CAREER: Fundamental Studies of Multidentate Halogen Bond Donors for Supramolecular Catalysis **P. I. Berryman**

Abstract for CAREER CHE-1555324

With CAREER support from the Macromolecular, Supramolecular and Nanochemistry (MSN) program of the NSF division of Chemistry, Professor Berryman is designing molecules that match the size and electronics of sulfur compounds. These new materials are being used to accelerate reactions involving sulfur and other polarizable molecules. This approach has not been demonstrated with sulfur compounds and this research is producing a new efficient way to make molecules containing sulfur. Sulfur compounds are found in nearly every aspect of our lives and this research will advance a number of fields including drug development, separation science, environmental remediation and crystal engineering. Additionally, this research is being used to inspire children to study STEM. To reach a broad underrepresented audience, 3D printing is being used to teach new chemical characterization techniques such as X-ray diffraction. In particular, three approaches are taken: 1) 3D printed models of X-ray crystal structures are used as an interactive learning tool at the spectrUM science museum and on native reservations. 2) High school students are understanding the concepts of molecular recognition and shape selectivity from 3D printed crystal structures. 3) University students are learning X-ray crystallography in their course work by using 3D printed crystal structures to teach concepts. This research is addressing whether interactions between molecules can be developed into a new genre of catalysis to inspire a new generation of scientists.

This proposal is answering the question whether multidentate halogen bonding receptors can selectively bind and catalyze soft substrates. The field of halogen bonding is currently experiencing an enormous amount of attention originating from seminal studies of donor /acceptor complexes of inorganic donors. However, the study of organic based halogen bond donors with soft Lewis bases is critically lacking. Since organic halogen bond donors are structurally and fundamentally different from traditional inorganic donors our motivation is that their applications are expected to be distinct. *The primary **intellectual merit** of this research is in demonstrating that organic halogen bond donors can be used as a predictable design strategy to target sulfur and other soft chalcogen and pnictogen containing compounds.* This objective is being met by obtaining a fundamental understanding of the strength, structure and nature of halogen bonding interactions between organic donors and soft chalcogen and pnictogen Lewis bases. *This research is being applied to catalysis by demonstrating that multidentate halogen bonding interactions are complementary and strong enough to activate sulfur substrates for reaction.* This research is addressing whether halogen bonding interactions can be developed into a new genre of organocatalysis.