DREXEL UNIVERSITY College of Arts and Sciences

Atmospheric Chemistry (Ezra Wood, PhD)

Research in Prof. Wood's atmospheric chemistry research group during the summer of 2021 will focus on development of analytical methods for quantifying several important trace compounds in the atmosphere. During most summers we conduct field work across the US. This upcoming summer we might be participating in an air quality project in New York City, but regardless we will also be working on developing new capabilities for our two main analytical instruments. Two likely laboratory projects are described below:

A. Our peroxy radical sensor "ECHAMP" (Ethane CHemical AMPlifier) is used to quantifyperoxy radicals like HOO, CH_3OO, C_2H_5OO, etc. These radicals are key species in the mechanism by which ozone, which is the main component of photochemical smog, is formed in the sampled air:

$HO_2 + NO \rightarrow OH + NO_2$
$NO_2 + h\nu\ (\lambda<400\ nm) \rightarrow NO + O\ O$
$+ O_2 + M \rightarrow O_3 + M$

The capability to quantify the concentrations of peroxy radicals (along w/ NO) enables us to calculate the rate at which ozone is formed, which is extremely useful for determining air pollution mitigation strategies in urban locations. Currently this instrument operates at atmospheric pressure, and attains a detection limit of approximately ~2 ppt. The instruments calibration is unfortunately sensitive to the relative humidity. We plan to characterize the instrument at reduced pressure, which should both increase the sensitivity and decrease the relative humidity dependence.

B. Our chemical ionization mass spectrometer analyzes highly oxygenated / polarizablecompounds via formation of adducts with iodide ions:

$X + I^- \rightarrow XI^-$ (X = HNO_2, HCOOH, HCN, HNCO, etc.)

These adducts are then detected with a time-of-flight mass spectrometer. No separation of compounds (e.g., w/ gas chromatography) is employed prior to ionization. This technique detects numerous compounds quite easily; the difficulty is calibrating for each compound as most compounds of interest are not stable enough to be prepared in a compressed cylinder. This summer we will work on developing calibration sources for nitrous acid (HNO_2). Additionally, we will work on developing methodology for detecting hydroxy hydroperoxides, e.g. $HOCH_2CH_2OOH$, which is formed by the atmospheric oxidation of ethylene under low-NOx conditions.

Studying the emissions, chemical transformations, and resulting concentrations of airborne pollutants is the major focus of Prof. Wood's research. All projects will be conducted working alongside members of the research group, comprising Prof. Wood and four graduate students. A student participating in these research projects will gain experience with gas-phase handling skills, trace pollutant calibration sources, and basic electronics, data acquisition, and data analysis methods. This summer experience will introduce a student to the field of atmospheric chemistry, which is and will continue to be of paramount importance in today's environment.

Materials Chemistry (Frank Ji, PhD)

Title: Atomic-Scale 1D Heteroarchitectures based on a Novel $M_aP_bX_c$ Material.

Significance:

The discovery of carbon nanotubes and the isolation of graphene from bulk graphite were individually responsible for launching entire scientific fields of inquiry into 1D and 2D nanomaterials, respectively. Graphene has been shown to be a gap-less semi-metal, however, and for many of the most compelling applications, including field-effect transistors, photodetectors, and solar cells, a band gap is required. Consequently, researchers are taking inspiration and insights from graphene and applying it to new or recently rediscovered 2D materials that do possess a band gap, such as molybdenum disulfide and, most recently, Black phosphorus (BP).

The allotrope known as black phosphorus (BP) is a layered material like graphene. Unlike graphene, BP possesses a band gap, a discovery that sparked a race to exploit its potential for optoelectronic applications in the last decade. However, the drawback of phosphorus-based devices is that pure phosphorus allotropes have the tendency to decompose or oxidize in air, especially when current passes through them.

The PIs have recently demonstrated the promising electronic properties of $Cu_2P_3I_2$, which is the first example of another class of phosphorus-based nanomaterials made of metal phosphorus halide ($M_aP_bX_c$). It was quickly followed with another, $SnPI_2$, published from Europe. Materials of this class have unique structures and are much more stable than pure elemental phosphorus. The results showed that $Cu_2P_3I_2$ devices are highly reproducible, flexible, stable and possess a short response time, which makes the compound a suitable candidate for commercialization as a new type of material for photodetectors. The structure of $Cu_2P_3I_2$ can be described as a 1D phosphorous nanotube inside a protecting CuI shell (Figure 1).

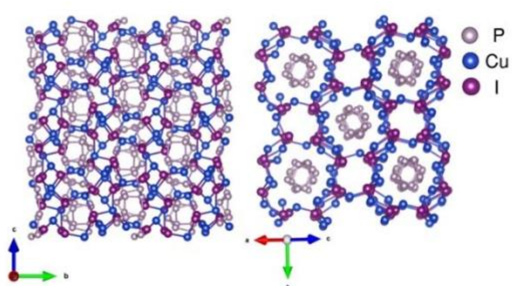

Figure 1. ***Crystalline structure of $Cu_2P_3I_2$, left: view along c-axis; right: view along the [101] direction to show the one-dimensional channels consisting of phosphorus tubes surrounded by copper and iodine. The crystal structures were plotted using VESTA.***

The objective of this project is to enable the synthesis of a series of nanostructures of stable, functional $M_aP_bX_c$ using chemistries selected for compatibility with wide-area optoelectronic device integration. The Maryanoff students will be involved in the synthesis and characterization of these materials.

Biophysical Chemistry (Reinhard Schweitzer-Stenner, PhD)

The **Biospectroscopy Group** is currently involved in researching the gelation of short peptides in water and water/ethanol mixtures. Short peptides fall into the category of low-molecular weight gelators. Gels of peptide have great potential for biotechnological use such as drug delivery and tissue repair because they are comparatively cheap. The work in the group is aimed at determining the parameters that govern the formation of peptide fibrils which are the building blocks for the sample spanning network which leads to the gelation of a sample Knowing this parameters is of utmost importance for the technical use oof peptide gelators. The work of the group has focused on so called GxG peptides where G represents glycine and x different nonglycine amino acids. Thus far, we have identified alanine (x=A), histidine (x=H), phenylalanine (x=F) and tryptophan (x=W) as powerful gelators. The Maryanoff student who will join the group in the summer of 2021 will work under the direct supervision of **Nichole O'Neill,** a graduate student who is currently working on the project. The group's principal investigator, **Prof. Reinhard Schweitzer-Stenner**, will oversee the project. He/she will use spectroscopic methods to probe the melting and reformation of gel phases as a function of sample composition. His/her will predominantly use the circular dichroism spectrometers in the Biospectroscopy and the departmental laboratory. Circular dichroism reflects the difference of how right- and lefthanded circular polarized light is absorbed by the sample, which is caused by the chirality of the formed molecular structures. The latter generally changes if a sample undergoes a transition from the gel into the solution phase and vice versa. The Maryanoff student will be subjected to a variety of learning experiences. He/she will learn the basics of peptide and protein biochemistry and dive into the vast literature on peptide self-assembly. He/she will become familiar with the theory which underlies circular dichroism and the kinetics of peptide self-assembly. Since this is a collaborative project the student will become familiar with what it takes to work in interdisciplinary teams. We expect candidates to be highly motivated to conduct meaningful research at a very early stage of their professional development.