Program Overview: Chemical Research Utilizing X-ray (CRUX)

[Video - Program Overview]

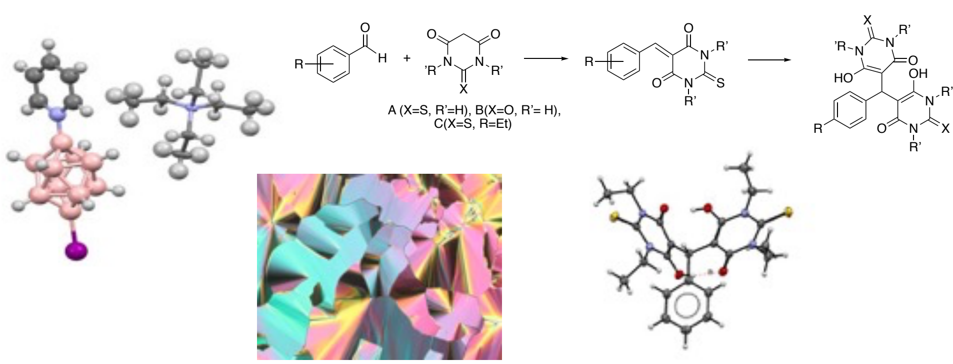
The CRUX-REU program is a community of undergraduate students who learn together about X-ray methods for characterization of materials. Each participant will synthesize or isolate new materials and work with at least one faculty member and their research groups, as well as our crystallographer. Most of the faculty are in the Department of Chemistry, and their research ranges widely from analytical methods development, to biochemical mechanisms, to organometallic catalysis, to organic and inorganic synthesis. Other common aspects of the program are field trips to Oak Ridge National Lab, Hudson Alpha Research Institute in Huntsville, Nashville downtown, regional natural areas, and other activities that the group selects.

CRUX REU Faculty Research Interests

Dr. Andrienne Friedli
Synthesis and Structure of Self-Organizing Materials

[Video - Friedli Research Areas]

Dr. Friedli works with highly colored donor-acceptor materials (yellow to purple) and also boron cluster derivatives, some of which self-organize into liquid crystals (LCs), films, or extended networks. Applications for these materials include sensors, electronics, or even quantum computers. Single crystal X-ray diffraction (SCXRD) and powder (PXRD) have identified unusual liquid crystalline phases, unexpected reactivity, and intermolecular interactions. Students will synthesize related series of these compounds, characterize with NMR, X-ray and other organic techniques to determine structure-property relationships.

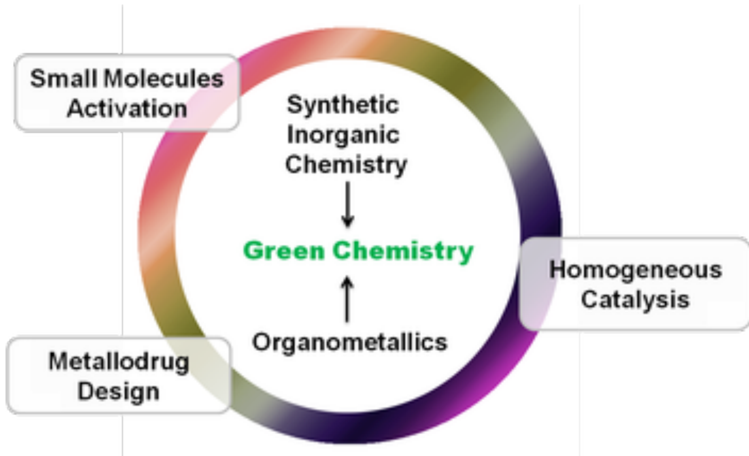


Left: [*closo*-$B_{10}H_{10}$-1-I,10-C_5H_5N]$^-$ NEt_4^+; B atom are pink, N is blue, I is purple. *Middle:* polarized microscopy of LC; *Right:* unexpected H-bonded side product accessible with some R groups.

CRUX-REU Faculty Research Interests

Video- Ding Research interests

Dr. Keying Ding "Green" Catalysts with Earth-Abundant Metals

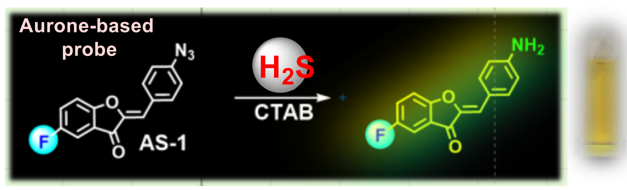


Our research revolves primarily around organometallics, catalysis and bioinorganic chemistry, solving challenging problems related to energy, environment and human health. The first project focuses on development of earth-abundant transition metal catalysts for small molecule activations and chemical productions important for drug discovery, agricultural science and advanced materials. In the second project, we are interested in main groups and transition metals catalyzed conversions of CO_2 into fuels such as methanol and methane. The third project targets on developing inorganic photocatalysts to be used for organic pollutants degradation under visible light. Through these multidisciplinary research projects, students are expected to obtain comprehensive research skills and learn innovative approaches for green and sustainable chemistry.

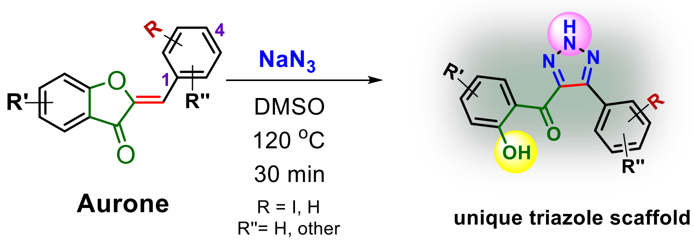
CRUX-REU Faculty Research Interests

Dr. Scott Handy Aurone Structure and Applications

Much of the work in the Handy group is centered on the aurone family. Aurones are natural products typically found in plants that produce golden-yellow flowers and are largely responsible for this color. From this golden starting point, we have been exploring its efficient synthesis, biological applications, conversion into other unusual structures, and most recently its application as a fluorescent probe or label to follow biological processes. Many of these aurones are nicely crystalline materials and some of the unusual aurone variants have proven difficult to characterize by any means other than X-ray analysis. Both synthetic and structural efforts are very much a part of everything that goes on in the Handy group.



Aurone-based fluorescent probe for H_2S detection

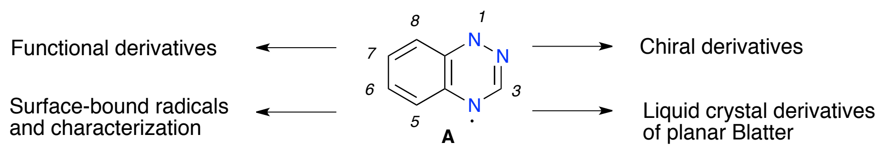


An unusual triazole synthesis from aurones

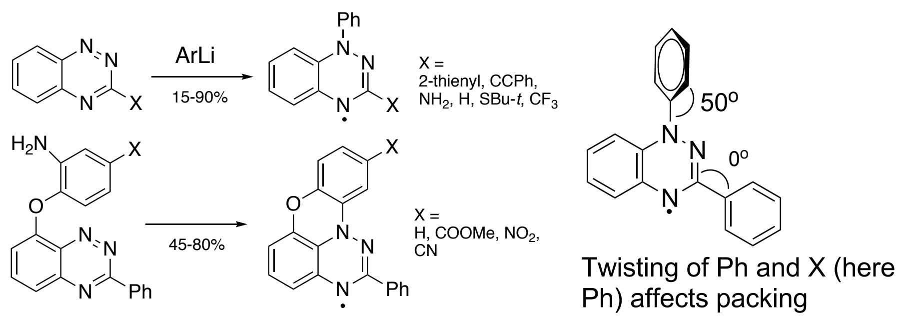
CRUX-REU Faculty Research Interests

Dr. Piotr Kaszynski Stable Radicals for Electronic and Magnetic Devices

Most molecules with unpaired spins are highly reactive intermediates. However, derivatives of molecular cores with unpaired spins like **A** are completely stable and have possible applications as molecular magnets, in addition to interesting fundamental science.



core of a stable radical

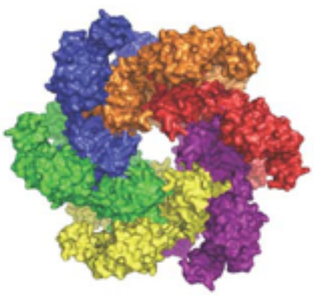


Chemistry to make standard (top) and bridged (bottom) derivatives is established, so students will be able to both synthesize and characterize new products, and analyze X-ray diffraction results for at least one compound, with an option to participate in magnetic measurements.

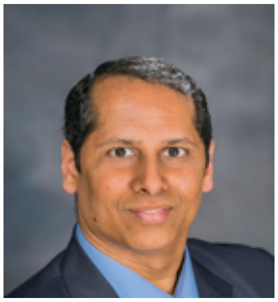
CRUX-REU Faculty Research Interests

Dr. Justin Miller Biochemical Mechanisms for Protease Activity

ATP-dependent proteases are molecular machines conceptually similar to paper shredders, where material is fed into an interior compartment and shredded. In the active state, Clp ATPases such as ClpA, ClpC, and ClpX, are assumed to form hexamers assembled from six of the same protein (shown below). The Miller group studies how the activity of an ATP-dependent protease is impacted by interactions with specific accessory proteins.



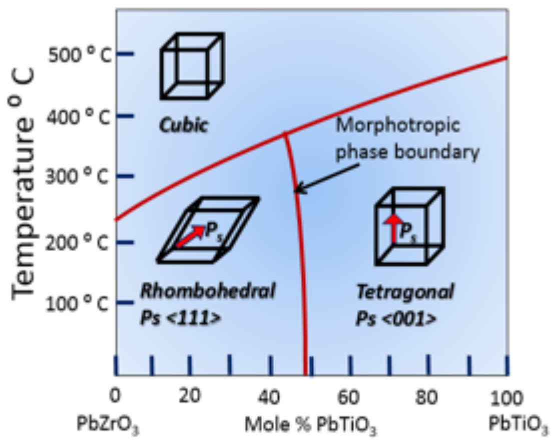
CRUX-REU Faculty Research Interests



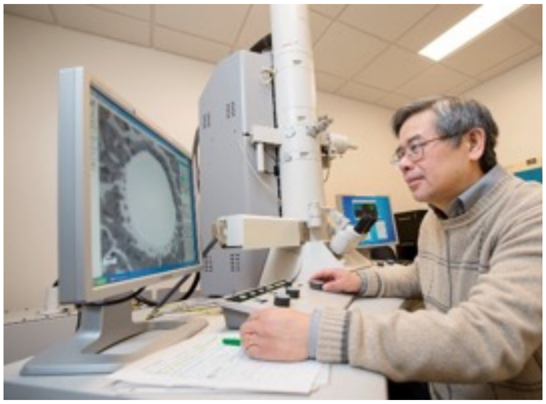
Dr. Vishwas Bedekar Piezoelectric Materials for Energy Harvesting

Piezoelectric polycrystalline materials are designed to enhance charge and voltage constants, thereby improving the energy harvested from ambient sources such as mechanical vibrations.

Dr. **Bedekar** will provide guidance to REU participants on synthesis of piezoelectric materials with various stoichiometries. They will generate a phase diagram with the help of PXRD.



CRUX-REU Faculty Research Interests



Dr. Ngee Sing Chong Catalysts for Biofuel Production

Calcination of shells has been used in the preparation of CaO catalysts that can achieve high yields in the conversion of triglycerides in seed oils to biodiesel via transesterification process. The performance of the CaO catalyst obtained from oyster shells was recently demonstrated in Dr. Chong's research group to be superior to that of eggshells and capable of achieving biodiesel yields of over 99% for methanol:oil reactant ratios of 6:1 through 12:1. Furthermore, using CaO as a heterogeneous catalyst will avoid the large volumes of wastewater needed to wash the biodiesel product when NaOH is used.

REU students will synthesize CaO-based catalysts from shells of oysters, clams, mussels, and crabs and analyze the elemental composition of the shell-based catalysts. The X-ray Fluorescence (XRF) technique will be used to evaluate the synergistic roles of transition metals in the shell-derived catalysts via quantitative metal analysis at the parts-per-million levels. The Scanning Electron Microscopy/ Energy Dispersion X-ray Analysis will be used to characterize the morphology of catalysts and the distribution of light elements such as carbon, oxygen, silicon, sodium, and phosphorus in different crystalline phases of the catalysts.

CRUX-REU Faculty Research Interests

Dr. Greg VanPatten   Quantum Dot Cation Exchange Reactions

The chemistry and applications of Cd-based nanocrystals or quantum dots (QDs) in solar cells and semiconductors is established, although Cd is toxic to the environment. Nanocrystals containing more environmentally friendly metal cations like Zn or Ag are not accessible in controlled size or quality. Therefore, Dr. VanPatten's group exchanges cations and measures the rates and structural effects of the exchange using X-ray methods (PXRD, TEM), and optical spectroscopy (UV and fluorescence). Cation exchange of Pb in PbS for Ag and Cd is demonstrated in the diagram below with UV (left column), PXRD (middle column) and TEM (right column).