2025 ROSETAS Project List

Contents

Project C1: Carbon Dioxide Incorporation into Organometallics
Project C2: Carbon Negative Materials Manufacturing2
Project C3: Carbon dioxide capture using electrochemical methods2
Project C4: Catalytic Conversion of Small Molecules to Value-Added Products
Project C5: Biofilm-Based Technologies to Upcycle Waste into Platform Chemicals and Bioplastics3
Project G1: Integrating Energy Justice and Disaster Resilience in the Energy Transition4
Project G2: Data-Driven Approach for Analyzing and Controlling Impacts of Electric Vehicles on Energy Systems
Project So1: Ground Supported Solar Arrays, Stability and Strength5
Project So2: Earth-Abundant Nanomaterials for Next Generation Solar Energy Harvesting
Project St1: ML-Driven Discovery of Disordered Materials for Clean Energy
Project St2: Chemical Stability Assessment of Cathode Materials in Solid-State Batteries through Spectroscopic and Electrochemical Techniques7
Project St3: Developing Electrodeposition as a Sustainable Technology to Fabricate Anodes for Aqueous Zn-ion Batteries
Project St4: Electrolyte Development for Advanced Lithium-Based Batteries8
Project W1: Exploiting a web-based wind farm database to understand and evaluate wind farm performance9

Project Area: Carbon

Project C1: Carbon Dioxide Incorporation into Organometallics

PI: Prof. Grace Panetti, Chemistry

Project Description: To tackle climate change, increasing the value of greenhouse gases like CO_2 by introducing new uses has the chance to have a beneficial impact on the economics of industries like carbon capture. To this end, finding new and exciting applications for CO_2 is of great value, particularly when paired with industrially relevant compounds like alkenes. To provide the templates for this reaction, transition metal ions offer a unique advantage to address this reaction. Students will investigate the ability of transition metals, alkenes, and CO2 to react and make new complexes.

Role of REU Student: The student will work with their mentor in the synthesis of new organometallic complexes derived from alkenes and CO₂. They will then characterize these compounds by x-ray diffraction, NMR techniques, and IR-spectroscopy under air-free conditions. The students will also investigate the reactivity of these complexes with other gases and reactants to determine their utility with their mentor.

Preferred Background & Skills:

- Studied Organic Chemistry
- Participated in an Organic Chemistry Lab Course
- Familiarity with NMR and IR spectroscopy

Project C2: Carbon Negative Materials Manufacturing

PI: Prof. Jonah Erlebacher, Materials Science and Engineering

Project Description: Carbon capture, utilization, and storage (CCUS) will undoubtedly play a significant role in achieving global emissions goals. Conversion of CO₂ to solid carbon introduced a wealth of opportunity in designing processes to achieve specific properties, either by directly synthesizing a target crystal structure or by engineering composite materials to achieve certain performance metrics. This project centers on developing different pathways towards the manufacture of carbon negative carbon materials, ranging from carbon negative cement to greenhouse gas-derived (GHG) carbon/carbon composites, and upgrading carbon pyrolysis products to form carbon negative aggregate.

Role of REU Student: Student will engage in experimental lab work focused on designing mixtures and chemistries to produce composite materials that contain some fraction of GHG-derived carbon. The work will focus on developing sample preparation and characterization, where variables of interest could include varying composition and constituent chemicals, heat treatments under different chemical environments, and post-processing. Materials characterization will include spectroscopic and x-ray techniques (XRD, Raman and FTIR). microscopy (Scanning Electron Microscopy), and mechanical properties (tensile and compression testing).

Preferred Background & Skills:

- Materials Science, Chemistry, Chemical Engineering (thermodynamics background)
- Experience/familiarity with materials characterization instrumentation (X-ray diffraction, Scanning Electron Microscopy)
- Experience/familiarity with mechanical testing (compression testing)
- Data analysis (Excel, MATLAB, etc...)

Project C3: Carbon dioxide capture using electrochemical methods

PI: Prof. Yayuan Liu, Chemical and Biomolecular Engineering

Project Description: Carbon capture is essential for mitigating anthropogenic carbon dioxide emissions, which is a critical part of the climate change mitigation plan. Compared to the conventional wet chemical scrubbing methods, electrochemical carbon capture utilizing redox-active sorbents is emerging as a more versatile and economical alternative. This project explores materials to enable carbon dioxide

removal from the air and ocean. Students will acquire knowledge across multiple length scales, such as electrochemistry, materials synthesis and characterizations, and device prototyping.

Role of REU Student: The REU student will work collaboratively with graduate students/postdocs to gain hands-on experience in conducting materials synthesis and characterization. Specifically, the student will conduct electrochemical analyses to understand the intrinsic properties of the redox-active carbon dioxide sorbents, develop and optimize formulations to afford high-performance sorbent electrodes, and construct prototypes to test the carbon capture performance.

Preferred Background & Skills:

- Electrochemistry/analytical chemistry knowledge/wet lab experience
- Interests in materials science and sustainability

Project C4: Catalytic Conversion of Small Molecules to Value-Added Products

PI: Prof. Sara Thoi, Chemistry

Project Description: This project is focused on the synthesis and characterization of novel metal catalysts for activating and converting small molecules such as carbon dioxide (CO_2), nitrogen (N_2), nitrate (NO_3^-), and other abundant compounds. One example is the development of metal-organic frameworks (MOFs) for transforming N_2 to ammonia (NH_3), an important fertilizer and nitrogen precursors for industrial and pharmaceutical chemicals.

Role of REU Student: The REU student will synthesize and characterize a variety of catalysts containing earth-abundant metal sites for activating small molecules. They will learn how to conduct electrochemical experiments, including cyclic voltammetry, chronoamperometry, and in situ vibrational spectroscopy. The REU student will correlate the various properties of the catalysts—structure, porosity, functional groups, identity of the metal—to their catalytic performance in terms of selectivity and activity. These structure-function relationships will elucidate mechanistic insights and provide a roadmap for further catalyst design.

Preferred Background & Skills:

- General Chemistry
- Electrochemistry
- Synthesis

Project C5: Biofilm-Based Technologies to Upcycle Waste into Platform Chemicals and Bioplastics

PI: Shilva Shrestha, Environmental Health and Engineering

Project Description: Biomanufacturing biochemicals and biopolymers from waste offers a sustainable alternative to fossil fuel-based products while also addressing growing waste management challenges. Chain elongation, an emerging biotechnology, can convert waste into medium chain carboxylic acids

(MCCAs). MCCAs are platform chemicals used in lubricants, fragrances, polymers, antimicrobial agents, and sustainable aviation fuel. Additionally, such waste can also be repurposed into microbial-based polyhydroxyalkanoates (PHAs), presenting an attractive alternative to conventional plastics. This project focuses on developing a biofilm-enhanced bioreactor to intensify MCCA and PHA production from brewery and dairy waste by promoting high mass transfer for microbial growth, retention, and efficient substrate utilization.

Role of REU Student: The student will learn to operate and monitor the biofilm bioreactor and liquidliquid extraction unit. They will conduct chemical analyses to evaluate MCCA and PHA production under different operational conditions. If interested, the student can also get involved in biofilm imaging and microbial analysis, specifically DNA and RNA extraction and sequencing data analysis. The student working on this project will gain knowledge on topics including but not limited to environmental and chemical engineering techniques tailored for the production and extraction of bioproducts and gain experience in handling lab-scale reactors, in addition to learning the core values of sustainability and biomanufacturing.

Preferred Background & Skills:

- Interest in sustainable energy
- Have some background in biology and chemistry
- Familiarity or willingness to learn analytical chemistry (HPLC and GC-MS)

Project Area: Grid

Project G1: Integrating Energy Justice and Disaster Resilience in the Energy Transition

PI: Prof. Yury Dvorkin, Electrical and Computer Engineering, Civil and Systems Engineering

Project Description: This project develops a novel modeling framework to integrate energy justice and disaster resilience into energy transition planning. By analyzing economic, environmental, public health, and reliability factors, we aim to ensure a fair and resilient transition to a decentralized, low-emission power grid. The research will focus on both normal and stressed grid conditions, emphasizing the impact of climate change on vulnerable communities and the equitable distribution of clean energy benefits.

Role of REU Student: The REU student will assist in developing and refining models that assess the fairness and resilience of the energy transition. They will gather and analyze data on socio-economic disparities, energy reliability, and the impact of extreme events on vulnerable communities. The student will also help evaluate how local renewable energy sources and storage can improve grid resilience, especially during natural disasters. By contributing to the integration of energy justice principles, the student will gain experience in applying quantitative methods to address critical challenges in energy systems and climate resilience.

Preferred Background & Skills:

• Python, Julia or equivalent

Project G2: Data-Driven Approach for Analyzing and Controlling Impacts of Electric Vehicles on Energy Systems

PI: Prof. Sijia Geng, Electrical and Computer Engineering

Project Description: Electric vehicles lead to a tighter integration between transportation and energy systems. It remains an open question how such an integration would affect the energy system, in terms of energy consumption, infrastructure resiliency, carbon emission, and social equity. This project aims to develop data analysis approaches to reveal the impacts of EVs on energy systems. We will develop computationally efficient optimization tools and control algorithms to determine the optimal design and operation of such integrated transportation-energy systems. Various emerging technologies, such as distributed renewable generation, DC fast charger, overhead and wireless charger, hydrogen generation and storage, will be evaluated.

Role of REU Student: The REU student will help develop the model of coupled transportation and energy systems, analyze data for EV customers and renewable generation, and develop optimization and control tools for design and operation of such nexus energy systems. Real geospatial data for transportation schedules, renewable generation, and meteorological information will be analyzed to provide valuable insights into decarbonization across sectors.

Preferred Background & Skills:

- Coding skill using Python or Julia language
- Mathematical skills: linear algebra, calculus
- Experience or interests in optimization and/or control problems
- Background or interests in renewable energy, power systems, or electric vehicles

Project Area: Solar

Project So1: Ground Supported Solar Arrays, Stability and Strength

PI: Prof. Ben Schafer, Civil and Systems Engineering

Project Description: Ground supported solar arrays are supported by a network of light steel structural members. Under wind and snow a large number of failures have occurred in solar farms that have not been properly designed. We have been experimentally and numerically investigating a new high-strength, light-steel, highly-optimized, cold-formed steel structural members for use as the pile foundation and for the torque tube in ground-supported solar. In addition, we are using these unique solutions to investigate improved methods for testing and designing these members.

Role of REU Student: The selected student will have the opportunity to learn about how structures support renewable energy and develop background and educational materials for the role of structures in ground supported solar array farms. The student will also have the opportunity to learn or exercise CAD skills in developing scaled drawings of typical and newly proposed structural systems for ground-mounted solar. The student will participate in ongoing experiments on the torsional strength of cold-

formed steel members utilized in solar arrays. Finally, the student will be supported in developing finite element (FE) models of the structural response of ground-mounted solar under wind and snow loads.

Preferred Background & Skills:

- Basic physics, strength of materials, or interest in same
- Computer aided drafting/design, or interest in same
- Hand tools, building, hands-on, or interest in same (if lab focused)
- Programming, hacking, or interest in same (computational focused)

Project So2: Earth-Abundant Nanomaterials for Next Generation Solar Energy Harvesting

PI: Prof. Susanna Thon, Electrical and Computer Engineering

Project Description: Next generation solar energy technologies should be tunable, flexible, and sustainable for installation in new contexts such as building-integrated photovoltaics, vehicular photovoltaics, and mobile power applications. Colloidal quantum dot (CQD)-based photovoltaics have all of these properties, but the highest-performing CQD solar cells are based on lead (Pb)-containing materials. We aim to develop new nanoparticles based on non-toxic and earth-abundant materials for applications in flexible photovoltaic and photobattery technology.

Role of REU Student: The REU student will learn to synthesis colloidal quantum dots. They will also assist in test device fabrication and characterization using techniques such as spin-casting, metals evaporation, solar simulator testing, and UV-vis spectrophotometry. The REU student will also participate in data analysis.

Preferred Background & Skills:

- Comfort with working in a chemical synthesis laboratory and/or willingness to learn chemical synthesis techniques.
- Comfort with basic mathematical analysis software (Matlab preferred) and/or willingness to learn.

Project Area: Storage

Project St1: ML-Driven Discovery of Disordered Materials for Clean Energy

PI: Prof. Corey Oses, Materials Science and Engineering

Project Description: The transition to a fossil-fuel-free energy future demands materials that can generate and store energy reliably, sustainably, and economically. A new class of materials, high-entropy ceramics, have demonstrated enhanced and emergent properties through disorder engineering. This design strategy has given rise to state-of-the-art solutions for clean hydrogen production, wasteheat recovery, and energy storage. The approach also offers far too many possibilities than can be tried experimentally. Can computational modeling and data-driven approaches be combined to realize even better performing materials faster? *Research Approach:* To reveal new relationships between a

material's composition/structure and its properties, we employ high-throughput first-principles calculations to generate large amounts of materials data that can be mined using machine learning (ML) algorithms.

Role of REU Student: Use and develop materials-modeling software and ML approaches to predict the stability and functional properties of disordered materials.

Preferred Background & Skills:

- Coding (python, c++); not necessary
- Chemistry, physics, materials science
- Machine learning algorithms

Project St2: Chemical Stability Assessment of Cathode Materials in Solid-State Batteries through Spectroscopic and Electrochemical Techniques

PI: Prof. Regina García-Méndez

Project Description: This project will explore the chemical stability of cathode materials when paired with solid ionic conductors in solid-state batteries. Using spectroscopic techniques (e.g., X-ray diffraction, Raman spectroscopy) and electrochemical methods (e.g., impedance spectroscopy), the student will investigate how the materials interact and degrade over time. The goal is to understand and improve the stability of these materials to enable the development of next-generation batteries with higher energy density, enhanced safety, and better performance. This research will contribute to the advancement of solid-state battery technology, a critical area in energy storage innovation.

Role of REU Student: The student will synthesize and process cathode and solid ionic conductor materials for solid- state batteries, followed by conducting materials and systems characterization using techniques such as X-ray diffraction, Raman spectroscopy, and electrochemical impedance spectroscopy. Literature reading will be expected to help guide the experimental approach and understand current research trends. The student will present regular updates to the principal investigator (PI) and the research group, collaborate with other researchers, and give a final presentation summarizing their work. This project provides hands-on experience in materials research, experimental techniques, and scientific communication.

Preferred Background & Skills:

- Passionate about sustainability and energy storage technologies
- Strong willingness to learn new techniques and concepts
- Eager to engage in hands-on experimentation, literature review, and collaborative research

Project St3: Developing Electrodeposition as a Sustainable Technology to Fabricate Anodes for Aqueous Zn-ion Batteries

PIs: Prof. Yuting Luo, Materials Science and Engineering

Project Description: "Beyond Lithium-ion" batteries of rechargeable aqueous zinc-ion batteries (AZBs), with their high theoretical capacity, low cost, geographically abundant, safety, and environmental friendliness, have risen as a promising candidate for next-generation energy storage system. However, current ZIBs suffer from low capacity, poor rechargeability and low Coulombic efficiency (CE) due to the formation of Zn dendrites, Zn corrosion and passivation. This project aims to strategically control crystal orientation on Zn anode surface by electrodeposition to mitigate the dendrite growth, enhancing reversible capacities and prolonging lifespan.

Role of REU Student: The electrodeposition setup has been established in our lab and different oriented Zn anode surfaces are synthesized. The role of REU student will be conducting electrodeposition experiment in aqueous solution to synthesize Zn anode with different experimental parameters; utilizing optical microscope to take images for morphology; learning to assembly coin cells; measuring electrochemical performances. With that, the REU student will learn hands-on experimental skills of material synthesis, battery assembly, material characterization as well as gain fundamental understanding of structure-performance relationship for batteries.

Preferred Background & Skills:

General chemistry

Project St4: Electrolyte Development for Advanced Lithium-Based Batteries

PI: Prof. Sara Thoi, Chemistry

Project Description: This project is focused on the design of electrolytes that can improve energy storage devices. We are particularly interested in Li metal batteries, owing to their high energy density and charge capacities. However, Li metal is very reactive and can lead to battery fires. We are thus focusing on electrolytes that can decrease the reactivity of Li metal to improve safety and longevity of the battery. One example is to apply a thin layer of a material that can serve as a protective coating for the Li metal during charging and discharging.

Role of REU Student: The REU student will synthesize and characterize new electrolytes and solid-state materials that improve the safety and performance of Li-based batteries. They will learn how to conduct electrochemical experiments, including cyclic voltammetry, chronoamperometry, and in situ vibrational spectroscopy. The REU student will correlate the various properties of the electrolyte—solubility, structure, functional groups, conductivity—to their battery cycling performance. These structure-function relationships will elucidate mechanistic insights and provide a roadmap for further electrolyte design.

Preferred Background & Skills:

- General Chemistry
- Electrochemistry
- Synthesis

Project Area: Wind

Project W1: Exploiting a web-based wind farm database to understand and evaluate wind farm performance

Pls: Prof. Dennice Gayme, Mechanical Engineering; Prof. Charles Meneveau, Mechanical Engineering

Project Description: Understanding the power output potential, maintenance needs and performance limits of large wind farms requires knowledge of the interactions between the turbulent flow field of the farm and the atmospheric/marine environment. This project will leverage an ongoing project that is generating a wind farm database based on large-eddy simulations. The database will contain hundreds of Terabytes of web-services accessible wind farm flow data over different on and offshore conditions. Diagnostic analyses of these data to explore correlations between flow phenomena in the turbine wakes and the upstream conditions and along individual blades will further our understanding of wind farm physics.

Role of the REU Student: The student will be exploiting the database and webservice tools to perform diagnostic analyses of the wind farm database to better understand the factors driving wind farm performance under a number of practical metrics. For example, the student will investigate various correlations between flow phenomena in the turbine wakes, blade forces and moments and the upstream atmospheric and met-ocean conditions. This understanding will be used to improve design-oriented wind farm models. At the end of the project students will have a general understanding of the some of the key interactions between turbulence in a wind turbine array, the turbine level forces/moments, turbine power output and the atmospheric boundary layer that influence wind farm performance. Students will also gain experience working with large amounts of data.

Preferred Background & Skills:

- Programming experience (preferably in Python)
- Basic Unix shell commands