**Research Interests**: Computational Atmospheric Chemistry, Computational Bioinorganic Chemistry, Computational Organometallic Chemistry, and Computational Physical Organic Chemistry

The study of atmospherically, biologically and industrially important chemical processes at the molecular level using modern computational methods is my primary research interests.

My current research projects in Prof. Joseph S. Francisco’s group at UNL are focused on understanding the role of sulfur chemistry in the formation of elemental sulfur aerosols in different environments, formation mechanism of hydroperoxy radical in troposphere, and carbon dioxide activation, and NOx reduction processes via metal free dual acid catalysis.

My previous research projects at [CEBC](https://www.cebc.ku.edu/), University of Kansas were focused on gaining an improved understanding of industrially important chemical processes, and involved extensive collaboration with Chemical Engineering groups of Professors [Bala Subramaniam](http://cpe.engr.ku.edu/faculty/subramaniam.html) and [Raghunath V. Chaudhari](http://distinguishedprofessors.ku.edu/professor/chaudhari-r). With Prof. Ward H. Thompson, and in close collaboration with Professor Subramaniam’s research group, I performed electronic structure calculations for finding the unconventional mechanistic pathways for the olefin ozonolysis that has not only received renewed attention as a means to break down long chain biomass molecules into more useful renewable chemical intermediates, but is also relevant in atmospheric context. With Prof. Jackson, and in extensive collaboration with Professor Chaudhari’s lab, I performed the quantum mechanical modelling of the rhodium-catalyzed hydroformylation process, which is one of the most important homogenously catalyzed industrial processes for the production of aldehydes and their derivatives.

During my PhD research work in Professor [Kozlowski’s lab](http://louisville.edu/chemistry/directory/faculty/pawel-m-kozlowski.html), I gained extensive experience in the application of ab initio quantum chemistry methods to the research problems of bioinorganic chemistry. Based on electronic structure calculations, we proposed a mechanism that can offer insight into the cobalt-carbon bond activation mechanism in B12-dependent mutases that catalyze a variety of complex chemical transformations. Our computational modeling studies of methyltransferases have predicted the existence of a new kind of interaction between the Co(I) ion of cob(I)alamin  and its axial ligands, and has led to the **"revision of the existing mechanism"** for the cob(II)alamin/cob(I)alamin redox process, which is a key chemical event in the this class of transferases.

