

2026 ROSETAS Project List

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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 CO₂ 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 CO₂ 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: Designing Modular Synthetic Microbial Consortia to Upcycle Waste into Platform Chemicals

PI: Prof. Shilva Shrestha, Environmental Health and Engineering

Project Description: Harnessing microbial consortia to upcycle organic waste into high-value chemicals represents a transformative opportunity to advance the U.S. energy and chemical sectors 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. Efficient conversion of complex waste to a target MCCA product requires specialized and carefully selected microbial consortia. This project will focus on rationally designing two- or three-member synthetic microbial consortia that are robust, resilient, and stable for biomanufacturing purposes.

Role of REU Student: The student involved in this project will gain hands-on experience in environmental and chemical engineering techniques tailored for the production of bioproducts, in addition to learning the core values of sustainability and biomanufacturing. They will learn anaerobic microbiology, molecular biology, and imaging techniques, including microbial growth studies, DNA/RNA extraction and quantification, PCR, and sequencing data analysis. Additionally, they will also perform chemical analyses to quantify metabolite concentrations using GC-MS and HPLC.

Preferred Background & Skills:

- Interest in sustainable energy
- Have some background in biology, microbiology, and chemistry
- Familiarity or willingness to learn microbiology and molecular biology techniques

Project C3: 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 (CO₂), nitrogen (N₂), nitrate (NO₃⁻), and other abundant compounds. One example is the development of metal-organic frameworks (MOFs) for transforming N₂ to ammonia (NH₃), 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 Area: Grid

Project G1: Extended Kalman Filter for Training of Physical-informed Neural Networks in Systems Engineering

PI: Prof. Jan Drgona, Civil and Systems Engineering

Project Description: Physics-informed neural networks (PINNs) are transforming systems engineering; they represent powerful framework for data-driven solutions and discovery of partial differential equations (PDEs). The success of PINNs depends on high-accuracy training via stochastic gradient descent (SGD). This project is concerned with alternative training strategy based on extended Kalman Filter (EKF). While EKF can obtain high-precision solutions in fewer iterations, SGD has won a victory with its lower computational cost and memory requirements, causing EKF to be forgotten. This project aims to develop a computation- and memory-efficient EKF-based optimizer for training PINNs, with applications in sustainable energy systems governed by spatio-temporal dynamics.

Role of REU Student: In this project, the selected REU student will be mentored by Prof. Jan Drgona and Dr. Liang Wu to: (i) gain foundational knowledge at the intersection of deep learning, control theory, and numerical optimization, and (ii) conduct numerical experiments (write code if possible) to validate the proposed modern EKF-based optimizer for training large-scale deep neural networks through numerical experiments.

Preferred Background & Skills:

- Strong motivation and interest in numerical computing and algorithmic development;
- Basic understanding of deep neural network training principles;
- Knowledge of Python programming.

Project G2: How Can Data Help Solve AI's Power Problem?

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

Project Description: This project examines how AI-driven data center growth affects U.S. grid infrastructure. Using regional operator data and data science, we analyze threshold effects where rapid capacity expansion significantly alters wholesale prices, volatility, and congestion patterns. We also investigate supply chain constraints—critical materials, manufacturing bottlenecks, and production capacity limits—that enable or constrain the ability to supply electricity from new generation resources. By linking demand-side pressures from digital infrastructure with electric supply, this research will analyze how AI's electricity needs reshape energy affordability, market dynamics, and the feasibility of timely capacity deployment across interconnected power systems.

Role of REU Student: The REU student will collect and analyze data on energy infrastructure suppliers, including company manufacturing capacity, factory locations, and production timelines. Using data mining and visualization techniques, the student will identify patterns and bottlenecks in the transformation of raw materials into key energy components (e.g., transformers, inverters, turbines). They will learn skills in data processing, validation, and integration across multiple sources (trade, industry reports, and government databases). The student will also contribute to building datasets that can be incorporated into ongoing capacity expansion models, providing hands-on experience at the intersection of supply chain analysis and energy systems planning.

Preferred Background & Skills:

- Interest in modeling, computing, energy and economics
- Basic skills in creating charts and graphs to identify patterns (any software, but we use Python or Matlab for visualization)
- Introductory programming for data analysis (or willingness to learn). Our group works with Python, Julia, R
- Proficiency in Excel or Google Sheets for data management

Project Area: Solar

Project So1: Materials Discovery of New Solar Cell Materials Using AI/ML

PI: Prof. Paulette Clancy, Chemical and Biomolecular Engineering

Project Description: We have a variety of projects underway that combine molecular simulation tools and/or machine learning algorithms that we've developed as a means to use existing small data sets to meet a pre-chosen objective that would otherwise be too time- and resource- intensive to undertake experimentally. This conserves energy use. Currently, we have ten such projects, engaging with faculty at Hopkins, Stanford, Georgia Tech, and Princeton. Here are two recent examples: Making stronger exotic metal alloys for spacecraft parts; making it easier to discover new metal halide perovskite materials for energy-saving room temperature synthesis. Come and be part of our team.

Role of REU Student: Learn to use computational tools that are the foundation of materials discovery, e.g., density functional theory, or Molecular Dynamics. Opportunity to use machine learning tools to characterize materials and optimize for a chosen property, like the best solvent to use for polymer processing, or the least corrosive material to use for orthopedic implants (both are examples of recent projects). Interact with a fun team of students and learn about conducting original research.

Preferred Background & Skills:

- Requires basic training in programming, especially Python coding (one course is sufficient or be self-taught)
- Assumes basic knowledge of chemistry as appropriate for the candidate's point of college progression (first year, sophomore, junior)
- Enthusiasm for a computational project

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, photobattery, and solar-powered carbon capture technology.

Role of REU Student: The REU student will learn to synthesis colloidal quantum dots and other nanomaterials and 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: Electrochemical Mining to Recover Critical Minerals from Water

PI: Prof. Yuting Luo, Materials Science and Engineering

Project Description: This project aims to develop sustainable electrochemical technologies for selective recovery of critical minerals directly from aqueous sources such as seawater, industrial brines, and mine wastewater. By integrating electrochemical separation with tunable electrode materials and interface engineering, we will establish ion-specific transport and redox mechanisms that enable efficient extraction of critical minerals such as Ni, Co and rare-earth elements. The proposed research advances circular mineral recovery, reduces environmental impacts of traditional mining, and contributes to securing the critical mineral supply chain for clean energy technologies.

Role of REU Student: REU student will conduct experiment with graduate student under PI's supervision. Specific experiments will include material synthesis, electrode integration and electrochemical testing. After collecting experimental data, REU student will work with graduate student to do data analysis and understand the electrochemical reactions and structure-performance relationship.

Preferred Background & Skills:

- General chemistry

Project St2: AI Materials Design for Energy

PI: Prof. Corey Oses, Materials Science and Engineering

Project Description: Meeting today's energy needs requires materials with superior performance and affordability. High-entropy ceramics, created through disorder engineering, exhibit unique properties for applications such as hydrogen production, waste-heat recovery, energy storage, and advanced nuclear systems including fusion and fission. However, the immense number of possible material combinations makes experimental discovery impractical. *Research Approach:* We integrate high-throughput first-principles computational modeling with autonomous, data-driven methods and artificial intelligence (AI) to generate and analyze large datasets, accelerating the discovery of high-performance, cost-efficient materials.

Role of REU Student: The student will use and develop materials-modeling software and data-driven algorithms to predict the stability and functional properties of disordered materials.

Preferred Background & Skills:

- Coding (python, c++)
- Chemistry, physics, materials science

- Machine learning algorithms

Project St3: From Chemistry to Configuration: Linking Battery Design to Deployment Cost Drivers

PIs: Prof. Magdalena Klemun, Civil and Systems Engineering

Project Description: Batteries are among the most scalable grid-scale storage options, yet limited research explores how their hardware characteristics shape deployment-related soft costs—non-hardware expenses such as site preparation, installation, permitting, and system operation. This project investigates how traits like form factor, energy density, thermal management, modularity, and cycle life influence these costs. Using lithium-ion systems as a baseline, the research develops dependency maps linking system design and battery chemistry attributes to soft cost components. These analyses support a generalizable framework for understanding how hardware traits interact with location-dependent deployment frictions, with applications to emerging chemistries such as sodium-ion and flow batteries.

Role of REU Student: The undergraduate researcher will support the expansion and management of a structured dataset of real-world battery storage projects by extracting, classifying, and standardizing data on system design features and soft cost components. These data will inform comparative analyses across technologies and deployment contexts to identify which design traits most effectively reduce soft costs in large-scale battery systems. Responsibilities include reviewing technical documentation, project reports, and databases; encoding and curating hardware and soft cost variables; contributing to the construction of dependency maps; assisting with preliminary data visualization; and synthesizing relevant literature on battery design and deployment economics.

Preferred Background & Skills:

- Background or interest in battery storage, techno-economic modeling, and sustainability
- Curiosity about how technology design affects deployment complexity
- Enthusiasm for data collection, cleaning, interpretation, and management
- Comfort working with structured datasets, collaborative tools, and basic programming skills
- Attention to detail and strong documentation habits

Project St4: *Operando* Microstructure Tracking in Functional Ceramics for Battery Applications

PI: Prof. Regina García-Méndez, Materials Science and Engineering

Project Description: Investigate how ceramic battery materials transform during processing using operando techniques. You will track the microstructure evolution upon processing and assist with the synthesis and characterization of your material/system. After processing, the microstructure will be correlated with properties using microscopy and spectroscopy techniques, including mechanical property testing and introductory electrochemical measurements. You will receive day-to-day mentorship from a graduate student, collaborate with group members at different stages in their

respective programs (Ph.D, M.S., undergraduate), participate in journal club and group meetings, and learn about your labmates' projects.

Role of REU Student: Assist with experiment setup, sample preparation, and real-time data collection and analysis upon material processing. Measure density using two analytical methods, prepare and polish cross sections for scanning electron microscopy, and document features systematically. Collect impedance spectra, extract basic parameters from Nyquist plots, and, with guidance, apply simple equivalent-circuit fits to link transport to microstructure. Maintain tidy spreadsheets, generate clear plots with uncertainty estimates, share interim updates during check-ins, and deliver a concise final summary of methods, results, and next steps.

Preferred Background & Skills:

- Experience with spreadsheets
- Interest in materials, electrochemistry, and batteries
- Collaborative attitude and curiosity

Project St5: 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: Team “Power”: When Data Centers, Wind, and Batteries Collaborate

PIs: Prof. Dennice Gayme, Mechanical Engineering; Prof. Yury Dvorkin, Electrical and Computer Engineering & Civil and Systems Engineering

Project Description: As electricity demand grows from data centers and electric vehicles, power grids struggle to satisfy this demand due to (i) lack of generation capacity and (ii) limited capacity to move power from the places where it is being produced to the places where it is consumed. This project focuses on addressing these two challenges by learning to coordinate generation, storage, and flexible loads (e.g., data centers) to reduce the scarcity of power generation. Tasks include: (1) modeling simple hybrid resource configurations (e.g., data center + storage; or data center + wind + storage), (2) comparing coordinated vs. independent operation using basic optimization and resource scheduling tool (e.g., degradation aware dispatch of storage or wake-enhanced modeling of wind farms), and (3) evaluating performance under different grid conditions (when the coordination makes sense and when independent operations can be justified).

Role of the REU Student: The student will work in a group of several Ph.D. students. Key responsibilities include: literature review of grid and data center literature; building components of models to simulate coordinated operation of generation, storage, and flexible loads; running optimization scenarios to compare system performance metrics (cost, reliability, efficiency); visualizing results through graphs and charts. The student will also have a chance to learn fundamental concepts in power systems, optimization, and data analysis. No prior energy systems knowledge required.

Preferred Background & Skills:

- Interest in modeling, computing, energy and economics
- Basic skills in creating charts and graphs to identify patterns (any software, but we use Python or Matlab for visualization)
- Introductory programming for data analysis (or willingness to learn). Our group works with Python, Julia, R
- Proficiency in Excel or Google Sheets for data management

Project W2: Wind Turbine Support Towers Under Combined Actions

PI: Prof. Ben Schafer, Civil and Systems Engineering

Project Description: The structural engineering of wind turbine support towers involves assessing the stability and ultimate strength of thin steel tubes. These towers are subject to several loading actions at once when the turbine is in operation; including axial, shear, moment, and torsion. To certify the towers for operation engineers commonly use design specifications and equations that account for each action in isolation. This research includes computational tools developed in the PI’s research group along with experiments conducted in the PI’s lab to explore the response when the actions are combined as in real towers.

Role of the REU Student: The REU student will learn about the structural engineering of wind turbine support towers and the role of structures in renewable energy. The student will have the opportunity to utilize the computational stability tools developed by the PI's group, and (if of interest) contribute to the user interface and visualization of these tools. In addition, the student will be able to contribute to experimental research where lab-scale thin steel tubes are scanned and then tested under combined actions to provide benchmark data for the studies.

Preferred Background & Skills:

- Interest in civil or mechanical engineering and energy structures
- Exposure or aptitude in CAD
- For computationally focused student, then Matlab (Python or Julia)
- For experimentally focused student, willingness to work with hands
- In general, we will teach the interested student what they need to know