October 2015

UNDERGRADUATE RESEARCH, CHEMISTRY 1710

Instructions:  Select areas that have the greatest appeal to you; then make appointments with the research directors to discuss the specific projects they have available.  [Undergraduate research is an important learning experience that should not be too time dependent.  However, since you are taking other classes, be sure to ask each research director approximately how much laboratory time per credit he/she will expect of you.]  After deciding upon the project you wish to undertake, check with the faculty member concerned to make sure he/she agrees to accept you.

Since a permission number is necessary for registering for Chemistry 1710 you must stop in Room 107 Chevron Science Center and see George C. Bandik or Regina Mahouski and also let us know whom you have selected as a research director; be sure to give the name of this individual.  We need this information so that a grade report can be issued at the end of the term.

<table>
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<th>Director</th>
<th>Research Area</th>
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| D. ACHARY     | Undergraduates can participate in two different research areas supported currently by the US-Department of Energy:  
                 1. Nuclear Magnetic Resonance (NMR) Spectroscopic investigations of novel materials for CO$_2$ capture. These materials include ionic liquids, polymers, microporous silica substrates and zeolites. Liquid and Solid state NMR spectroscopy will be used to characterize and also study molecular level interactions between $^{13}$CO$_2$ and these materials.  
                 2. Computational discovery and investigations of potential CO$_2$ capture materials. Quantum chemical calculations will be performed to probe inter- and intra-molecular interactions in commercial and custom synthesized Ionic liquids. Information gained from calculations will be correlated to physical properties obtained experimentally to establish a database for structure activity correlation for ionic liquids specific for carbon capture.  
                 [http://www.chem.pitt.edu/people/damodaran-krischan-achary](http://www.chem.pitt.edu/people/damodaran-krischan-achary) |
| (450 CHVRN-48403) | damodak@pitt.edu                                                            |
| S. AMEMIYA    | Bioanalytical Chemistry and Electrochemistry: Development, miniaturization and theory of electrochemical sensors, and application of these as a probe of scanning electrochemical microscope in order to understand molecular transport at biological membranes.  
                 [http://www.chem.pitt.edu/people/shigeru-amemiya](http://www.chem.pitt.edu/people/shigeru-amemiya) |
| (803A CHVRN-41217) | amemiya@pitt.edu                                                             |
                 [http://www.chem.pitt.edu/people/sandy-asher](http://www.chem.pitt.edu/people/sandy-asher) |
| (701 CHVRN-48570) | asher@pitt.edu                                                              |
K. M. BRUMMOND
(807 CHVRN-41955)
kbrummon@pitt.edu
Our group is focused on reaction discovery for the ultimate application to biologically relevant compounds. In particular, we apply these reactions towards the preparation of covalent modifiers of proteins targets and smart fluorophores; areas that are of great importance to human health.
http://www.chem.pitt.edu/people/faculty/kay-brummond

L. T. CHONG
(331 EBERL-46026)
lchong@pitt.edu
Computational Biophysical Chemistry. We apply computer simulations to study the structure, dynamics, and function of proteins at the atomistic level. Systems of interest include natively unfolded proteins, molecular switches, and their ligand binding interactions. Especially interested in undergraduates who would like to do research for at least a year, including full-time research during the summer.
http://www.chem.pitt.edu/people/faculty/lillian-chong

R. COALSON
(321 EBERL-48261)
rob@ringo.chem.pitt.edu
Theory of chemical dynamics, with applications to optical spectroscopy (absorption, Raman scattering, photo-dissociation processes), tunneling, isomerization, optical fiber design, neutron scattering cross sections, and other experimentally observable phenomena. Emphasis is on using measured spectra and cross sections to unravel microscopic mechanisms.
http://www.chem.pitt.edu/people/faculty/rob-coalson

D. P. CURRAN
(1101 CHVRN-48240)
curran@pitt.edu
New strategies for the total synthesis of structurally interesting and/or biologically active natural products and the development of new synthetic methodology. Radical chemistry. Fluorous chemistry.
http://www.chem.pitt.edu/people/faculty/dennis-curran

A. DEITERS
(903 CHVRN-45515)
deiters@pitt.edu
Chemical Biology: We are developing new chemical tools to study biological processes relevant to human health. Our multidisciplinary research program involves organic synthesis, cell and molecular biology, protein engineering, nucleotide chemistry, amino acid chemistry, photochemistry, as well as medicinal and organometallic chemistry.
http://www.chem.pitt.edu/people/faculty/alexander-deiters

P. E. FLOREANCIG
(1203 CHVRN-48727)
florean@pitt.edu
http://www.chem.pitt.edu/people/faculty/paul-floreancig
CO₂ ABSORPTION BY IONIC LIQUIDS: Global warming from fossil fuel use is a major threat to the environment. Currently technologies to capture CO₂ from the exhaust of fossil-fuel burning power plants are economically infeasible. Ionic liquids might change that. Ionic liquids are fluids made exclusively of cations and anions, and whose properties can be tuned for particular tasks. Ionic liquids are being developed to capture CO₂ more efficiently, but progress is limited by our poor understanding of the molecular interactions between the CO₂ and the ionic liquid. To address the fundamental interactions between CO₂ and the ionic liquids, we use vibrational spectroscopy of the antisymmetric stretch of CO₂. To explore these issues, students will load CO₂ into a series of ionic liquids and measure FTIR spectra. The students will diagnose cooperative interactions with the cation and anion by determining if the vibrational frequency shifts of the CO₂ across a series of ionic liquids that vary the cation and anion are or are not additive. The project will advance our understanding of how this potentially useful class of solvents absorb CO₂.

http://www.chem.pitt.edu/people/faculty/sean-garrett-roe

Spectroscopic and laser studies of reactions of atmospheric importance, including those of electronically excited atoms and small molecules. Computer-assisted-instruction in General and Physical Chemistry.

http://www.chem.pitt.edu/people/faculty/michael-golde

Research in the Horne lab is focused on the design, synthesis, and study of synthetic analogues of proteins. These non-natural species can provide insight into the behavior of proteins found in nature and can also act as scaffolds for the design of molecules with interesting structures and functions. Our research takes place at the interface between organic chemistry, biochemistry, biophysics, structural biology and materials science.

http://www.chem.pitt.edu/people/faculty/seth-horne

Our group develops new materials, as well as microscale and nanoscale functional devices literally from the bottom up. We focus on building electronic materials from molecular subunits, both organic and inorganic, using a variety of techniques to rationally design the desired properties. This encompasses chemical synthesis, characterization (both physical and chemical), combined with theoretical modeling and simulation. Areas of research cover: Materials and Nanoscale Chemistry. Computational Materials Design. Rational Design and Materials Synthesis. Electronic Materials. Nanoscale Dynamics.

http://www.chem.pitt.edu/people/faculty/geoffrey-hutchison
K. D. JORDAN  
(330 EBERL-48690)  
jordan@pitt.edu  
Theoretical studies of molecular structure and reaction mechanisms. Computer simulations with emphasis on hydrogen-bonded systems, chemical reactions on surfaces, and characterization of biomolecules. We are also applying computer simulations to address a range of problems in the energy area.  
http://www.chem.pitt.edu/people/faculty/kenneth-jordan

K. KOIDE  
(1201 CHVRN-48767)  
koide@pitt.edu  
Integrated approaches to medical and environmental problems: We design, synthesize, and apply synthetic organic molecules for various problems. For example, we chemically synthesize complex natural products and study them in biological systems. In addition, fluorescent probes are being developed for biological imaging, critical medicine, and environment.  
http://www.chem.pitt.edu/people/faculty/kazunori-koide

D. S. LAMBRECHT  
(322 EBERL-48912)  
qclab@pitt.edu  
Quantum Chemistry: We develop reduced-scaling computational methods that facilitate calculations on larger and more complex systems than ever before. One aim is to develop a bottom-up understanding of catalyst-support interactions, which is essential to be able to control the stability and activity of supported nano-particles - which are widely used in catalysis. Another aim is to understand structure-spectra correlations for IR, ESR, and NMR spectra of (bio) molecules to aid in the elucidation of the structure and ultimately function with atomic resolution.  
http://www.chem.pitt.edu/people/daniel-s-lambrecht

H. LIU  
(201 EBERL-42062)  
hliu@pitt.edu  
Research in the H. Liu lab is focused on the chemistry and applications of nano-materials. We are interested in a wide range of organic and inorganic materials, including but not limited to DNA, graphene, carbon nanotubes, and colloidal nanocrystals. Current projects include the use of DNA nanostructures to pattern silicon wafer, the synthesis and chemical modification of graphene and single walled carbon nanotubes, and the mechanistic study of colloidal nanocrystal synthesis. Haitao Liu received his BS from the University of Science and Technology of China, his PhD from University of California at Berkeley, and completed postdoctoral work at Columbia University.  
http://www.chem.pitt.edu/people/faculty/haitao-liu

P. LIU  
(225 EBERL-35065)  
pengliu@pitt.edu  
Computational Organic Chemistry: The Liu group use computational tools to study organic and organometallic reactions. We use quantum mechanical calculations to study how reactions occur, factors controlling rates and selectivity, and provide theoretical insights to help develop improved catalysts and reagents. We are also developing a multi-scale computational screening protocol to facilitate the discovery of new catalysts.  
http://www.chem.pitt.edu/people/faculty/peng-liu
Our research program resides at the interface of chemistry, biology, medicine and material and concerns the study of broadly defined template-independent biological processes in living systems. The current research focus of our laboratory is in the context of the biogenesis and signal transduction event related to polysaccharide, polypeptide and polyprenylated small molecule natural product. The goal is to understand these biological processes at a detailed molecular level and transfer the knowledge acquired to facilitate the discovery of novel therapeutics for the treatment of cancer, autoimmune, neurodegenerative and infectious diseases, as well as the creation of new environmentally friendly biomaterials for biomedical applications. To achieve these goals, a highly interdisciplinary approach is adopted. While our strength lies in synthetic organic chemistry, protein biochemistry and enzymology, we also effectively integrate microbiology, cell biology, biophysics and bioengineering into our research program that will complement and accelerate our problem solving process.

http://www.chem.pitt.edu/people/faculty/xinyu-liu

Polymers and Materials. The synthesis and characterization of Repeating Sequence Copolymers (RSCs) for electronic and biomedical applications. The design and preparation of stimuli-responsive hydrogels. Especially interested in undergraduates who would like to do research for two semesters or more.

http://www.chem.pitt.edu/people/faculty/tara-meyer

Electroanalytical Chemistry: construction of ultramicro electrodes; monitoring dynamics of neuro-chemical events, development of enzyme electrodes; development and electrochemical characterization of redox polymers.

http://www.chem.pitt.edu/people/faculty/adrian-michael

Inorganic and Materials Chemistry; Nanomaterials; Surface and Colloid Chemistry. Whether they will be used in catalysis or artificial limbs, nanoparticle surfaces influence every aspect of their behavior. For example, the ligand shell of a nanocrystal can determine its luminescence, its performance in a solar cell, or its clearance from the human body. In the Millstone group, we are interested in synthetically controlling both the crystallographic and chemical composition of the nanoparticle surface, in order to develop new nanoparticle architectures that will have applications in fields ranging from catalysis to medicine.

http://www.chem.pitt.edu/people/faculty/jill-millstone
S. G. NELSON  
(1401 CHVRN-44290)  
sgnelson@pitt.edu  
http://www.chem.pitt.edu/people/faculty/scott-nelson

R. A. S. ROBINSON  
(111 EBERL-48167)  
rena@pitt.edu  
Our research goal is to develop high-throughput proteomics technologies which can be used to understand what occurs at the molecular level in aging and in the aging immune system using human tissues and/or mammalian models. We are also working on the development of novel hybrid ion mobility spectrometry and mass spectrometry instrumentation. These research projects take advantage of biochemistry, analytical, and bioinformatics tools.  
http://www.chem.pitt.edu/people/faculty/renã-robinson

N. L. ROSI  
(1018 CHVRN-43987)  
nrosi@pitt.edu  
Nanoscience and Materials Chemistry. We employ a variety of techniques from the traditional disciplines of modern chemistry to develop new methods of assembling and organizing molecular and nanoparticle building blocks into functional materials, such as catalysts, sensors, and gas storage containers.  
http://www.chem.pitt.edu/people/faculty/nathaniel-rosi

S. K. SAXENA  
(711 CHVRN-48680)  
sksaxena@pitt.edu  
Biophysical Chemistry: Conformational dynamics in proteins, and protein interactions and structures are studied using Fourier Transform electron spin resonance. New spectroscopic methods and instrumentation are also developed.  
http://www.chem.pitt.edu/people/faculty/sunil-saxena

A. STAR  
(112 EBERL-46493)  
astar@pitt.edu  
Star group research interests are in areas of molecular recognition at nanoscale and nanotechnology enabled chemical and biological sensing. This research, in addition to basic understanding of chemical and biological processes, will yield a prospect of building novel detection methods for widest possible range of chemical and biological analytes. Our group is currently working with a commercial partner to develop a disposable nanoelectronic sensor for the measurement of carbon dioxide (CO₂) and nitric oxide (NO) in human respiration. These disposable nanoelectronic sensors will extend the reach of the gas monitoring into emergency medicine and point-of-care settings.  
http://www.chem.pitt.edu/people/alexander-star
D. H. WALDECK  
(G-10 CHVRN-48430)  
dave@pitt.edu  
http://www.chem.pitt.edu/people/faculty/david-waldeck

M. WARD  
(107 CHVRN-48064)  
muscat@pitt.edu  
Undergraduates can participate in research related to the development of new curriculum for upper-level analytical laboratory courses.  
http://www.chem.pitt.edu/people/faculty/michelle-ward-muscatello-0

S. G. WEBER  
(603A CHVRN-48520)  
sweber@pitt.edu  
Fundamental and applied electrochemistry. Application of these to bioanalytical problems; trace determination of neuroactive and other peptides, biosensors and micro extractors for drugs and hormones. Application of molecular recognition to analytical chemistry.  
http://www.chem.pitt.edu/people/faculty/steve-weber

P. WIPF  
(758 CHVRN-48606)  
pwipf@pitt.edu  
Organic chemistry: Total synthesis and study of biologically important structures and novel, reactive functionalities. Design of peptide mimetics. Development of metal-based catalytic systems for asymmetric synthesis.  
http://www.chem.pitt.edu/people/faculty/peter-wipf