JMU REU Research Project Descriptions

We offer a diversity of research opportunities, which are conducted solely by undergraduate students, in collaboration with faculty. While faculty expertise spans all sub-disciplines of chemistry, strength and synergy lie in the areas of synthesis, materials and biophysical chemistry. These strengths are highlighted in the research summaries below. Not all faculty involved in our REU program are listed. The details of their research projects may be found on the Departmental website (**http://www.jmu.edu/chemistry/people/**).

*** = faculty member who has previously mentored D/HH student(s)*

Ashleigh Baber (Materials). ***Role of Surface Modifications on Molecular Binding and Transformation.*** Surface science studies take a simplified look at complex heterogeneous catalysts to better identify active sites and reaction pathways. Our group investigates how molecules interact with each other on metallic surfaces, as well as how low concentration defect sites important in high surface area catalysts influence molecular binding. We are also interested in controlling the chemical reactivity and selectivity of titania-modified gold surfaces. By altering the titania nanoparticle size and oxidation state, we can control the selectivity of the transformation of alcohols to aldehydes or alkenes. The discoveries made under ultrahigh vacuum conditions using model catalysts can be applied to the design of highly selective catalysts on the industrial scale. **Intellectual merit:** We aim to understand the fundamental interaction between molecules and surfaces to design better heterogeneous catalysts.

Christopher E. Berndsen (Biochemistry)** ***Describing protein complexes involved in sugar metabolism.*** The chemistry of digesting food to produce energy referred to as metabolism is complex! There are hundreds of proteins called enzymes involved in the process, but somehow it happens in an orderly and controlled fashion. How? In part, these processes are controlled by having the enzymes interact to form complexes which allow the enzymes to coordinate their separate activities. These complexes are largely undescribed despite their critical role in human and plant metabolism because of the difficulty in identifying the binding partners, purifying the proteins, and studying their arrangement in the complexes. The lab team is currently working to describe complexes from plants and humans which are involved in the storage and use of sugars and their conversion into energy. We purify protein targets and study their activities in and out of the complex and then use X-ray scattering along with computational methods to describe the structure. Additionally, we are describing the chemistry and structure of the sugar substrates as to gain further understanding into what these complexes "see" in the cell. **Intellectual merit:** Our work will inform how sugar metabolism is controlled and lead to opportunities to improve biotechnological efforts such as improving starch yield and accessibility in crops.

Brycelyn M. Boardman (Organometallic Synthesis/Materials).** ***Developing Hybrid Copolymers from Polymerizable Cobalt Chalcogenide Clusters.*** Hybrid systems containing polymers and inorganic particles have been investigated for a wide range of applications. These systems offer the benefits of each component to achieve the next generation of light weight, low cost, flexible optoelectronics. Our work has focused on designing new polymerizable thiophene based ligands that can be incorporated into cobalt chalcogenide clusters. These clusters then undergo mild polymerization conditions to produce hybrid copolymers with covalent attachment of the inorganic and organic components. Our work has shown that there is improved charge transfer in these hybrid copolymers when compared to the simple mixtures. Current studies involve varying the ratio of cluster to the other comonomers as well as synthesizing new ligands containing other conjugated polymer monomers to investigate how copolymer structure impacts charge transfer properties in these materials. **Intellectual merit:** Understanding the fundamental interactions

between the polymers and inorganic particles in new hybrid systems will lead to a variety on new optoelectronic materials.

Kevin L. Caran** **(Synthesis/Materials)** ***Polycationic Amphiphiles & Polymers: Synthesis, Aggregation, Bioactivity and Foam-Forming Ability*****.** In the Caran lab, students design, synthesize, and purify novel amphiphiles and polymers to develop self-assembled soft materials (colloids) with well-defined properties. Subsequently, a range of tools are used to measure the colloidal properties and to understand the modes of self-assembly of aqueous aggregates formed by these compounds. The Caran lab has made more than 100 new amphiphiles with non-traditional architecture, including those with two to six cationic headgroups and one or more non-polar tails. After synthesis and colloidal analysis, antibacterial activity is measured against Gram-positive and Gram-negative bacteria. We also test the ability of these amphiphiles to form aqueous foams. Ongoing directions include the preparation and study of polycationic amphiphiles with an ever-expanding structural base and cationic polymers with structures designed to impede the formation of pathogenic bacterial biofilms. **Intellectual merit:** An understanding of relationships between structure, antibacterial activity, colloidal activity, and foam-formation is essential in the development of tools to combat pathogenic bacteria.

Christine A. Hughey** **(Analytical/Food Chemistry).** ***Beer Processomics: Molecular monitoring of volatile and nonvolatile compounds during brewing.*** Beer is a complex mixture consisting of volatile and nonvolatile compounds that evolve throughout the brewing process (mashing/boiling, hops addition, fermentation, and conditioning). The Hughey lab uses targeted and untargeted mass spectrometric-based techniques to monitor how these compounds change as a function of brewing time. Beers studied are produced in the Madison Academic Brewery housed within the Department of Engineering at JMU. Volatile flavor compounds are monitored with SPME GC/MS; while non-volatile compounds are monitored with LC/MS. Targeted metabolomics uses known *Saccharomyces Cerevisiae* biochemical pathways to monitor the nonvolatile metabolites that produce volatile flavor compounds. Untargeted metabolomics wholistically looks at differentially expressed compounds at each stage of brewing. Collectively, the use of GC/MS and LC/MS with targeted and untargeted metabolomic techniques provides an unprecedented, molecular-level look into the “processomics” of small molecules throughout the beer brewing process. **Intellectual merit:** A molecular-level understanding of how flavor compounds are produced from their nonvolatile precursors will afford brewers the ability to select ingredients (malt, hops and yeast) that produce the exact flavor profile desired.

Debo Ogunjirin** **(Medicinal Chemistry, Gallaudet University)** ***Discovery of small molecules for the treatment of nicotine addiction.*** Nicotinic acetylcholine receptors (nAChRs) play a crucial role in a number of clinically relevant mental and neurological pathways, as well as autonomic and immune functions. The development of subtype-selective ligands for nAChRs therefore is potentially useful for targeted therapeutic management of conditions where nAChRs are involved. Dr. Ogunjirin uses computer-aided software to design new analogs of pyridyl ether compounds, studying how small structural modifications can change selectivity for a particular nAChR subtype. Candidate molecules are then synthesized, isolated and characterized by NMR, IR and mass spectrometry. **Intellectual Merit:** This work will advance our knowledge of how small nicotine-like organic molecules can be used to manage nicotine addiction and other neurological disorders

Gretchen Peters** **(Organic Chemistry) Research summary:** ***Crosslinker cooperativity in polyvinyl alcohol gels.*** Gels are useful a wide range of applications, including environmental remediation, tissue engineering, and drug delivery. The diol-rich polymer polyvinyl alcohol (PVA) can be effectively crosslinked with boric acid (BA) or a diboronic acid to form soft materials and gels. While the complexation of PVA by BA has been extensively studied, the possibility of cooperativity between BA and diboronic acids has yet to be explored. Our initial studies suggest that the

introduction of a linear diboronic acid crosslinker to a PVA-BA organogel improves the physical properties (thermal stability and stiffness) of the material, while a non-linear diboronic crosslinker has little to no effect. Currently, we are investigating how structural variations in the diboronic acid crosslinkers (linker length and flexibility) impact the morphology and material properties of the PVA-BA gel. We rationalize that a well-developed understanding of these processes will allow us to develop stimuli-responsive materials with easily tunable physical and morphological properties. **Intellectual merit:** Cooperative crosslinking is a novel mechanism that can be used to manipulate and tune the material properties of gels to suit specific applications.

Barbara Reisner (Inorganic and Materials Chemistry). ***Composite materials to remove contaminants from water.*** Is my water safe to drink? That's a question we don't have to ask at JMU because we have access to safe and reliable water sources. However, there are many places where water contains ions that we want to extract because we have a safety concern (lead) or because the ions are rare and are needed for other applications (gold). In this project, we will synthesize composite materials consisting of a biopolymer and a porous material such as a metal-organic framework (MOF) or zeolite. We are comparing the efficacy of different composites on the uptake of Pb^{2+} and dyes to better understand how the nature of the composite influences ion adsorption and how we can selectively remove ions from solution. We are also using the results from this work to generate projects for a classroom undergraduate research experience (CURE) laboratories. **Intellectual Merit:** Understanding how composite composition impacts ion uptake can help us design selective adsorbents for water remediation.

Isaiah Sumner ** **(Computational Chemistry).** ***Research summary: Computational Analysis of the Ubiquitination Mechanism.*** Ubiquitination - the process by which the small protein, ubiquitin, is attached to a target - regulates many cellular processes including inflammation response and DNA repair. Ubiquitination is catalyzed by a series of enzymes, the families of which are dubbed E1, E2 and E3. The E2 family directly catalyzes the transfer of ubiquitin to a lysine in the target protein, whereas the E3 ligase assists in the transfer. Previous work in my lab has focused on understanding the chemical step of the E2 enzyme. Current work in the lab is focused on the E3 enzyme. Our approach is twofold. First, we are using MD to examine how the local environment changes in the enzyme active site when the E3 is present and to examine the amount of strain placed on the thioester bond between the transferring ubiquitin and the ubiquitin conjugating enzyme. (This bond breaks during the ubiquitination reaction.) Second, we are using QM to quantify how much strain is required to account for the observed increase in rate - one hypothesis for the E3 mechanism is that it places strain on the thioester, which makes it easier to break. **Intellectual merit: Understanding of the chemical mechanism in ubiquitination in eukaryotes** will help pave the way for designing therapeutics.

Nathan Wright ** **(Biochemistry).** ***Defining the role of obscurin in epithelial and muscle cells.*** The cytoskeleton provides cellular scaffolding yet also allows cells to move. One protein, termed obscurin, helps balance these competing demands of strength and motion by acting as a molecular spring, anchoring discrete targets and tethering them to other cellular structures. Obscurin is linked to cell adhesion and mobility in epithelial cells, and sarcomere organization in striated muscle. Over the past several years, our lab and others have discovered the downstream signaling profile of obscurin, however obscurin effectors remain unknown. We now hypothesize that obscurin is activated not through biochemical mechanisms, but through physical changes such as being stretched. We are currently using FRET-based tension sensors placed inside of obscurin to measure its tensile load inside live cells in a variety of different conditions. We also model how obscurin acts on an atomic level using both MD and solution structure methods (SAXS; NMR) to describe how obscurin behaves when relaxed and under tensile strain on the atomic level. This multi-scale work establishes a novel mechanism through which cells sense their environment. **Intellectual merit:** These studies explore a mechanism through which cells monitor their physical

environment, which has fundamental implications in our understanding of eukaryotic cellular homeostasis.