Chemistry Research Opportunities at UWSP

Analysis of Blood Alcohol Content in Mice using Gas Chromatography - Headspace Analysis

(PI) Dr. Dave Snyder, Professor of Chemistry, and (Co-PI) Dr. Sean Mooney-Leber, Assistant Professor of Psychology dasnvder@uwsp.edu

Description: This work supports a psychology project examining the influence of genetics on the long-term impacts of adolescent alcohol exposure in mice. Our partners in the UWSP Department of Psychology are utilizing a well validated model in which the mice selfadminister the ethanol, which creates some individual mouse variation. They are assessing behavioral outcomes and our group is conduct the chemical analysis of blood samples.

Techniques: Gas Chromatography and Head Space Analysis General Requirements for Students: Completion of CHEM 248 Number of new students: 2-3 Project Timeline: Fall

Chemical Analysis of Hemp

Professors Dr. Shannon Riha (PI), Dr. Laura Cole (Co-PI), Dr. Brian Barringer (Co-PI), Dr. Ann Impullitti (Co-PI), and Dr. Brvant Schrenbroch (Co-PI) 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

Development of Greener Methods for Quantifying Nitrogen in Agricultural Runoff

(PI) Dr. Dave Snyder, Professor of Chemistry, and (Co-PI) Juli Bowling, UWSP Water and Environmental **Analysis Lab** dasnvder@uwsp.edu

Description: Nitrogenous compounds in agricultural runoff can be toxic to aquatic life and can lead to eutrophication of surface water. Current analytical methods are time-consuming and involve the use of toxic catalysts during the digestion process. Total Nitrogen (TN) analysis offers a possible alternative to these methods that involve minimal sample prep and does not produce toxic waste. The objective of this work is to develop a method of TN analysis that is comparable to current methods.

Techniques: Total Organic Carbon (TOC), Total Nitrogen (TN), and Turbidity Analysis. **Environmental Data Analysis**

General Requirements for Students: Completion of CHEM 106 and concurrent enrollment or completion of CHEM 248 Number of new students: 1-2 Project Timeline: Fall

Filtration of PFAS Utilizing Porous Solids

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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 metalorganic 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

(PI) Dr. Jason D'Acchioli

Professor of Chemistry

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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

Isolation of Bioactive Molecules from Mushrooms

Dr. Katie McGarry, Associate Professor of Chemistry, and Dr. Matt Rogge 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

Organic Electrochemistry

Dr. Robin Tanke Professor of Chemistry rtanke@uwsp.edu

Description: Organic Chemist routinely carry out oxidation and reduction reactions, many times those reactions involve highly specialized reagents and generate a far amount of waste. To carry out reactions in more economical and environmentally friendly ways, organic chemist have begun using electrochemical cells in order to carry out reactions. However, many of the skills needed to carry out reactions using electrochemical series are not familiar to organic chemists including myself. This project will explore the use of electrochemical equipment and the control of voltage and current

to carry out oxidation and reduction reactions.

Techniques: Organic Synthesis, work up and characterization as well as electrochemistry **General Requirements for Students:** Basic laboratory safety and documentation skills **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

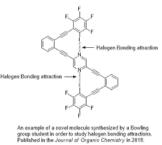
Description: Chalcogenide perovskites are materials with the chemical formula, ABX3, where element A is a cation with a +2 charge, element B is a cation with a +4 charge, and element X represents S, Se, or Te. Recently, theoretical studies have suggested that chalcogenide perovskites have potential for 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

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

Synthesis of Polymerization Catalysts

Dr. Dana Haagenson Associate Professor of Chemistry dhaagens@uwsp.edu

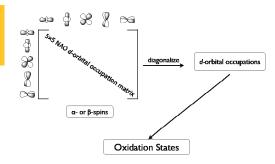
Description: Catalysts are used in the yearly production of hundreds of millions of tons of plastic. New catalysts are continually being developed to more efficiently make plastics and/or modify their properties. Our group designs and synthesizes inorganic ligands which are used to prepare compounds of titanium, zirconium, and other metals. These metal compounds are potential active catalysts for the polymerization reactions used in the manufacturing of plastics.

Techniques: Air-free synthesis, product purification and characterization (NMR) General Requirements for Students: Completion of Chem 105/106 Number of new students: 2-4 Project Timeline: Fall and spring



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)I be enrolled in Chem 106. Number of new students: 1 Project Timeline: Fall

Quantification of n-alkanes to quantify nutrient supplies in large herbivores

Dr. Dave Snyder, UWSP Chemistry, dasnyder@uwsp.edu and David Jaramillo, USDA Marshfield

Description: n-alkanes and other plant-wax compounds can be used as markers to quantify the nutrient supply to large herbivores. The USDA would like us to quantify these compounds in fecal material from cows as a part a local project they are conducting.

Techniques: Automated Solvent Extraction, GC/MS, GC/FID General Requirements for Students: Prefer students who are currently enrolled or have completed quantitative analysis Number of new students: 3-4 Project Timeline: Fall and spring

