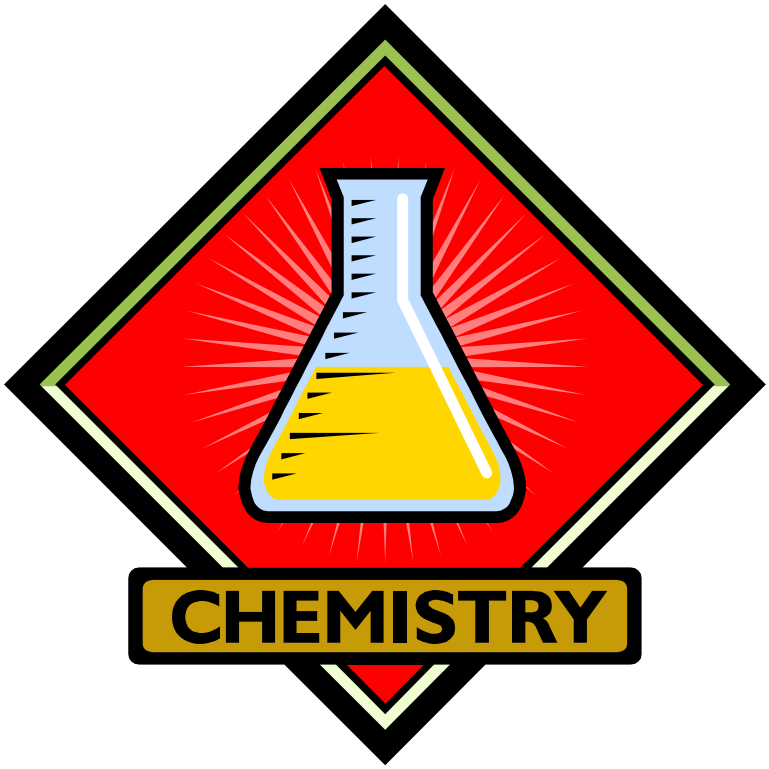
University of Cincinnati



Undergraduate Research Topics

2023-2024

Dr. Noe Alvarez

Office: 418T Rieveschl
Telephone: 513-556-9370
Email: Noe.Alvarez@uc.edu

The ***Alvarez Lab*** research is focused on carbon nanomaterials synthesis and assembly into macroscopic materials for sensor applications. We synthesize and assemble carbon nanotubes ***(Fig 1)*** into fibers and films and use them for physiological and electrochemical sensors, as well as energy storage devices. Besides of the fundamental chemistry such as synthesis and electrochemistry, students in the Lab are exposed to engineering aspects of nanomaterials development.

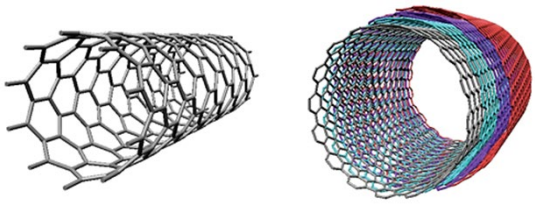


Fig. 1: *Single a and 4-walled carbon nanotubes*

Physiological Sensors: We are developing microelectrodes suitable for physiological applications such as recording extracellular activity for neuroscience research and the ability to stimulate neurons in a targeted fashion. Brain related treatments like epilepsy and Parkinson's disease, require microelectrodes implants that are flexible, biocompatible and reliable electrodes. This research is focused on a bottom-up approach that allows us to combine carbon nanotubes (CNTs) into macroscopic flexible electrodes that can be adjusted to application-specific requirements. Electron transfer rates are currently under study using Electroretinogram (ERG) for signal recording and electrical stimulation. Biocompatible polymer coatings and control over their porosity and stiffness are topics of interest in neuroscience as implants to prevent damaging brain tissue.

Electrochemical Sensors: Detection of heavy metals in our drinking water has become high priority for our societies, particularly for people living in cities where water infrastructure was built more than 50 years ago. This research intents to develop an electrochemical sensor based on CNTs to detect toxic metals such as Pb, Cd and Hg that have been detected in drinking waters. The sensor will quantify trace levels of multiple heavy metal ions simultaneously and should operate autonomously. Current electrochemical approach employs anodic stripping voltammetry and can detect nanomolar concentrations, however the sensitivity heavily depends on the material characteristics. Besides of the material, miniaturization of the electrodes allows the fabrication of small sensors that can potentially assist human wellbeing.

Energy Storage Devices: Miniaturized, flexible and wearable electronics devices are topics of growing interest. Powering these devices needs for compatible energy storage units that can exhibit similar mechanical strength and flexibility. Fiber-based energy storage devices that are light-weight, and flexible can be easily integrated into textiles. The large surface area, electrical conductivity, and mechanical strength of CNTs makes their fiber assemblies an ideal material for fiber supercapacitors and batteries. This research is oriented to the development of microns thick energy storage devices based on CNTs and thin films in combination with polymers.

Dr. Neil Ayres

Office: 704C Rieveschl
Telephone: 513-556-9280
Email: Neil.Ayres@uc.edu

Research in the Ayres Lab is focused on synthetic polymer chemistry for applications in biomaterials. We have ongoing projects investigating polymer biomimics for blood-contacting biomaterials, reversible gels with self-healing properties, and shape memory polymers. The experiments we perform are rooted in organic synthesis, but no prior knowledge of polymer science is required, and we welcome undergraduate student participation, especially from transfer students.

One of the main project areas we have in the Ayres lab is the synthesis of porous polymer materials known as polymerized high internal phase emulsions, or polyHIPEs. These porous materials have applications in acoustic materials, biomaterials, and as low mass-density engineering materials. In this work we prepare a two-phase emulsion, where the continuous phase contains polymerizable molecules, typically polyurethane or polysiloxane prepolymers. We use a rapid photochemical polymerization reaction to obtain the final materials. Students working on this project will gain experience in small molecule and polymer synthesis, polymer and materials characterization, and training in polymer and surfactant chemistry.

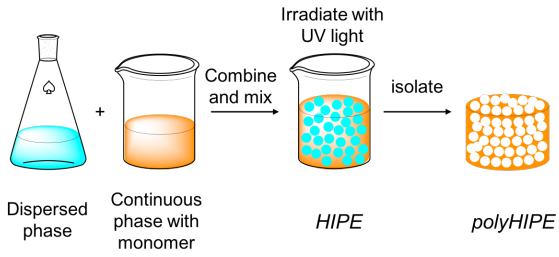


Figure 1. Synthesis of porous materials using an emulsion template.

The second major research area in our lab is in stimuli-responsive hydrogels. We are preparing hydrogels that can swell or shrink upon exposure to different stimuli, which results in different potential applications including as in vitro extra-cellular matrix models and as biomimetic actuators by compositing different hydrogels together. We use a variety of polymerizations mechanisms and small molecule chemistry to achieve this chemistry. Students working on this project will gain experience in polymer chemistry, hydrogel preparation and characterization, and training in polymer and network chemistry.

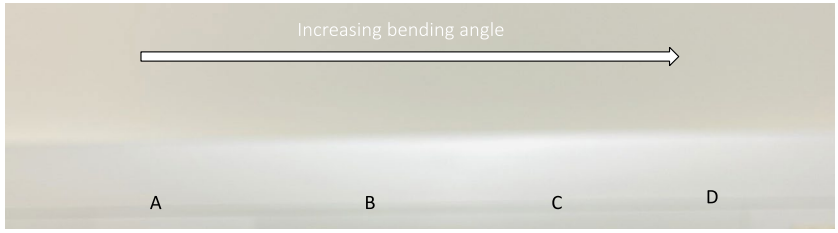


Figure 2. Hydrogel composites showing spontaneous curvature due to differences in swelling in the composite layers.

Undergraduate researchers in the Ayres group can contribute to these projects in many different ways. To learn more about our research please contact Dr. Ayres at neil.ayres@uc.edu or visit our website at ayreslab.squarespace.com.

Dr. Neil Ayres

Office: 704C Rieveschl
Telephone: 513-556-9280
Email: neil.ayres@uc.edu

Undergraduate researchers in the Ayres group can contribute to these projects in many different ways. To learn more about our research please contact Dr. Ayres at neil.ayres@uc.edu or visit our website at ayreslab.squarespace.com.

Dr. Michael J. Baldwin

Office: 302 Crosley
Telephone: 513-556-9225
Email: Michael.Baldwin@uc.edu

Undergraduate Research Opportunities in the Baldwin Group

Our research group is interested in designing new transition metal complexes that may have useful applications, and are inspired by bioinorganic systems, but are not limited to biologically available components. For example, one project in our group uses Ni(II), which is generally unreactive with O_2, to catalyze oxidation of various organic compounds using O_2 as the oxidant. Catalysis of aerobic substrate oxidations like this is considered to be environmentally friendly "green chemistry". This chemistry is accomplished by choosing ligand donor groups, oximates, which form a remarkable metal-organic redox hybrid with the nickel. This kind of redox hybrid is used in nature by various metalloenzymes, including the copper-containing galactose oxidase and amine oxidases, which catalyze the same kind of chemistry as our nickel complex. Another project in our group involves the development of bio-inspired, light-activated metal transport agents. These complexes bind Fe(III) very tightly, but release it as Fe(II) upon photolysis by an appropriate wavelength of light. Among the potential applications of these "siderophore mimics" is site-specific delivery of an activating metal to a metal dependent pharmaceutical, such as a chemotherapy agent that would be activated by the light-triggered release of an appropriate metal only at the tumor site.

A typical undergraduate project in any of these areas would involve synthesis of a new ligand designed for the particular application, characterization of its metal complex (with nickel, iron, or other appropriate metal), and screening the new complex for the desired chemistry. This will provide the student with experience in organic and inorganic synthesis, a variety of spectroscopic and analytical methods, and the evaluation of useful new chemistry. Several undergraduates working on these projects have become co-authors on published papers based on their research.

Dr. Ruxandra Dima

Office: 304 Crosley
Telephone: 513-556-3961
Email: ruxandra.dima@uc.edu

Bioinformatics methods for targeted drug-design:
Our group is developing and applying database mining approaches and other bioinformatics methods to the determination of binding motifs at interfaces between various biological molecules; the goal of this research is to build a repository of specific and non-specific interactions between macromolecules which can be used for targeted drug-design.

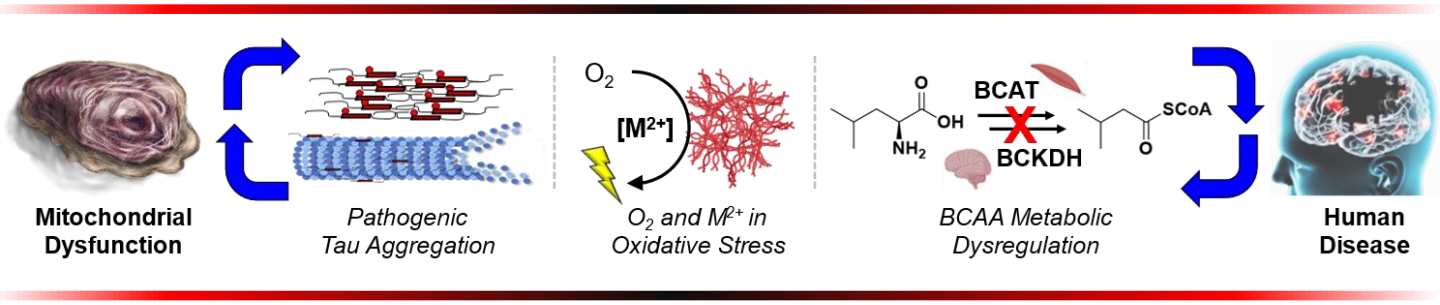
Computer modeling of biological macromolecules dynamics and function:
We are studying the conformational space in proteins using simplified methods that encode specific characteristics of the polypeptide chain; an example of a project is to target the metastable states that represent obligatory intermediates on the pathway of folding of a protein from a fully unfolded state to its native functional form. Knowledge of all the relevant intermediates for the reaction from the unfolded to the folded form of a molecule can be used to gain insight into the details of its function.

Anthony Grillo
www.GrilloLabUC.com

Office: 902 Crosley
Phone: (513) 556-1034
Email: grilloas@ucmail.uc.edu

Elucidating the Molecular Mechanisms of Mitochondrial Dysfunction in Disease

Overview: Research in the Grillo Lab focuses on the *molecular understanding* of how genetic, age-related, or environmental-induced mitochondrial dysfunction alters metabolism through molecular O_2 pathogenicity, amino acid metabolism, and metal-mediated proteostatic failure in neurologic disease. Mitochondria are increasingly recognized as more than just the "powerhouse of the cell", but play central roles in metabolism, proteostasis, nutrient regulation, and other physiological processes. However, mitochondrial failure is a central hallmark of aging, and is causative in many genetic diseases. Our research at the *interface of biochemistry, metabolic physiology, and medicine* employs multiple *in vitro* and *in vivo* models to investigate the basic biochemistry and molecular mechanisms of inborn errors of metabolism (e.g. Leigh Syndrome) and age progressive neurodegenerative diseases (e.g. Parkinson's and Alzheimer's Disease) caused by mitochondrial dysfunction.



Project 1: Age is the greatest risk factor in acquiring most mortality causing diseases such as Alzheimer's Disease, heart disease, and diabetes. Mitochondrial dysfunction through deactivation of Complex I of the mitochondrial Electron Transport Chain remains one of the earliest features in many of these diseases. However, there remains an *urgent need to better understand the influence of mitochondrial dysfunction on the molecular determinants that elicit biologic decline*. Age-related reductions in ETC activity cause metabolic O_2 imbalances, microvascular aging, and neuroinflammation in dementia and movement disorders. Our lab probes the etiological implications of mitochondrial dysfunction in proteotoxicity and illuminate the molecular underpinnings of Complex I deficiencies in neurometabolic diseases. To achieve this, we use a variety of cellular and animal models with the goal of discovering novel pharmaceutical interventions to treat biological decline with normative aging.

Project 2: Mitochondrial dysfunction with age promotes metal deposition and reduces oxygen utilization, which may contribute to the oxidative stress that accompanies normative aging. Oxidative damage is widely implicated in explaining disease pathophysiology, however, there is *a dire need to better understand the underlying molecular chain of events that cause this oxidative damage*. Our lab investigates the pathophysiology of divalent metal and O_2-mediated oxidative damage caused by mitochondrial dysfunction by identifying oxidized proteins that accumulate with age, determine which sites are vulnerable to metal-mediated oxidation, elucidate the fundamental biochemical principles that dictate metal binding, and probe their importance in biologic decline in normative aging. More broadly, we aim *to unravel the largely uncharted metalloproteome*, and uncover how O_2 and metal imbalances influence the ~30% of the proteome that can bind metals.

Project 3: There is a longstanding interest to understand the regulation of mitochondrial metabolism and the cross-talk between these complex pathways. Furthermore, there is a dire need to better understand alterations in metabolism in disease. Branched chain amino acid (BCAA) accumulation is implicated in age-related diseases (e.g. diabetes) and inborn errors of metabolism (e.g. maple syrup urine disease). Improper BCAA catabolism in mitochondria initiates early-onset muscle wasting and progressive brain degeneration in mice and patients. Severe nutritional BCAA restriction helps manage this disease, but there is *a marked paucity of effective pharmacological interventions*. Our lab aims to better understand the pathobiology of diseases associated with defective branched chain amino acid metabolism in mitochondria. This mechanistic-based approach will further enable the discovery of novel treatments for diseases such as Maple Syrup Urine Disease.

Dr. Hairong Guan

Office: 822 Rieveschl
Telephone: 513-556-9239
Email: hairong.guan@uc.edu

The research in the Guan group lies at the interface between inorganic and organic chemistry focusing on the development of homogeneous catalysts based on first-row transition metals such as nickel, cobalt, iron and copper. Such efforts are motivated by the fact that precious metals, which are widely used today in catalysis for synthesizing commodity and specialty chemicals, are expensive, limited in supply, and sometimes difficult to remove from organic products. The challenge of using first-row transition metals for catalysis starts with the difficulty in identifying ligands that can not only bind tightly to the metals but also promote precious metal-like reactivity or de-emphasize metal's role. Our investigation of pincer-ligated metal hydrides has led to the discovery of nickel and iron based catalysts for the hydroboration of CO_2 to methanol derivatives and the hydrogenation of fatty acid methyl esters to fatty alcohols. Our ongoing projects build on these initial successes and focus more on the improvement of catalytic efficiencies through further modification of the catalyst structures. Students involved in these projects will learn various synthetic techniques including the handling of air- and moisture-sensitive compounds. They will also be trained to conduct mechanistic studies using NMR spectroscopy, X-ray crystallography, and chemical kinetics. Furthermore, the research projects will teach students the concept of increasing energy efficiency by performing catalytic reactions and the notion of sustainability by using renewable feedstock and readily available materials.

Dr. Anna D. Gudmundsdottir
http://www.anna-research.com

Office: 821 Rieveschl
Telephone: 513-556-3380
Email: annag@uc.edu

Photodynamic Crystals

Crystal's natural beauty is captivating, and consequently colorful and aesthetically pleasing crystals have been used as ornaments and jewelry from the beginning of the time. Crystals, however, are not only visually appealing, they have been applied in numerous practical ways over the centuries. We are studying photoinitiated release of gas molecules from various crystal lattices. The release of gas molecules from the crystal lattice is distinctive for each compounds. For example, some crystals tolerate a build-up of large gas bubbles within the crystals before cracking, whereas others release gas concurrently with light exposure. Some crystals shatter fiercely upon exposure to light, whereas others leap around and gradually break apart. We are elucidating how the crystal packing arrangement affect the release. Understanding how the crystal lattices control the photodynamic behavior of organic molecules, will contribute towards the field of materials science, and aid in developing various devices, which are based on light can be converted into motions, such as actuators and sensors. In addition, the release of N_2 from organic azido crystals makes it possible to be develop light-initiated air inflating devises or explosives, similar to what is used to inflate airbags in automobiles

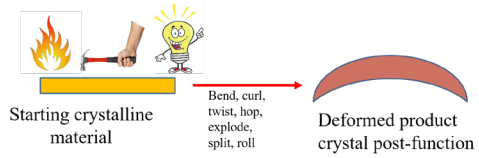
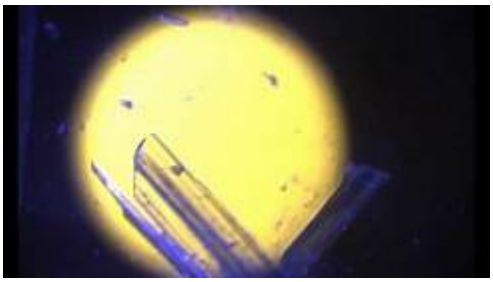


Figure 1. Dynamic behavior of crystals



https://www.youtube.com/watch?v=YSFFrv3uCNA
Figure 2. Example of photodynamic behavior: Cinnamic aid exposed to light

An undergraduate project would focus on preparing various derivatives of an organic azido compound and investigate if they release nitrogen gas upon exposure to light. The undergraduate student working on this project will gain experience in carrying out simple synthesis and how to purify the starting material by column chromatography. The student will learn to use 1H-NMR, IR and MS spectroscopy to characterize the starting materials. The student will also learn how to record and analyze the movements of the crystals upon exposure to light.

Dr. Jianbing Jiang

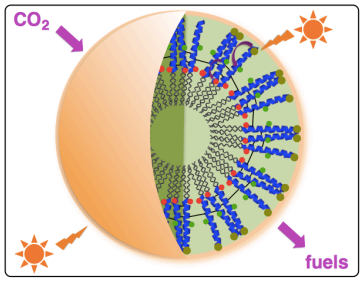
Office: 717 Rieveschl
Telephone: 513-556-1952
Email: Jianbing.Jiang@uc.edu

Statement of Research in the Jiang Group

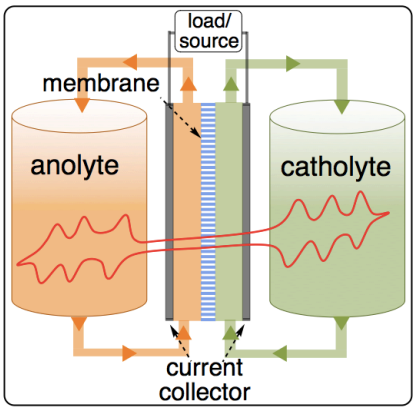
The interdisciplinary research in the Jiang group involves expertise in a wide variety of areas (materials science, renewable energy, molecular engineering, and spectroscopy). Undergraduate students in our group will have options to work on various project(s) based on their expertise and research interests.

Our research interests center on the development of advanced materials with novel properties to address the main question in the renewable energy field. Leveraging synthetic and molecular engineering techniques, we will design and synthesize a series of model materials to understand the molecular interactions underpinning renewable energy storage. Our research is focused in two areas: catalysis for renewable fuel production and rechargeable battery for energy storage, as briefly described below.

Photo- and electrocatalysis for renewable fuel production. Photocatalytic nanoreactors have the advantage that substrates and catalysts are confined in a nanosized compartment for improved compatibility and catalytic performance. Our group will design and construct self-assembled, hybrid nanoreactors as a platform for photocatalysis of various substrates, with special interest in CO_2 photocatalytic reduction to renewable fuels. Each of the photosynthetic components (photosensitizers and catalysts) is positioned at specific sites within the nanoreactor to allow efficient energy transfer from the chromophores to the catalytic centers. The modular hybrid architecture facilitates the molecular engineering for overall efficiency improvement. Metrics of success include product selectivity, catalyst stability, and electrochemical (over)potentials.



Next-generation rechargeable batteries for stationary and mobile energy storage. Redox flow batteries (RFBs) have received increasing attention as a large-scale stationary energy storage technology due to their safety, cost efficiency and scalability. Enhancing energy density is one of the most pressing issues in the development of RFBs. Our group focuses on the development of highly soluble, multielectron-active, polymeric metal complexes with tunable redox properties for improved overall battery performance. Synthetic tools will be used to prepare a series of metal complexes with variations on metal centers, peripheral ligands, and polymer backbones and side chains. Electrochemical and mechanistic studies will then be performed to elucidate the structure-function relationships to provide information to design, synthesize and characterize the next generation of polymeric metal complexes with combining desirable properties. The identified candidates will be tested in flow batteries, and the feedback obtained will facilitate iterative development of polymeric metal complexes with improved performance.



Fast-growing demand for high power-density batteries for electronic devices and electric cars has motivated the exploration of energy storage devices with high charge capacity and stable cyclability. The lithium-sulfur battery has a high theoretical specific capacity yet has been retarded by the loss of active sulfur species during charge/discharge cycles. Our group will design and synthesize a saccharide-based polymer cathode material to (1) entrap the sulfur material in the cathode region by covalent bonding; (2) increase the battery practical capacity; (3) enhance the charge/discharge cyclability; and (4) reduce the cost. The carbon nanotubes (CNTs) are electronically conductive and will be used as a structural and electronically conductive support to improve the conductivity of the glycopolymer. The degree of sulfur loading will be optimized to improve the performance of the cathode material. Sulfur redox reactions and confinement mechanisms will also be studied at the molecular level, the results of which will in turn guide iterative material designs for better performance.

Dr. In-Kwon Kim

Office: 802 Crosley
Telephone: 513-556-1909
Email: in-kwon.kim@uc.edu

Poly(ADP-ribosy)lation (PARylation) is a reversible post-translational modification that regulates DNA repair, gene expression, and cell fate. Targeting poly(ADP-ribose) (PAR) metabolism and signaling emerges as a promising strategy for tumor-specific therapy and precision cancer medicine. Research projects in our lab are focused on understanding the structure, mechanism, and function of a PAR turnover enzyme PARG, a PAR-dependent tumor suppressor CHFR, and PAR signaling proteins. We are particularly interested in developing small-molecule modulators of those proteins as novel anticancer therapeutics. Students will use multidisciplinary research tools, including X-ray crystallography, time-resolved fluorescence resonance energy transfer (TR-FRET), small-angle X-ray scattering (SAXS), high-throughput screening, various biochemical assays, and chemical synthesis, to investigate 1) how proteins and domains communicate for their specialized functions, and 2) how they specifically recognize small-molecule ligands and substrates.

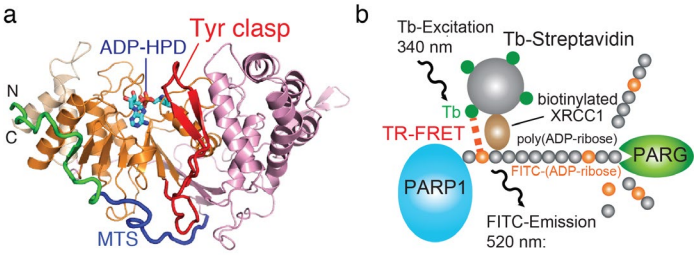


Fig. 1. Structural biochemistry of poly(ADP-ribose) glycohydrolase (PARG). (a) Structure of PARG bound to its substrate mimic ADP-HPD (Kim *et al*., *Nat. Struct. Mol. Biol.* 2012) (b) Schematic of a high-throughput TR-FRET PARG activity assay (Kim *et al*., *J. Biol. Chem*. 2015).

Project 1. Structural biology of PAR turnover and signaling proteins**:** Poly(ADP-ribose) metabolism is essential for maintenance of genomic integrity and downstream DNA damage response. PAR glycohydrolase (PARG) is a primary enzyme that turns over PARylation and thereby counteracts the PAR synthesis by PARP1. Using X-ray crystallography and SAXS, we are investigating the structure and protein-substrate/inhibitor interactions of PARG and downstream PAR signaling & DNA repair enzymes. This structural work (***project 1***), along with a high-throughput assay (***project 2***), will be a framework to develop novel chemical modulators/probes (***project 3***) for these bio-medically important enzymes.

Project 2. Development of a high-throughput TR-FRET assay for PAR turnover and signaling proteins**:** We are using a Time-Resolved Fluorescent Resonance Energy Transfer (TR-FRET) as a primary assay system. TR-FRET assay can be developed in a 384-well format that is suitable for high-throughput screening, and is a convenient mix-and-read type of assay with very low background signal. We are currently using or developing a TR-FRET assay for PARG, CHFR, DTX3L, and DNA ligase III for biochemical analysis of their enzymatic activities and for high-throughput screening.

Project 3. Cancer drug discovery through a high-throughput screening and a structure-based lead optimization**:** We aim to discover and develop new cancer therapeutics by targeting PAR metabolism and signaling pathways. Once we establish a TR-FRET assay (***project 2***), we actually run a pilot screening or medium- to high-throughput screening *in house* to identify new chemical scaffolds. We will optimize our lead compounds through a structure-activity relationship and a high-resolution crystal structure of protein-ligand complex.

Dr. Wei Liu

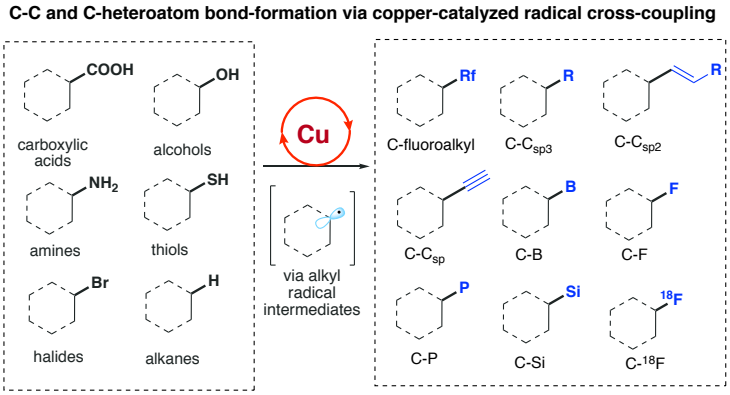
Office: 430 Rieveschl
Telephone: 513-556-5865
Email: liu2w2@uc.edu

The Liu Group @ UC

Overview

The overarching goals of the Liu group are dedicated to the discovery of practical catalytic reactions and understanding the mechanisms of these reactions. My research interest can be divided into two areas of research:
1. Development of new catalytic methods for the synthesis of biologically active molecules
2. Investigate the reactive intermediates in transition-metal catalysis
Our research program will be multidisciplinary and students in our lab will gain extensive training in organic and inorganic synthesis, methodology development, compound characterization, electrochemistry, medicinal chemistry and radiochemistry.

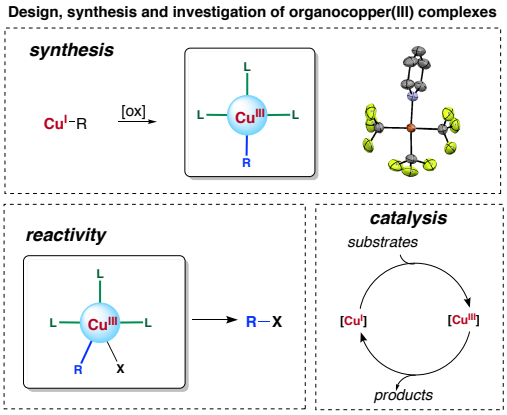
1) Development of Copper-Catalyzed Radical Cross-Coupling Reactions



Cross-coupling reactions are powerful tools for the construction of carbon–carbon and carbon–heteroatom bonds. Despite the advantageous properties of copper, copper-catalyzed cross-coupling reactions remain largely underdeveloped. The limited capability of copper to catalyze cross-coupling reactions has been attributed to the slow oxidative addition rates of Cu^{I} complexes. Our group will address this challenge by developing and advancing copper-catalyzed radical cross-coupling reactions. We hypothesize that a single electron transfer from a Cu^{I} catalyst with an alkyl electrophile could lead to the formation of an alkyl radical and a Cu^{II} intermediate, which could recombine to form an organocopper(III) complex. This high-valent Cu^{III} complex reductively eliminates to form the product. Our research group will explore different reaction parameters, including electrophiles, nucleophiles, and ligands, to develop novel copper-catalyzed reactions, which will allow for the facile construction of a variety of C-C and C-heteroatom bonds. Our interest in this field includes:

- The development of novel copper-catalyzed C-C bond and C-heteroatom bond-forming reactions
- The rational design of new ligands/catalysts guided by detailed mechanistic studies
- The merging of copper-catalyzed radical coupling with electrochemistry

2) Design, Synthesis and Investigation of Novel High-Valent Organocopper(III) Complexes



High-valent organocopper(III) compounds have long been considered key intermediates in copper-catalyzed reactions. However, reactive organocopper(III) complexes with well-defined structures remain limited. As a result, considerable controversy remains over the involvement of Cu^{III} species in these catalytic reactions. Therefore, development of methods for the synthesis of structurally defined organocopper(III) complexes and investigations of their reactivity complexes will be vital toward the progress of Cu-based organometallic chemistry and catalysis. Our research group will rationally design and synthesize high-valent organocopper(III) complexes in order to directly investigate their reactivity toward catalytically relevant bond-forming reactions. The fundamental understanding of these reactions will guide the optimization of known copper-catalyzed reactions as well as drive the development of novel catalytic systems. Our interest in this field includes:

- The design, synthesis and investigation of catalytically-relevant organocopper(III) complexes
- The mechanistic investigation of the fundamental reactions of organocopper(III) complexes
- The development of novel copper(III)-catalyzed group transfer reactions

Dr. James Mack

Office: 831 Rieveschl
Telephone: 513-556-9249
Email: james.mack@uc.edu

Green Chemistry

The chemical community has recently been concerned with green chemistry. These concerns have led to an increasing interest in chemical waste minimization. One of the primary sources of chemical waste is volatile organic compounds (VOCs). Many VOCs have been targets of waste minimization since the Clean Air Act Amendments of 1990. In research laboratories organic solvents generally comprise most of the waste involved in a reaction. Common practice has been to use milligram quantities of reagents and gram quantities of solvents. At the conclusion of such reactions the small amounts of reagents are recovered, and the large volumes of solvent discarded. VOCs such as carbon tetrachloride and benzene both appear on several of the EPA's minimization priority lists. Carbon tetrachloride has been shown to be an ozone depletion chemical, while benzene is a known carcinogen. Although both of these chemicals have a history of environmental disdain they are continually used in the research laboratory as well as in industrial processes, especially in the area of radical chemistry. Benzene has been cited in more than 1,400 publications as the solvent for various reactions in 2002. Likewise, carbon tetrachloride, given its tag as an ozone depletion chemical and its mark up in price over the past several years has been used as a solvent in more than 400 publications in 2002. We are interested in exploring solvent-free reactions utilizing high-speed vibrational milling. HSVM is a procedure in which solid reactants (crystals or powders) are placed inside a steel vessel along with ball bearings. The vessel is sealed and placed inside the milling apparatus whereby it is vigorously agitated. The high speed agitation (60 Hz) forces the ball bearings to pulverize the reagents, causing them to react. Reactions under HSVM conditions potentially will have large impact in organic synthesis with little to no solvent waste.

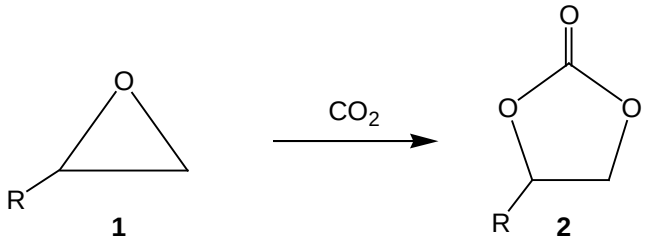
Dr. Allan R. Pinhas

Office: 602 Crosley
Telephone: 513-556-9255
Email: allan.pinhas@uc.edu

The Conversion of an Epoxide to a Cyclic Carbonate

Several years ago, we discovered the very easy and synthetically useful conversion of an aziridine (a three membered ring compound with nitrogen in the ring) to an oxazolidinone (a five membered heterocyclic system) using carbon dioxide (CO_2). This stereo- and regiospecific reaction may be done using THF or water as the solvent, and it also may be done in the absence of any solvent. This reaction uses common salts, such as LiI, KBr, and NH_4I, as the catalyst.

Our goal is to extend this chemistry to the conversion of an epoxide (**1**) to a cyclic carbonate (**2**) using similar reaction conditions.



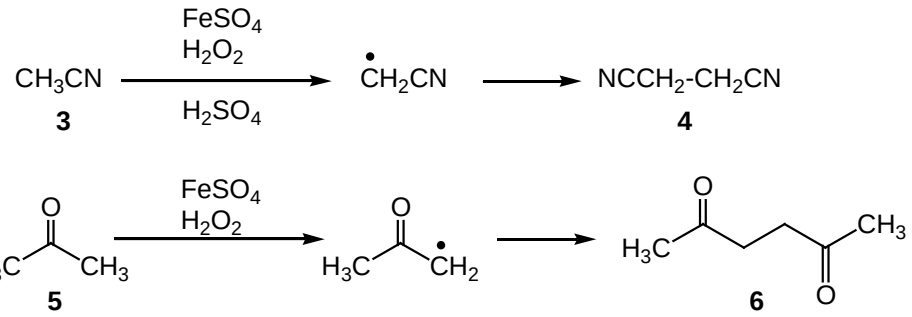
1 **2**

An undergraduate student will investigate various substitution patterns on the epoxide, different solvents, and different salts as potential catalysts. In addition, our goal will be to determine the regio- and stereochemistry of the conversion of compound **1** to compound **2**.

Generation of Carbon-Carbon Bonds with Water as the Solvent

Fenton's Reagent ($FeSO_4$ and H_2O_2 in water) is well known for its ability to remove a hydrogen atom from DNA and cause the double helix to unravel. It also causes the degradation of other biological systems, such as proteins and lipids. In contrast, we have studied the use of Fenton chemistry not to destroy a molecule, but rather to create new carbon-carbon bonds. Specifically, we have investigated the radical coupling of acetonitrile, acetone, and acetophenone using water as the solvent.

Two molecules of acetonitrile (**3**) couple to give succinonitrile (**4**) in good yield. However, the coupling of two molecules of acetone (**5**) only occurs in very low yield. Surprisingly, when acetone and acetonitrile are mixed, the acetone coupling product **6** predominates.



3 **4**

5 **6**

An undergraduate student will investigate ways to improve the yield of the coupling of ketones and also will investigate the coupling of various other functional groups.

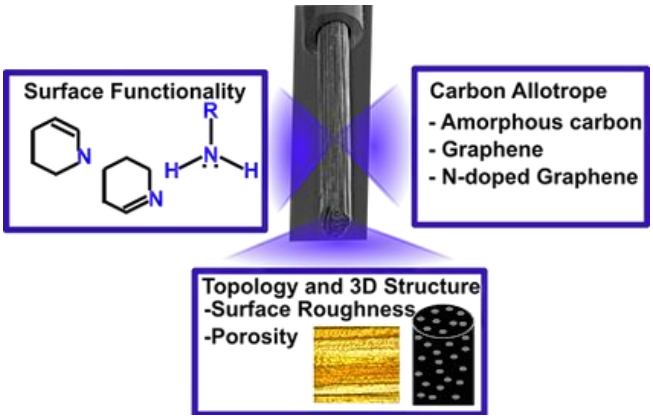
Dr. Ashley Ross

Office: 418 Rieveschl
Telephone: 513-556-9314
Email: Ashley.ross@uc.edu

Research in the Ross lab focuses on developing methods to probe signaling within and between the brain and the immune system. Our lab primarily uses a combination of electrochemistry, microfluidics, and fluorescence microscopy to reveal the intricate signaling network across these organs. We are specifically interested in understanding the mechanism of how neurotransmitters are regulating important "danger signals" within the brain and how this communication is extended into the immune system during autoimmunity. Undergraduates are required to commit to a minimum of 2 semesters in the Ross lab so that adequate learning of the analytical methods and contribution to the overall goals of the lab (discussed below) are achieved. Students will have the opportunity to aid in the following projects:

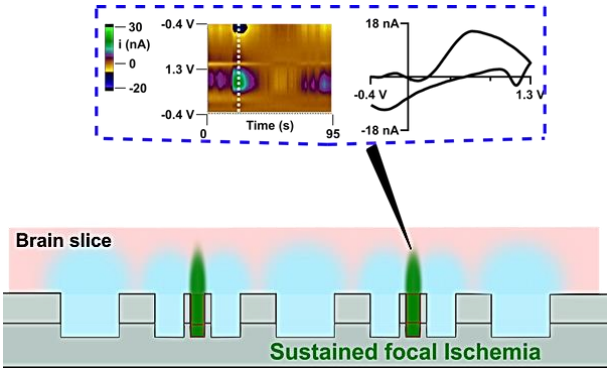
(1) Novel Carbon Surfaces

Carbon-fiber microelectrodes are common electrode materials for FSCV detection. Our lab is interested in investigating and designing novel carbon materials and developing new carbon-fiber microstructures and functionalizations to improve electrochemical detection of a variety of important neurochemical analytes. We focus on the fundamental interactions at the electrode-analyte interface to drive carbon surface design. Projects in this area are focused on fundamental electrochemistry, materials science, electrode surface characterization, and computational simulations of analyte-electrode interactions.



(2) Microfluidics

Microfluidics allows precise control over small volumes with exquisite spatial resolution. The brain is a complicated organ of the central nervous system, composed of several sub-regions ranging from a few microns to several hundred microns in size. Likewise, the central organ of the immune system (the lymph node) is fairly heterogeneous. The ability to better replicate complicated in vivo signaling but with precise control within and between organs along the gut-brain-immune axis would significantly advance our understanding of a host of inflammatory and neurodegenerative diseases. Our lab focuses on designing microengineered platforms to more precisely study the effects of stroke and neural communication between the brain and immune system.

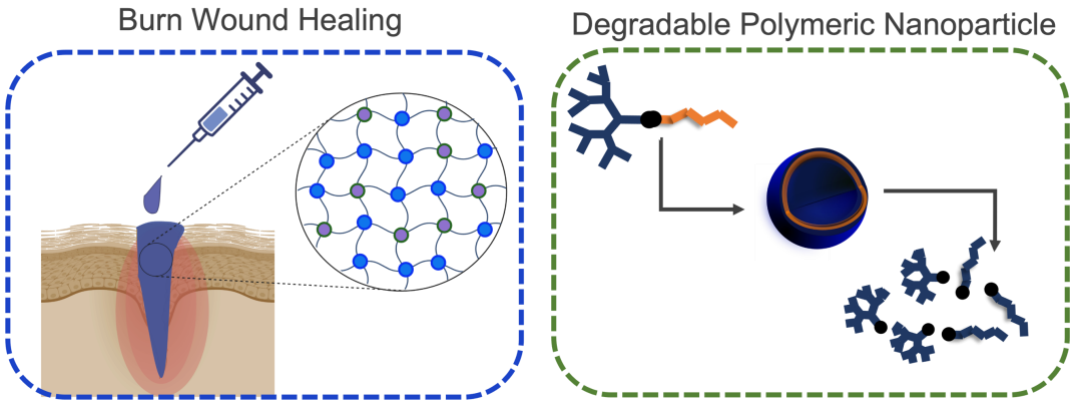


(3) Monitoring neurochemical signaling in real-time

Traditional neurotransmitters and neuromodulators, like catecholamines and indolamines, can be released from not only neuronal cells, but also immune cells to aid in inflammatory modulation. The extent to which these neurochemicals are signaling within the immune system is not well understood. Fast-scan cyclic voltammetry (FSCV) coupled to carbon-fiber microelectrodes is an electrochemical technique widely used to study neurotransmitter release in the brain and provides the necessary temporal resolution needed to monitor rapid changes. Our lab is focused on developing methods to characterize and monitor rapid signaling within both the brain and immune system. Projects in this area focus on developing and applying new methods to study purine signaling in the brain during ischemia and neurochemical signaling in organs along the gut-brain-immune axis.

Simms Lab of Functional Biomaterials

Overview: Research in the Simms Lab of Functional Biomaterials focuses on the strategic design of bio-interactive materials that directly addresses health equity concerns from a chemistry and biomedical engineering perspective. Currently, we are developing polymeric biomaterials for applications in wound healing and therapeutic delivery. If you have special interests in conducting interdisciplinary research that bridges synthetic organic chemistry, biochemistry, and biomedical engineering in a dynamic learning environment, this might be the lab for you! For more information regarding the current research in our lab or becoming a lab member feel free to contact Dr. Simms at: simmsbl.ucmail.uc.edu.



Project 1:

According to the American Burn Association, 11 million burns (of all types) occur annually. Unfortunately burn injuries are more prevalent in vulnerable communities (considering socioeconomic status, disabilities, and the elderly). Current methods of treating burn wounds include skin grafting (requiring healthy skin with an immune match) or polymeric dermal substitutes (which often lack the dermal components to encourage tissue regrowth). We believe that injectable, polymeric hydrogels are the solution to promoting burn wound healing and tissue regeneration. With these things in mind, we aim to design and develop a hydrogel scaffold for applications in burn wound healing.

Burn wounds are classified by the depth of penetration within the skin caused by extreme heat, electrical, or chemical means. One of the reasons that tissue engineering has become a rapidly growing field is to close the gap between the supply and demand for tissue and organ transplantation. As it pertains to skin, tissue engineering aims to assist the physiological healing of epithelium and induce the regeneration of skin and its components. The development of hydrogels for use as tissue engineering scaffolds has proven to be a useful strategy for promoting the growth and formation of the desired tissue after a burn. The specific challenges we will address are 1) developing a library of injectable hydrogel scaffolds with varying physical and mechanical properties that match that of various skin types, and can be injected into irregular shaped wounds, 2) develop a scaffold that allows for the delivery of therapeutic agents and cell infiltration for tissue regeneration, and 3) address differences in skin pigmentation by encouraging melanogenesis (formation of melanin) within the skin.

Project 2:
There are lots of health-related challenges that can result in someone taking a significant amount of pills/medications over a prolonged period of time. What if there was a way that all of the medication for a given time period was administered simultaneously in one simply injection? This is the premise of another project area in the Simms Lab of Functional Biomaterials.

Polymeric nanoparticles are a favorable vehicle for the delivery of therapeutics. Although some polymeric materials have made their way to clinical settings, there is still significant room for improvement in the realm of overall stability, drug loading capabilities, targeted delivery, and drug release. To this end, our lab will be designing, and synthesizing Janus-type dendrimer-based amphiphiles that can self-assemble into nanosized-carriers. The specific challenges we will address are 1) design a library of fully degradable nanoparticles, 2) integrate a timed-release system into established particle systems 3) introduce specified targeting moieties to understand targeting pathways.

Contact Information:
Principle Investigator:
Briana L. Simms, Ph.D.
Email: simmsbl@ucmail.uc.edu

Dr. David Smithrud

Office: 603 Crosley
Telephone: 513-556-9254
Email: david.smithrud@uc.edudu

Our research group designs, synthesizes, and authenticates novel organic molecules for biological and physical applications.

Dr. George Stan

Office: 1501B Crosley
Telephone: 513-556-3049
Email: george.stan@uc.edu

Research in Stan's group is focused on computational modeling of biological nanomachines involved in essential protein quality control mechanisms of protein folding assistance and degradation.
We develop and apply computational molecular modeling tools, such as the widely used program CHARMM, in combination with extensive data mining of protein databases. This is an opportunity to acquire a diverse set of computational skills and apply them to problems of biomedical interest. In addition, our supercomputer cluster provides a chance to learn about designing and maintaining high-performance computers for data intensive applications.

Molecular modeling of chaperonin-assisted protein folding
Chaperonins are biological nanomachines that employ a spectacular mechanism to assist protein
folding. During the chaperonin cycle, concerted, large scale, rigid body conformational changes, ultimately driven by ATP hydrolysis, result in a dramatically expanded chaperonin cavity serving as folding chamber. Currently, very little is known about the annealing action of eukaryotic chaperonins. Questions that we are trying to address are what are the chaperonin binding sites for substrate proteins, how does protein folding assistance take place in the absence
of a change in chemical environment and how does the sequential opening of the eukaryotic chaperonin promote protein folding.

Computational models of protein degradation by bacterial proteases
Protein quality control such as degradation mechanisms prevent deleterious off-pathway reactions of misfolding or aggregation. In the degradation pathway, AAA+ (ATPases associated with various cellular activities) nanomachines, such as bacterial Caseinolytic protease (Clp) ATPases, unfold and translocate SPs through narrow central pores as a prerequisite for the ultimate destruction of the polypeptide chain within the peptidase chamber. We focus on probing the dependence of the Clp ATPase unfoldase function on the direction of application of mechanical force. Multiscale modeling of Clp-mediated unfolding of SPs with discernible mechanical anisotropy will yield detailed information of these properties. We propose to probe mechanisms of unfolding and translocation along the restricted direction of the N-C termini. The substrate proteins to be studied will involve wild-type and variants of proteins probed in single-molecule experiments. Unfolding and translocation patwhays obtained in these studies will be contrasted with those in multidirectional pulling geometries, which mimic the cellular environment.

Pietro Strobbia

Office: 201 Crosley
Telephone: 513-556-5883
Email: strobbpo@ucmail.uc.edu

Overview

The research in our group is largely directed towards bridging the gap between current state-of-the-art sensing technologies and the actual requirements for their application in clinical settings or in the field. To this end, we leverage expertise in optics, plasmonics, surface-enhanced Raman scattering (SERS) and sensing. We are a multidisciplinary lab and follow all the steps in the development of these technologies, from the chemical transduction mechanism to the optical detection and the development of deployable prototypes. Our long-term goal is to benefit the developing and developed world through the dissemination of new cost-effective and practical analytical tools.

Undergraduate students will have the opportunity to be involved in different aspect of this work depending on their interests. Possible research tasks include optimization and synthesis of nanoparticles and other plasmonic-active substrates; test the analytical performance of sensing assays *in vitro* and in environmental samples; and aid the integration of sensing technologies into an automated device.

These tasks will contribute to the following projects:

DNA nanotechnology for ultrasensitive detection of viral targets

One of the “Holy Grails” of medical diagnostic applications are liquid biopsies, the detection of disease-specific biomarkers from peripheral body fluids (e.g., blood or nasal and oral swabs) for pre-symptomatic and non-invasive identification of a diseases. To this end, SERS-sensors are ideal due to their ability in the simultaneous detection of many biomarkers and their high diagnostic accuracy. The challenge in the application of these sensors for liquid biopsies is the requirement of extreme sensitivities (i.e., fM-range limit of detection). Reaching this detection range remains a challenge for the implementation of SERS-sensors. Innovative technologies are needed to enable applications to liquid biopsies.

The aim of this project is to develop SERS-sensors capable of detecting fM concentration of target nucleic acid sequences. We will achieve this goal by combining homogenous SERS sensors based on nanostars with a DNAzyme (DNA-enzyme) isothermal amplification mechanism. Such sensors will be capable of detecting numerous analytes simultaneously without sample preparation and at clinically relevant concentrations. This project will also involve the integration of the sensors and the sensing mechanism into a portable device. Undergraduate students can be involved in the synthesis of metallic nanoparticles used in this project (i.e., silver-coated nanostars). Additional opportunities are expected in the fabrication and optimization of the device, as well as on its validation.

Fiber sensors for *in situ* monitoring of toxic contaminants in water systems

A rising issue in ground water and freshwater supplies is the contamination by pesticides. These contaminants often reach groundwater through the runoff and drainage in farmland. Minimizing runoff of pesticides in the agricultural process is key to keep safe the current limited drinking water supplies. Current standard methods to detect water contaminants require large instruments, specialized personnel, multi-step sample preparation and are performed in a centralized lab, to which samples are shipped. There is a critical need for technology that could permit quantitative analysis of multiple contaminants directly in the field.

In this project, we will develop a field-ready plasmonic sensing system to directly detect pesticides in water for environmental applications, to detect water contaminants without the need of sample preparation and laboratory testing. These sensors are called aptamer-based inverse molecular sentinels (AiMS). The AiMS nanosensors consist of plasmonic nanoparticles equipped with functional nucleic acid sensing receptors that will change conformation in the presence of the target molecule through a competition assay. The nanosensors are immobilized at the end of optical fibers to permit remote sensing, directly in the water. Undergraduate students will be involved in the fabrication of the sensors, as well as on the evaluation of sensor performance in different media.

Dr. Yujie Sun

Office: 722 Rieveschl
Telephone: 513-556-0227
Email: Yujie.Sun@uc.edu

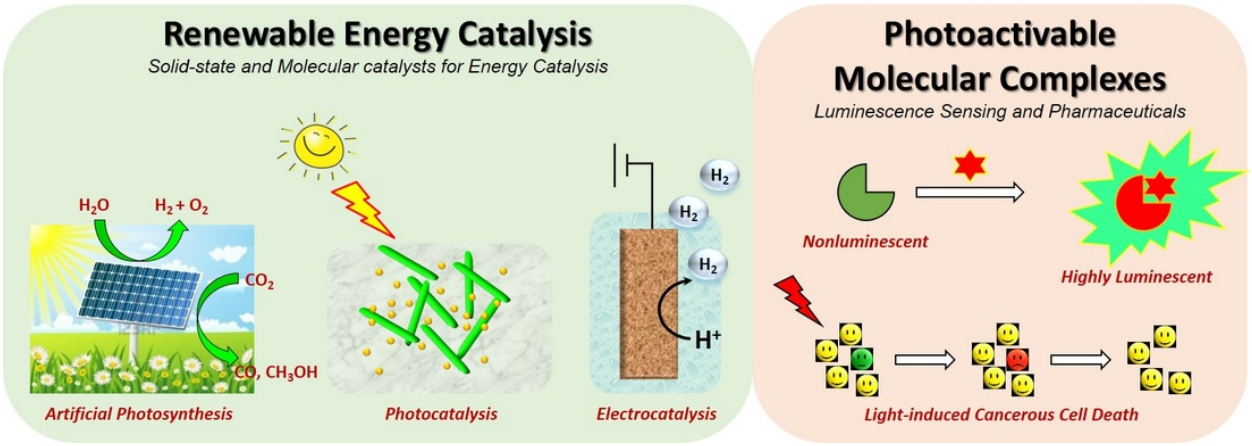
Undergraduate students are encouraged to join our group to participate in a variety of multidisciplinary research projects. The overall theme of our laboratory is to use our expertise in coordination chemistry, materials science, electrochemistry, and photochemistry to address two frontier challenges: energy and health. Students will be trained in a broad set of skills and inspired to become critical-thinking scientists with a passion on solving urgent problems from a fundamental science perspective.

Currently, we are interested in the following directions:

(**1**) Inexpensive solid-state materials for renewable energy catalysis and organic transformation, including water splitting, H_2 oxidation, N_2 reduction, and biomass valorization.

(**2**) Bioinspired molecular catalysts for small molecule activation, such as O_2 evolution.

(**3**) Photoactivable complexes and materials for luminescence sensing and phototherapy.



Dr. Pearl Tsang

Office: 701 Crosley
Telephone: 513-556-9239
Email: pearl.tsang@uc.edu

Undergraduate research in the Tsang laboratory involves introduction and analysis of the structure and function of important biochemical molecules such as proteins and nucleic acids. The research is focused upon understanding how essential proteins involved in protein biosynthesis recognize and interact with their cognate RNA molecules using techniques such as gel electrophoresis, spectroscopy and fluorescence.

Dr. Ryan White

Office: 418-B Rieveschl
Telephone: 513-556-4369
Email: Ryan.White@uc.edu

The White Group @ UC

Overview

Our research lies at the intersection of nanoscience, electrochemistry and the biological interface. Research interests in our group focus on the development of new (bio)analytical methods to probe chemical and biological systems with unprecedented spatial and temporal resolutions afforded by working at the nanoscale. The scope of this research is quite broad, ranging from studies of fundamental chemical and biological phenomena to the development of applied sensor technologies. As such, students in the group can expect to gain valuable interdisciplinary laboratory experience.

Electrochemical Biosensors and Bioanalytical Chemistry

The White Group @ UC develops electrochemical biosensors to tackle a wide variety of bioanalytical applications ranging from single cell analysis to biomedical diagnostic devices. As such, undergraduate students can become involved in different aspects of biosensor developing. The projects include fundamental studies of the electrochemical behavior of the sensor readout, biomolecular engineering and design of nucleic acid-based recognition elements, and the development and use of protein channels for single molecule sensors. Sensor development is always rooted in the application of the sensor and students will have opportunities to then apply their developed sensors to different biological systems.

Nanoelectrodes and Sensors

In line with our bioanalytical applications, we aim to develop small-scale sensors that are amenable to single cell analysis and electrochemical imaging. Undergraduates working in this area can become involved in new ways to make small electrodes, electrode characterization, sensor fabrication, and ultimately electrochemical imaging using scanning ion conductance or electrochemical microscopy.

Dr. Peng Zhang

Office: 702 Crosley
Telephone: 513-556-9222
Email: peng.zhang@uc.edu

Dr. Peng Zhang's group

Nanoscience is at the unexplored frontiers of science and engineering, and it offers one of the most exciting opportunities for innovation in technology. One of the hopes for nanoscience and technology is that the combination of a number of areas - from physics and chemistry to material science and biology - will create a new area and lead to major advances both in understanding of science and in their applications in technology. Key to this new era is research across many disciplinary interfaces. The central theme of this research program is the development of various types of nanomaterials and their applications in sensing and therapeutics.

Development of nanoparticle-based photosensitizers for photodynamic antibacterial therapy

We are developing nanoparticles as photosensitizers to be used in photodynamic antimicrobial therapy. The particle sizes range from <10 to 100 nm. The versatility of such nanoparticle-based photosensitizers lies in the fact that the surface of these nanoparticles can be modified to have either positive or negative charges so as to be specific to a class of bacteria, or be coated with antibodies specific to a certain type of bacterium. Experiments are underway to test the efficacy of these photosensitizers towards several bacteria, such as P. fluorescens, E. coli., and S. epi.

Development of chemical and biochemical sensors

There are various activities along this theme: 1) Develop nuclear relaxation-based sensor for detection. 2) Develop colorimetric detection schemes for point-of-care applications. 3) Develop SERS-tag for Raman imaging. 4) Design and develop oligonucleotide sensors based on photon upconversion nanoparticles.