Chemistry Research Opportunities at UWSP

Chemical Analysis of Hemp

Professors Dr. Shannon Riha, Dr. Laura Cole, Dr. Brian Barringer Dr. Ann Impullitti, and Dr. Bryant Scharenbroch
sriha@uwsp.edu

Description: Environmental factors can play a significant role in the quality of hemp and its products (CBD, fibers, etc.). This research targets the analysis of hemp phytochemistry by means of chromatography and spectroscopy. In particular, we analyze how the growth environment may influence the production of cannabinoids and terpenes, which are chemical compounds that give hemp its medicinal applications. Another area of research in our group investigates where and to what extent toxins (e.g., heavy metals and PFAS) are sequestered within the hemp plant tissue.

Techniques: Digestions and extractions, high performance liquid chromatography, inductively coupled plasma-optical emission spectroscopy, liquid chromatography-mass spectrometry
General Requirements for Students: Motivated and reliable, can work independently and safely in a laboratory setting, completed CHEM248 or PI/Co-PI recommended
Number of new students: 2-3
Project Timeline: Fall and spring

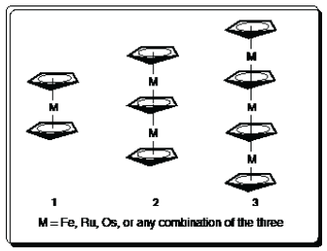
Filtration of PFAS Utilizing Porous Solids

Dr. Joe Mondloch
Associate Professor of Chemistry
jmondloc@uwsp.edu

Description: Poly- and perfluoroalkyl species (aka PFAS) are ubiquitous man-made chemicals that are persistent in the environment and been shown to cause adverse human health effects. Strategies are needed to remove PFAS from the environment as well as industrial waste streams. Our research focuses on making porous solids called metal–organic frameworks (MOFs) that are capable of removing PFAS from water. Understanding how the mechanism(s) by which this process works is a crucial aim of our research.

Techniques: Powder X-ray Diffraction, NMR & IR Spectroscopy, SDT, Nitrogen Adsorption
General Requirements for Students: Students should have completed Chem 105 and have at least 3 hours/week to commit to research
Number of new students: 4
Project Timeline: Fall or spring

Electronic structure of multidecker metallocenes



Dr. Jason D'Acchioli
Professor of Chemistry
jdacchio@uwsp.edu

Description: Metallocenes have captured the imaginations of synthetic chemists and theoreticians ever since the accidental preparation of ferrocene (1 below, M =Fe) in 1951. A variety of metallocenes based on complex 1's motif has been synthesized over the years, and there has been recent interest in triple-decker complexes such as 2 and the as-yet-unrealized quadruple decker complex 3. Indeed, what would happen if we hand an n-decker complex, a "molecular wire" based on a metallocene motif, extending infinitely in 2-dimensions? How would such complexes be synthesized, and what would their electronic properties be? My group will be collaborating with Professor Eric Watson at Seattle University to attempt to answer those exact questions. Professor Watson's team of undergraduates will be synthesizing novel triple-decker complexes, as well as working towards making a tetra-decker complex. My research group will use density functional theory (DFT) to study the electronic structure of the complexes, both synthesized and imagined, in an attempt to better understand the fascinating chemistry of this group of organometallic species.

Techniques: Computational chemistry including density functional theory; group theory; fundamental aspects of inorganic structure and bonding
General Requirements for Students: Students should have taken Chem 105 and (ideally) I be enrolled in Chem 106.
Number of new students: 2
Project Timeline: Fall

Department of Chemistry and Biochemistry
College of Letters and Science
University of Wisconsin-Stevens Point

Isolation of Bioactive Molecules from Mushrooms

Dr. Katie McGarry, Associate Professor of Chemistry
Dr. Matt Rogge, Associate Professor of Biology
kmcgarry@uwsp.edu, mrogge@uwsp.edu

Description: The rise in antibiotic-resistant microorganisms creates a serious threat to public health. To address this critical issue, finding new and effective antimicrobial substances is a top research priority. Mushrooms are known to release several bioactive compounds and present an untapped resource for discovery. Students on this project will utilize biological testing to drive the development of appropriate extraction and isolation methods of bioactive compounds, leading to the isolation and identification of specific substances that may prove valuable to the medical community.

Techniques: Extraction, Chromatography, Antimicrobial Testing
General Requirements for Students: Ideally students have taken Chem 325 and Biol 333, but at a minimum Chem 106 and Biol 111
Number of new students: 2-4
Project Timeline: Fall and spring

Nitrogen Heterocycle Formation

Dr. Katie McGarry
Associate Professor of Chemistry
kmcgarry@uwsp.edu

Description: Nitrogen heterocycles are prevalent in many biologically active natural products and pharmaceuticals. Improved synthetic methods which introduce nitrogen into a carbon scaffold or achieve formation of a Nitrogen heterocycle could provide more efficient access to known molecules or new derivatives that may prove medicinally useful. Research on this project focuses on developing new pathways to accessing these structures.

Techniques: Schlenk line technique, rotary evaporator, NMR
General Requirements for Students: Open to learning, have completed one semester of organic chemistry (Chem 325)
Number of new students: 1-2
Project Timeline: Fall and spring

Studying How Ligand Binding Impacts Protein Stability

Dr. Amanda Jonsson
Associate Professor of Chemistry
ajonsson@uwsp.edu

Description: Serum albumins are the major soluble protein in the bloodstream and have many functions, including binding to a wide variety of small molecules, including many drugs. Understanding how compounds interact with serum albumin proteins can help us understand how drugs and other small compounds behave in the body. We will be using bovine serum albumin (BSA) as our model protein and exploring how different small molecules bind to the protein and whether ligand binding impacts the stability of the albumin protein.

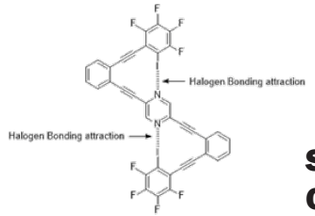
Techniques: UV-vis and fluorescence spectroscopy, DSC
General Requirements for Students: Completion of Chem 106
Number of new students: 1-2
Project Timeline: Fall

Synthesis and Characterization of Novel Solar Cell Materials

Dr. Shannon Riha
Associate Professor of Chemistry
sriha@uwsp.edu

Description: Chalcogenide perovskites are materials with the chemical formula, ABX3, where element A is a cation with a +2 charge, element B is a cation with a +4 charge, and element X represents S, Se, or Te. Recently, theoretical studies have suggested that chalcogenide perovskites have potential for optoelectronic applications, such as thin film solar cells. In this project, you will explore solid-state and/or colloidal synthetic routes to make the chalcogenide perovskite, BaZrS3.

Techniques: Air-free synthesis methods, solid-state reactions, powder x-ray diffraction, Raman spectroscopy
General Requirements for Students: Can work independently and safely in a laboratory setting, good lab notebook skills, motivated and reliable, three semesters of college chemistry lab experience
Number of new students: 2-4
Project Timeline: Fall and spring



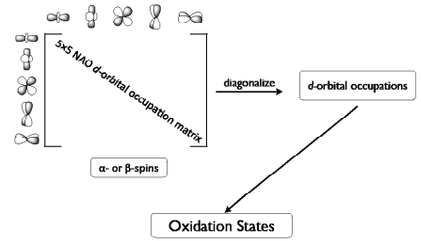
An example of a novel molecule synthesized by a Bowling group student in order to study halogen bonding attractions. Published in the *Journal of Organic Chemistry* in 2018.

Synthesis of Novel Conjugated Molecules

Dr. Nate Bowling
Professor of Chemistry
nbowling@uwsp.edu

Description: Our group makes molecules that have never existed in order to study and design specific electronic properties into the molecules.

Techniques: Organic Synthesis, Purification/Chromatography, Characterization/NMR Spectroscopy
General Requirements for Students: Minimum of B in Chem 325 and Chem 326 or exceptional performance in Chem 105/106
Number of new students: 1-8
Project Timeline: Summer



Theoretical Determination of Oxidation States

(PI) **Dr. Jason D'Acchioli**
Professor of Chemistry
jdacchio@uwsp.edu

Description: Oxidation state assignments are critical for explaining the reactivity of compounds in chemical reactions. Even though they are critically important there is no simple, general, agreed-upon way of computing oxidation states from theoretical models. We are in the process of developing a method of determining the oxidation state of transition metals in molecular systems, which we believe will satisfy the aforementioned criteria of "simple" and "general". We utilize quantum chemistry packages including Gaussian16 and ORCA, as well as natural bond orbital (NBO) theory to gather the raw electronic information from these systems. We then utilize the program GNU Octave to analyze the results of the calculations, attempting to gain insight into the oxidation states of the target transition metals.

Techniques: Computational chemistry including density functional theory; group theory; fundamental aspects of inorganic structure and bonding
General Requirements for Students: Students should have taken Chem 105 and (ideally)l be enrolled in Chem 106.
Number of new students: 1
Project Timeline: Fall

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