Chemistry Department
2018 Summer Research Program

Shields-Temelso Research Group

As a computational chemistry group, our research focuses on the application of efficient computational methods to understand the structure and dynamics of hydrogen-bonded systems ranging from water clusters to sulfate aerosols in the atmosphere.

I. Structure and Stability of Small Water Clusters:

Water is the most fundamental molecule on earth and it plays a key role in many processes. However, developing a water model that can describe all its unusual and crucial properties has proven difficult. To contribute to the development of better models, we study the structure and thermodynamic stability of small water clusters, (H2O)n, n=2-20. The most stable water clusters we predict under different conditions are then compared with experimental results from broadband rotational spectroscopy.

II. Thermodynamics of Sulfate Aerosol Formation:

Aerosol particles in the atmosphere serve as seeds for cloud formation and have a net cooling effect on the global climate, in contrast to greenhouse gases that warm the climate. Sulfate aerosols in particular have a large cooling effect, but their formation pathways in the presence of different component vapors, temperature and pressure conditions as well as their size and distribution in the atmosphere remains unclear. To answer some of these questions, we model the formation of sulfate aerosols at a molecular level. The end goal is to explain the growth of nanoscale small gas phase clusters to large aerosols and cloud droplets in the micrometer range. That will minimize the large uncertainty associated with the role of aerosols in the global climate and refine models used to understand the severity of global warming and aerosols’ possible role in mitigating it.

In both water clusters and sulfate aerosols, the molecular clusters are held together by weak and dynamic hydrogen bonds. That makes the kinds of structures they can form and their relative stability very hard to determine. We develop and apply different tools to 1) sample the large number of configurations these clusters can adapt efficiently and 2) determine which ones are important.