The efficient capture of CO₂ from industrial power generation sources is a major challenge. Current studies are investigating the adsorption of CO₂ into ionic liquids (ILs). Imidazolium-based ILs have received a great deal of attention for CO₂ capture due to their unique physical properties. However, it has recently been reported that imidazoles – neutral counterparts to imidazolium-based ILs – can offer enhancements in viscosity, cost and CO₂ capacity. However, the lack of thermophysical property data for neutral imidazole substitutions and chemical permutations makes it difficult to identify and develop future candidates for specific gas processing applications without having to obtain extensive experimental datasets. Using *ab initio* and molecular mechanics methods, we are elucidating the thermodynamic and structural properties of a variety of N-functionalized imidazole compounds. *Ab initio* calculations are used to determine parameters (such as partial charges) for the all-atom Optimized Potentials for Liquid Simulations (OPLS-AA) force field, followed by simulations using the molecular dynamics package Gromacs. We are making comparisons with our experimentally-synthesized compounds (Prof. Jason Bara), providing guidance towards new synthesis targets.

This project will expose the REU student to advanced molecular simulation tools, including molecular dynamics and Monte Carlo techniques. Many thermodynamic concepts will be reinforced, and students will become familiar with statistical mechanics, data analysis techniques, and visualization software.

Excluded volume analysis is used to determine the void space available for gas adsorption. Experimental results indicate that the void volume is the primary predictor of CO₂ adsorption, versus specific chemical interactions. The structural analysis can be used to predict gas selectivity and total adsorption capacity.