine the atomic structure of semiconductor nanocrystal surfaces. Specific systems of interest include CdSe and PbS. The SULI student will learn how to perform solid-state NMR experiments that can reveal the precise ordering and arrangement of atoms at the surface of nanocrystals (see, https://pubs.acs.org/doi/full/10.1021/jacs.1c03162 and

https://pubs.acs.org/doi/full/10.1021/jacs.5c18223). They will learn how to perform dynamic nuclear polarization (DNP) enhanced NMR experiments using commercial 263 GHz/400 MHz and 395 GHz/600 MHz instruments that are present at Ames lab. They will also learn other standard characterization techniques for nanocrystals including solution NMR spectroscopy, microscopy and UV-Vis absorption spectroscopy.

Project Name: Nanoparticles

Title: Assembling and crystallization of nanoparticles **PI:** David Vaknin

Description:

We use X-ray diffraction techniques to determine the structures of assembled nanoparticles (NPs) either at the liquid/vapor interface or in bulk. To assemble NPs, we modify their surfaces by grafting various polymers (water- or solvent-soluble). We then modify the conditions of the solvent (pH, salinity, temperature, etc.) to explore conditions under which the NPs aggregate in an ordered structure. We use various synchrotron X-ray diffraction and spectroscopic techniques to determine the structures and the viable parameters that lead to high-quality crystallization. The student will conduct X-ray scattering with the group (if the synchrotron beamtime allocation coincides with the SULI program) and will be involved in the structural analysis of the X-ray results using Python routines and Jupyter notebooks.

Mechanical Engineering

Project Name: Magnetic regenerators

Title: Active regenerators for magnetocaloric cooling **PI:** Julie Slaughter

Description:
Caloric materials change temperature in response to externally applied fields (magnetic, stress, electric) and are very promising for replacing conventional vapor-compression systems in cooling applications. Caloric refrigeration has the potential to improve efficiencies while also eliminating the risk of leakage inherent to gaseous refrigerants. Our team at Ames Laboratory has been instrumental in driving the advance of magnetocaloric technologies. One area that needs additional research is fabrication and manufacturing methods for active magnetic regenerators (AMR) made of magnetocaloric materials. In order to realize the potential of magnetic cooling, the active regenerator needs fine feature sizes for efficient heat transfer, low fluid-flow pressure losses, and efficient magnetization. The research project will focus on AMR designs and fabrication methods to achieve these goals and advance the overall state of the technology.

Nanotechnology

Project Name: Terahertz scanning microscopy

Title: Quantitative near-field light-matter interaction in scanning terahertz microscopy
PI: Richard Kim

Description:
Scanning near-field microscopy has emerged as an essential experimental technique for probing high-momentum, light-driven nanoscale phenomena in a wide range of materials. At its core, this technique exploits the strong, geometrically enhanced electromagnetic near-field generated at a sharp metallic probe, which interacts locally with the polarizable sample beneath it. Despite its widespread use, the field still lacks a comprehensive quantitative electromagnetic description of the full tip-sample geometry. This gap is primarily due to the vastly different length-scales (nanometer length scales of the near-field to hundreds of micrometers for the far-field scattering problem) of the structures involved in the experimental setup, especially when operated in the terahertz frequency domain. This project will develop analytical techniques and boundary-element-method numerical simulations to obtain realistic, high-fidelity solutions for the tip-sample interaction and terahertz scattering beyond the resolution limits of conventional full-wave finite-element approaches. The theoretical and numerical results will be validated against experimental data acquired through hands-on measurements using a state-of-the-art terahertz scanning near-field microscope at Ames Laboratory.

Project Name: Bioinspired Metamaterials

Title: Bioinspired metamaterials **PI:** Surya Mallapragada

Description:
This project focuses on developing fundamental bioinspired approaches to create self-assembled mesoscale 2D and 3D structures that can serve as functional metamaterials. We are investigating mechanistic questions related to dynamic and tunable creation of these nanostructures and their hierarchical assemblies. We are developing bioinspired bottom up synthesis approaches with macromolecular templates for metallization to create nanoresonators and to enable their higher-level 2D and 3D mesoscale organization and alignment. The main goal is to devise approaches to controllably assemble these individual meta-atoms/nanoresonators into 2D and 3D mesoscale superstructures to create optical metamaterials. These goals will be achieved through an interdisciplinary collaborative and integrated approach combining experiment (synthesis and advanced characterization techniques,including electron microscopy) and predictive theory (meta-atom design, function and assembly).

Project Name: Nanoparticle Assembly

Title: Engineering Nanoparticle Systems for Photonic Crystals **PI:** Alex Travesset

Description:
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. Recently, we have demonstrated that NCs functionalized with end charged groups can be assembled into many open lattices, including simple cubic and diamond. The case of diamond is particularly relevant as it can be shown that describes a photonic crystal. The system we are interested consists of generic core, i.e gold, silver, etc.. functionalized with Polytehylene glycol terminated with carboxylic and amine groups, whose charge is regulated by electrolytes. In this internship, the student will perform Molecular Dynamics of nanoparticles with water as solvent with the additional effect of electrolytes, including pH. The goal is to understand how charge can be regulated and optimize the parameters to assemble nanoparticle materials with applications in a wide range of areas. Some experience with Python, including numpy and matplotlib is a plus.