Zeolites are crystalline structures made of oxygen, silicon, and sometimes aluminium (or other metallic cations). The zeolite framework has features called pores, channels, and windows. In these channels smaller molecules (such as CO₂ or N₂) can interact with the zeolite walls and be adsorbed.

My research involves studying how gaseous molecules are adsorbed, explore, and interact with the walls of the zeolite and the other adsorbed molecules. Specifically I will be studying the effects of pore loading and the molar fraction of N₂ to CO₂ in ITQ-3 on the diffusion coefficients of the adsorbed species.

A molecular dynamics (MD) simulation is used to determine the positions and energies of atoms over time. This type of simulation uses Newton’s equations of motion iteratively over a short timestep (a femtosecond) to determine the position of each atom. Forces are calculated based on Lennard-Jones (LJ) and Coulombic potential energy equations.

By running MD simulations with varying CO₂ and N₂ concentrations, we have discovered that only CO₂ concentration has a significant effect on either CO₂ or N₂ diffusion rates in ITQ-3.

Previously, we had run MD simulations and recorded the frequency at which molecules visited each position in the UC and determined the most favored sites in the UC.

In order to better understand diffusion, we ran extended simulations with only one molecule of CO₂ and displayed its position over time.

We noticed that the CO₂ molecule spent an unexpectedly large amount of time in the narrow windows that connect ITQ-3’s spherical pores and also that when the CO₂ molecule was in the pores, it did not spend an equal amount of time on all surfaces of the pore.

There is a strong correlation between the depth of the PE wells for CO₂ and the amount of time that a typical CO₂ molecule spends in the narrow windows that connect ITQ-3’s spherical pores and also that when the CO₂ molecule was in the pores, it did not spend an equal amount of time on all surfaces of the pore.

Within the green volumes are the most favorable sites (PE < -3 x 10⁴ K) for the center of mass of a CO₂ molecule within the pink volumes are the most favorable sites (PE < -1.5 x 10⁴ K) for the center of mass of an N₂ molecule.

There is an agreement between the minimum configurations at that position which provides the average and minimum PE for a CO₂ molecule at that position. This process was also performed on N₂.