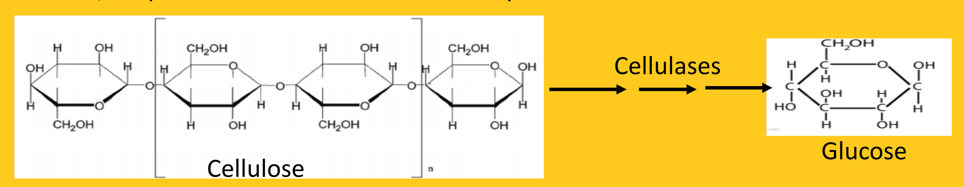
Canisius College Department of Chemistry and Biochemistry Research

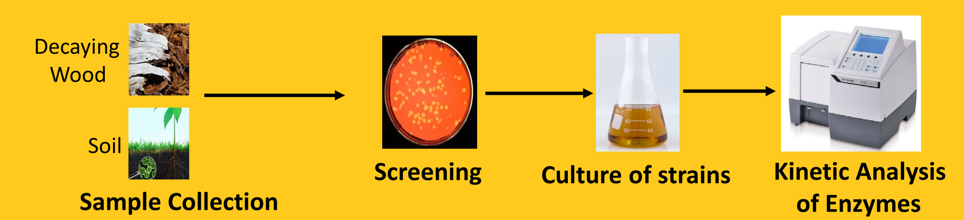
Dr. Zeenat Bashir
Biochemistry

Discovery and Metabolic Engineering of Novel Enzymes

Dr. Bashir's research group is interested in the discovery of novel enzymes, particularly cellulases from microorganisms, that degrade cellulosic biomass, a renewable resource on Earth, for production of biofuels or a variety of chemicals.



The aim is to discover novel cellulases and design the most efficient cellulase systems in a bioengineered strain of bacteria or yeast. The approach for the discovery of enzymes will involve different ways of screening microorganisms from decaying wood and soil samples collected at different locations in WNY. Further, the focus of the metabolic engineering will be on the enzymes that show higher catalytic activity on the synthetic substrates.

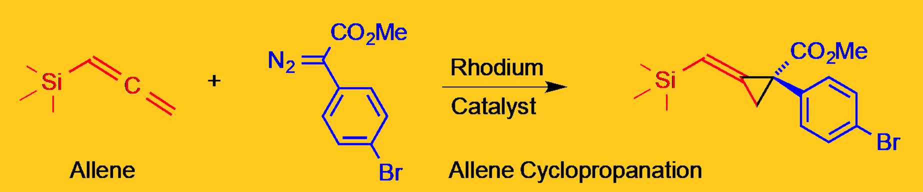


Our research may provide an alternative solution for the development of sustainable bioprocessing and economical production of biofuels or chemicals.

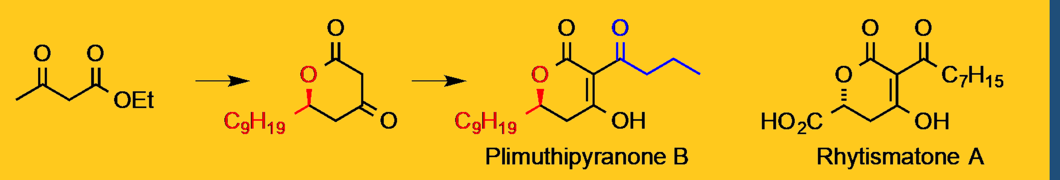
Dr. Timothy Gregg
Organic Chemistry

Organic Reaction Mechanisms and Synthesis

Dr. Gregg's group is interested in the reactions of carbenes and their use in the synthesis of novel types of chemical products. In past publications, we have demonstrated the use of rhodium catalysts for enantioselective cyclopropanation of allene substrates.



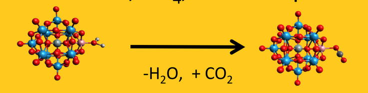
Our exploration of new reactions and molecular structures helps the scientific community in the development of new medicines and materials. We also develop synthesis routes that allow preparation of interesting natural compounds, including anti-fungal and antibacterial compounds.



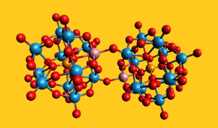
Dr. Mariusz Kozik
Inorganic Chemistry

Transition-Metal Substituted Polyoxotungstates (TMSPOTs) as Catalysts for Carbon Dioxide Reduction

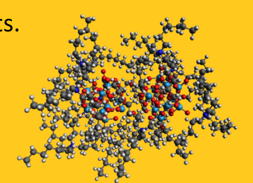
The goal of Dr. Kozik's research group is the one-step, multi-electron reduction of carbon dioxide (greenhouse gas) to methane (fuel) using TMSPOTs as electrocatalysts. In nonpolar solvents, the transition metal in the TMSPOT loses its coordinated water molecule, and becomes susceptible to reactions with other ligands (for example with CO_2). The CO_2 bound to cobalt can receive multiple electrons from a reduced TMSPOT, possibly becoming reduced to methane, CH_4, which requires multiple electrons.



We also discovered and proved by 2D DOSY NMR that TMSPOTs dimerize in very dry nonpolar solvents.



Recently we used Density Functional Theory (DFT) to study structures of TMSPOTs. DFT calculations showed that dimers of TMSPOTs in nonpolar solvents are more stable than their monomers. TMSPOT anions are surrounded by tetraheptylammonium cations, $[(C_7H_{15})_4N]^+$, in nonpolar solvents.



We are also working on theoretical predictions of 31-P NMR chemical shifts in paramagnetic TMSPOTs by DFT computations.

Dr. Peter Schaber
Analytical Chemistry

Heavy Metal Pollutants in Samples Collected Along the WNY Waterways

Dr. Schaber's research group is interested in developing and utilizing analytical tools to identify heavy metal pollutants in water and soil. Most recently, soil samples in and around the waterways of WNY have been collected and analyzed for lead (Pb) and cadmium (Cd) using a newly acquired instrument, Inductively Coupled Plasma Mass Spectrometer (ICP-MS). The aim of these investigations is to identify and locate the sources of contamination.

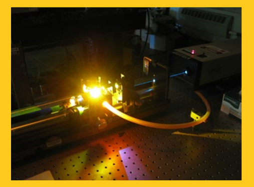
Buffalo River Soil Samples

Number	North	West	Lead (Pb) ppb SOIL	Cadmium (Cd) ppb SOIL
1	43° 51.678'	78° 49.582'	4.89	0.00
2	42° 51.778'	78° 49.322'	4.09	0.00
4	42° 51.857'	78° 49.195'	N/A	0.00
5	42° 51.893'	78° 49.175'	63.81	0.00
6	42° 51.972'	78° 49.120'	17.71	0.00
12	42° 51.964'	78° 52.110'	40.94	0.00
13	42° 51.823'	78° 48.629'	42.83	0.00
14	42° 51.979'	78° 52.439'	101.60	0.00
15	42° 52.276'	78° 52.708'	100.53	0.00

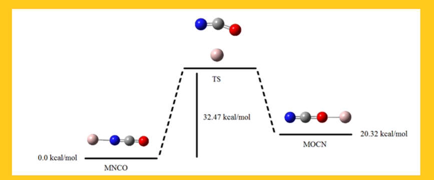
Dr. Phillip Sheridan
Physical Chemistry

Spectroscopy of Metal-Containing Molecules

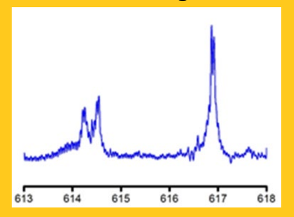
Dr. Sheridan's research group is interested in the characterization of small, metal-containing molecules in the gas phase.

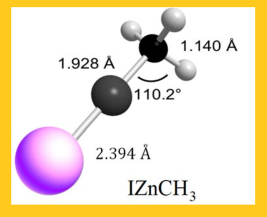


A combination of laser excitation spectroscopy, rotational spectroscopy, and computational chemistry methods are used to study these molecules, which consist of a metal atom bonded to a single ligand.



The goal is to determine the geometric and electronic structure of these molecules in order to understand the metal-ligand bond at a fundamental level.

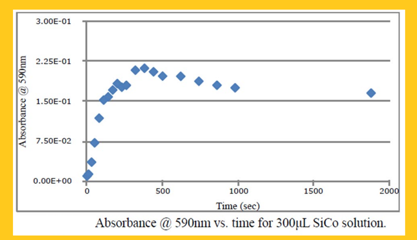


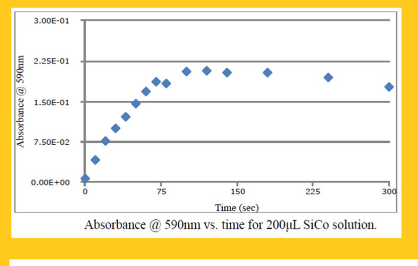


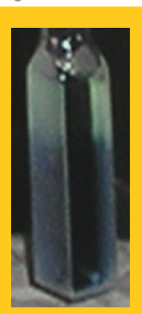
Dr. Steven Szczepankiewicz
Analytical/Environmental Chemistry

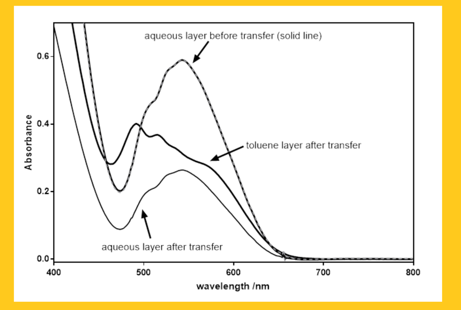
Inorganic Photosynthesis and Environmental Analysis

Dr. Szczepankiewicz's research group is interested in developing rugged photoactivated catalysis capable of reducing small, stable molecules such as CO_2. We've developed a strategy to prepare the catalyst in favorable reaction conditions and determined the photoactivation mechanism. We're now investigating the products of CO_2 fixation.









Dr. Szczepankiewicz's group also investigates the prevalence of persistent environmental pollutants in local aquatic habitats and fish populations.