October 2019

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.*

<u>Director</u> <u>Research Area</u>

S. AMEMIYA (803A CHVRN-41217) amemiya@pitt.edu

Bioanalytical Chemistry and Electrochemistry: Development, miniaturezation 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/person/shigeru-amemiya

S. A. ASHER (701 CHVRN-48570) asher@pitt.edu Development of new laser spectroscopic techniques and optical devices. Resonance Raman and vibrational studies of peptide and protein folding. Development of new smart materials for chemical sensing, nonlinear optics and display devices.

http://www.chem.pitt.edu/person/sandy-asher

K. M. BRUMMOND (807 CHVRN-41955) kbrummon@pitt.edu

Research in our laboratory focuses on the discovery and development of synthetic transformations to facilitate and overcome the challenges posed by the preparation of molecularly complex bioactive compounds.

http://www.chem.pitt.edu/person/kay-m-brummond

L. T. CHONG (331 EBERL- 46026) ltchong@pitt.edu Computational Biophysical Chemistry. We apply computer simulations to study the mechanisms of complex biological processes such as protein binding and switching at the atomistic level. Areas of interest include: (i) development of weighted ensemble methods and software for extending the timescales of the computer simulations, (ii) development of more accurate simulation models, (iii) rational design of protein-based sensors for detecting ligands of interest, and (iv) estimating rate constants for receptor-ligand unbinding processes. 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/person/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/person/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/person/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.pitt.edu/~deiters/

P. E. FLOREANCIG (1203 CHVRN-48727) florean@pitt.edu

Organic chemistry: Development of methodology for the construction of carbon-carbon bonds and unusual functionality. Synthesis of small molecules designed to elucidate mechanistic details of biochemical phenomena. Natural products synthesis. http://www.chem.pitt.edu/person/paul-floreancig

S. GARRETT-ROE (216 EBERL-41283) sgr@pitt.edu

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/person/sean-garrett-roe

R. HERNÁNDEZ SÁNCHEZ (1113 CHVRN-84218) raulhs@pitt.edu

We are a research group focused in combining supramolecular, inorganic, and materials chemistry to synthesize functional systems that bridge the gap between nanoscale materials and molecular chemistry. https://www.chem.pitt.edu/person/raul-hernandez-sanchez

W. SETH HORNE (1405 CHVRN-48700) horne@pitt.edu 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/person/seth-horne

G. HUTCHISON (316 EBERL-80492) geoffh@pitt.edu

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/person/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/person/kenneth-jordan

K. KOIDE (1201 CHVRN-48767) koide@pitt.edu

We design, synthesize, and apply synthetic organic molecules for various problems. For example, we chemically synthesize complex natural products and study them in cancer. In addition, we develop fluorescent chemosensors for biological imaging in cells and animals and for the quality control of drinking water, environment, and discoveries of precious metals.

http://www.chem.pitt.edu/person/kazunori-koide

J. LAASER (1212 CHVRN-30125) j.laaser@pitt.edu The Laaser lab works at the boundary between polymer chemistry and polymer physics, exploiting both controlled synthesis methods and physical and optical characterization techniques to understand how molecular-level interactions between polymer chains dictate the bulk properties of these materials. We are particularly interested in polymer systems containing dynamic bonds, which can break apart and re-form on timescales relevant for e.g. self-healing materials, and in polymer systems that respond to external stimuli like light. Depending on current projects, opportunities may be available for undergraduate researchers interested in polymer synthesis, polymer characterization, and/or spectroscopy.

http://www.chem.pitt.edu/person/jennifer-laaser

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/person/daniel-s-lambrecht

H. LIU (201 EBERL-42062) hliu@pitt.edu Research in the H. Liu lab is focused on the chemistry and applications DNA and carbon materials. DNA Nanotechnology: we use DNA to prepare well-define nanoscale objects and explore their use in nanoscale patterning. The targeted applications are the fabrication of nanoelectronics and antifouling/self-cleaning surfaces. Carbon Materials: we study the intrinsic surface properties of carbon materials. Our recent work showed that many surface properties of carbon materials are masked by surface contamination by airborne volatile organic compounds. Removing these contaminations resulted drastic improvement in material performances. We are exploring the effect of surface contamination on applications related to environmental science, energy storage, and composite materials.

http://www.chem.pitt.edu/person/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 multiscale computational screening protocol to facilitate the discovery of new catalysts.

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

X. LIU 1005A CHVRN-46932 xinyuliu@pitt.edu

Our research program resides at the interface of chemistry, biology, medicine and material and concerns the study of broadly defined templateBindependent 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/person/xinvu-liu

T. Y. MEYER (1003 CHVRN-48635) tmeyer@pitt.edu

Polymers and Materials. The synthesis and characterization of Repeating Sequence Copolymers (RSCs) for electronic and bio-medical 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/person/tara-meyer

J. MILLSTONE (1006 CHVRN-84153) jem21@pitt.edu 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/person/jill-millstone

S. G. NELSON (1401 CHVRN-44290) sgnelson@pitt.edu

Natural Products Total Synthesis and Asymmetric Catalysis. Development of new synthetic methodology for the rapid and efficient construction of therapeutically relevant natural products. Design and execution of new asymmetric catalytic procedures for stereoselective carbon-carbon bond constructions.

http://www.chem.pitt.edu/person/scott-nelson

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/person/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/person/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 ($\rm CO_2$) and nitric oxide ($\rm NO$) 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/person/alexander-star

D. H. WALDECK (G-10 CHVRN-48430) dave@pitt.edu

Experimental Physical Chemistry, with applications to electron transport and electron transfer in nanometer scale assemblies. Our group is using electrochemistry, photochemistry, and electrical measurements to examine how the chirality of molecules and materials affect the charge and spin current in electron transfer processes. This work has implications for spintronics, enantioselective chemistry, and homochirality in biology. http://www.chem.pitt.edu/person/david-waldeck

Y. WANG (505 CHVRN-40028) ym.wang@pitt.edu Organic synthesis, organometallic chemistry and catalysis. The Wang group works on the development of new catalysts, reactions, and reagents for the synthesis of high-value molecular building block from readily accessed starting materials.

https://www.chem.pitt.edu/person/yiming-wang

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. www.chem.pitt.edu/person/michelle-m-ward

S. G. WEBER (603A CHVRN-48520) sweber@pitt.edu

We address the challenges of acquiring chemical information of living systems through devising and applying measurement concepts with unique attributes. Much of our work involves a need to understand or control mass transport by diffusion, convection, and electroosmosis/electrophoresis. Recently, we have created systems for making quantitative measurements of neurotransmitters *in vivo* by microdialysis/fast capillary LC, for electroosmotically perfusing tissue to determine neuropeptide hydrolysis rates. Core analytical techniques are electrochemistry and liquid chromatography. http://www.chem.pitt.edu/person/steve-weber

P. WIPF (758 CHVRN-48606) pwipf@pitt.edu Organic chemistry: Total synthesis and study of biologically important molecules and novel, reactive functionalities. New technologies, including the use of 3D printing of synthesis cassettes and blue LED powered photochemistry in-flow.

http://www.chem.pitt.edu/person/peter-wipf