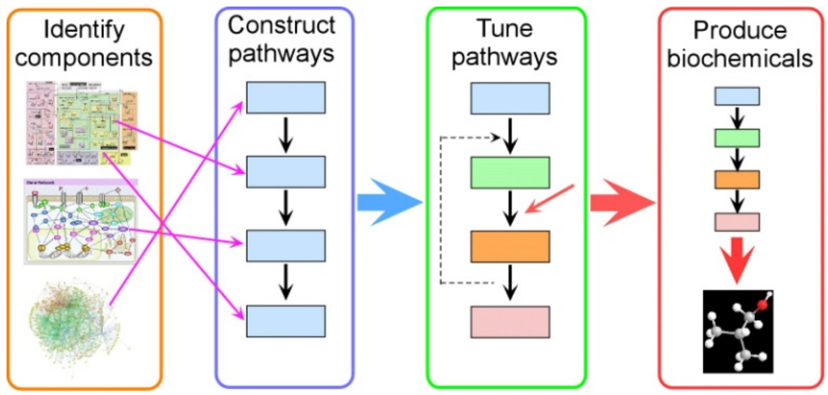
ChemEnergy NSF REU - Faculty Mentors and Examples of Research Projects

Descriptions of proposed projects (arranged alphabetically by the last name of the faculty).

Protein Engineering and Synthetic Biology for Biofuel Production (Prof. Shota Atsumi)

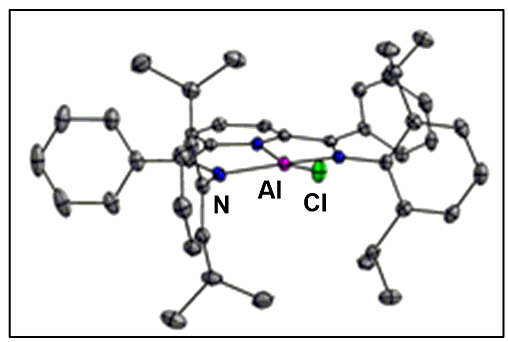
An REU student will identify enzymes to engineer biosynthetic pathways that will develop and improve biofuel production from engineered microorganisms. In a representative project, the student will improve isobutyl acetate production from *Escherichia coli* with protein engineering and synthetic biology approaches. Isobutyl acetate is used as a flavoring agent, solvent, and fuel. A student will develop skills in molecular biological and microbiological techniques including PCR, gene manipulation, plasmid construction, bacterial cell culture, and small molecule analysis with HPLC and GC.



http://chemistry.ucdavis.edu/faculty/department_faculty/shota_atsumi.html

Catalysts for Electrocatalytic Reduction of CO_2 and N_2 into Liquid Fuels (Prof. Louise Berben)

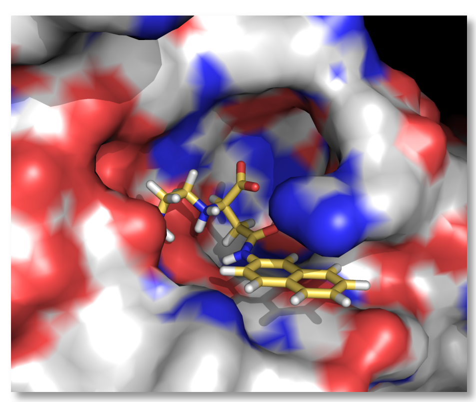
To access preferred products and to reduce the energy input required by operating catalysts at low potentials, multielectron processes are desirable over one electron processes. This idea applies to reactions such as CO_2 reduction to formate or methanol, and to N_2 reduction into NH_3 which is a 6e and 6H^+ process. The NSF REU project will develop the fundamental chemistry of Al(III) with a focus on generation and reactivity of ligand-based hydrides. This will lower barriers to future adoption of main group catalysts. Proton and electron transfer reactions will be used to generate hydride equivalents that can be used in formation of H_2 or of C-H or N-H bonds with various substrates. The chemistry of redox-active ligand complexes of aluminum (III) has previously been reported by the Berben research group and we will build on this expertise (Figure 1). In a ten week research experience, a student will be involved in the synthesis of Al(III) coordination complexes. In completing this project the student will learn how to use inert atmosphere synthetic techniques including Schlenk line and glove-box manipulations. Characterization skills learned will be NMR and IR spectroscopy and basic cyclic voltammetry experiments.



http://chemistry.ucdavis.edu/faculty/department_faculty/louise_berben.html

Structure Characterization of Enzymes for Sulfur Metabolism (Prof. Andrew Fisher)

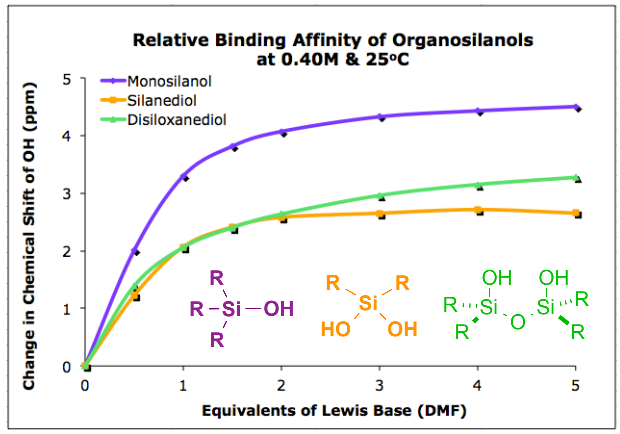
An REU student will use X-ray crystallography, biochemistry, and enzyme kinetics to characterize the structure-function relationship of enzymes involved in sulfur metabolism, specifically from the organism *Mycobacterium tuberculosis* with the long-term goal to identify inhibitors of enzymes that may serve as lead compounds for tuberculosis treatment. In a representative REU project, a student will express, purify and crystallize an enzyme in this pathway and, time permitting, determine the atomic resolution structure.



http://chemistry.ucdavis.edu/faculty/department_faculty/andrew_fisher.html

Catalysts for Selective Organic Synthesis (Prof. Annaliese Franz)

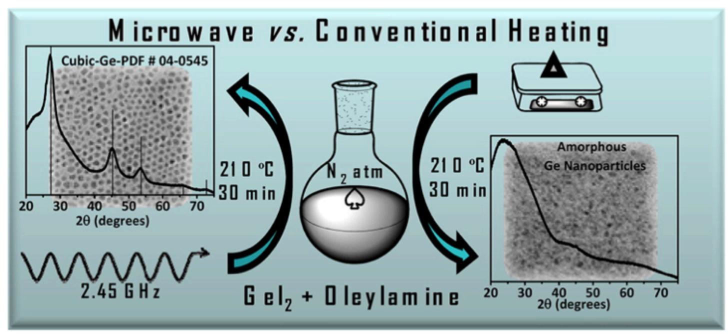
An REU student will design and synthesize new catalysts and ligands based on either hydrogen-bonding or metal catalysis. In a representative project, the student will synthesis and compare homogeneous and heterogeneous catalysts for selective organic transformations (such as Michael addition and Diels-Alder reactions), and gain experience with organic synthesis, mechanism, metal-binding and/or hydrogen-bonding studies using MS, NMR, spectroscopic, and computational methods, and analyze selectivity by NMR, GC and HPLC.



http://chemistry.ucdavis.edu/faculty/department_faculty/annaliese_franz.html

Synthesis & Characterization of Novel Thermoelectric Materials (Prof. Susan Kauzlarich)

An REU student will synthesize new nanostructured materials for the conversion of thermal energy directly into electrical energy. In a representative project, the student will compare two approaches to preparing nanostructured phases: 1) nanoparticle composites, and 2) nanocrystalline inclusions in a bulk phase. A student will develop skills to handle air-sensitive reagents, characterize nanostructured products using single crystal and powder X-ray diffraction, SEM, TEM, FTIR, Raman Spectroscopy, UV-Vis, and photoluminescence.



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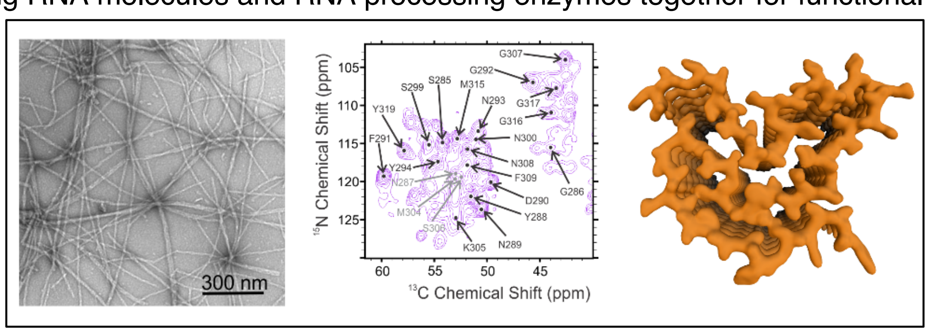
Protein Assembly Processes in RNA Metabolism (Prof. Dylan T. Murray)

An REU student will perform experiments aimed at understanding the role of multiprotein nanostructures in regulating biochemical reactions in RNA metabolism. In a representative project, the student will prepare a macromolecular assembly of an RNA-binding protein and characterize the structural, thermodynamic, and kinetic properties of the assembly process. The student will learn to make quantitative measurements using solid state nuclear magnetic resonance, fluorescence, electron microscopy, and calorimetry, in addition to learning fundamental laboratory practices for the expression and purification of proteins using bacterial expression systems. The results will provide insight into the role of RNA-binding proteins in bringing RNA molecules and RNA processing enzymes together for functional activity.



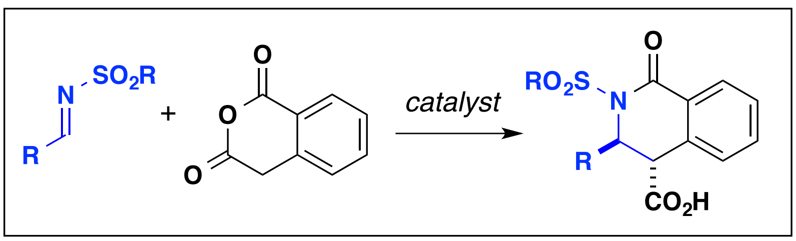
http://chemistry.ucdavis.edu/people/dylan-murray

Photocatalysts for Sunlight to Fuel Conversion (Prof. Frank Osterloh)

An REU student will synthesize an inorganic photocatalyst and test it for solar energy conversion into hydrogen fuel. In a representative project, the student will synthesize a metal oxide powder and then a thin film will be prepared to measure its thickness and optical properties with optical absorption spectroscopy and profilometry. The student will measure photochemical charge separation properties using surface photovoltage spectroscopy and the photocatalytic function for artificial photosynthesis will be evaluated in irradiation experiments. The student will develop skills in inorganic synthesis, design of photocatalysts, thin film preparation, thickness measurements, optical characterization, photophysical and gas chromatography measurements.
http://chemistry.ucdavis.edu/faculty/department_faculty/frank_osterloh.html

Catalysts for Multicomponent Reactions (Prof. Jared Shaw)

An REU student will perform experiments aimed at discovering new catalysts and methods to efficiently assemble organic molecules with high selectivity. In a representative project, the student will explore conditions for catalyzing reaction such as the anhydride-Mannich reaction to access new amino acids as building blocks for the synthesis of medicinal compounds and materials. The student will develop skills in catalyst development, purification, HPLC analysis, NMR spectroscopy and mass spectrometry.



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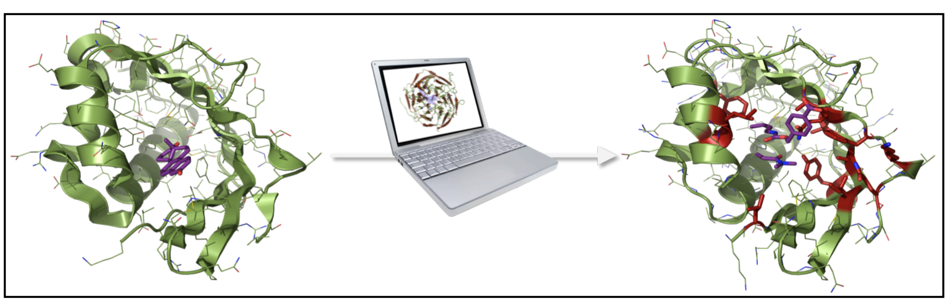
Computational Design of Novel Enzymes (Prof. Justin Siegel)

An REU student will utilize computational tools to engineer and assay enzyme activity to identify novel enzymes. In a representative project, the student will reengineer β-glucosidase, a ubiquitous enzyme with important roles ranging from sugar utilization to antioxidant activation. The student will build large data sets in which hundreds of computationally engineered mutations are designed, built, and experimentally characterized in terms of k_{cat} and K_M. This fundamental study will elucidate the intricacies of this enzymes structure-function relationship, enabling the rapid redesign for new applications. A student will develop skills in enzyme engineering, molecular modeling, molecular biology, microbiology, protein purification, enzymology, and computer science.



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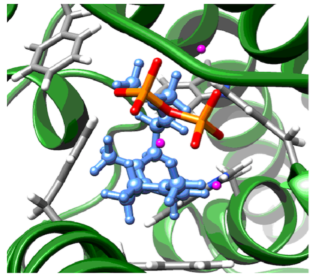
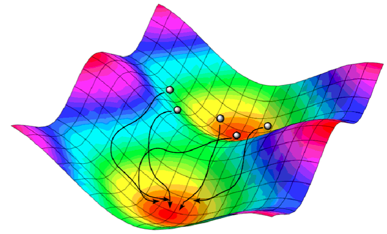
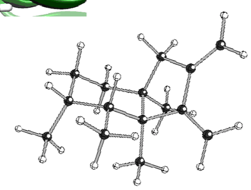
Computational Studies of Energy Surfaces and Reaction Dynamics
(Prof. Dean Tantillo)

An REU student will utilize quantum chemical calculations to investigate factors that control the reactivity and selectivity of organic compounds. In particular, the roles of potential energy surfaces, entropy and non-statistical dynamic effects will be explored. The student will develop skills in multiple types of molecular modeling and will gain experience with performing calculations within a scientific computing environment.







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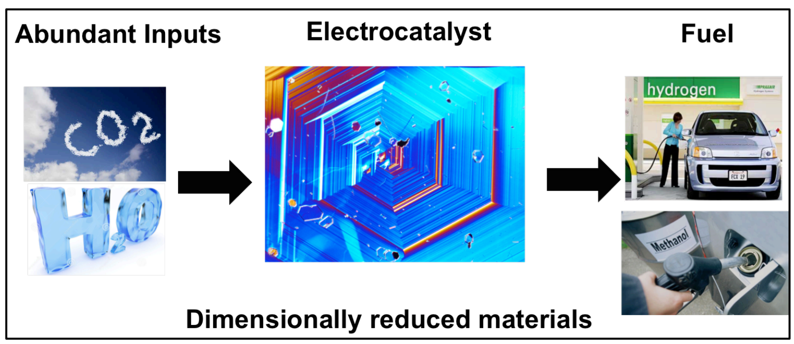
Synthesis and Characterization of Heterogeneous Electrocatalysts for Energy Conversion
(Prof. Jesús M. Velázquez)

An REU student will focus on the synthesis and electroanalytical characterization of heterogeneous catalysts for the reduction of CO_2 to liquid fuels. The student will have the opportunity to learn synthesis of thin films via the vapor-liquid-solid, thermal conversion or solid-state chemistry methods. The student will have the option to choose among the research group targeted materials; such as 2D metal carbides, mesoporous metal oxides or metal nitrides. In addition, the student will learn how to monitor the formation of liquid fuels from CO_2 by combining various analytical techniques including electrochemistry, NMR spectroscopy, and gas chromatography.



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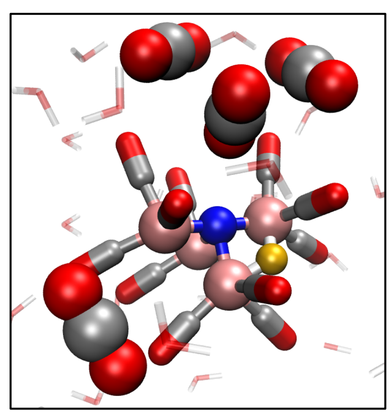
Molecular Dynamic Simulations for CO_2 Reduction Catalysts
(Prof. Lee-Ping Wang)

An REU student will apply first-principles molecular dynamics simulations to investigate the mechanism of CO_2 reduction in a molecular electrocatalyst. In a representative project, a student will simulate the interactions of a CO_2 molecule with a reduced form of a Fe_4N-containing transition metal catalyst (developed in the Berben lab) to investigate the mechanism of hydride transfer to CO_2 to yield formate ion. The student will develop skills using electronic structure and molecular dynamics simulation software, as well as Linux and scripting languages (e.g., Bash, Python) for task automation and data analysis. The student will develop skills to perform calculations within a scientific computing environment.



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