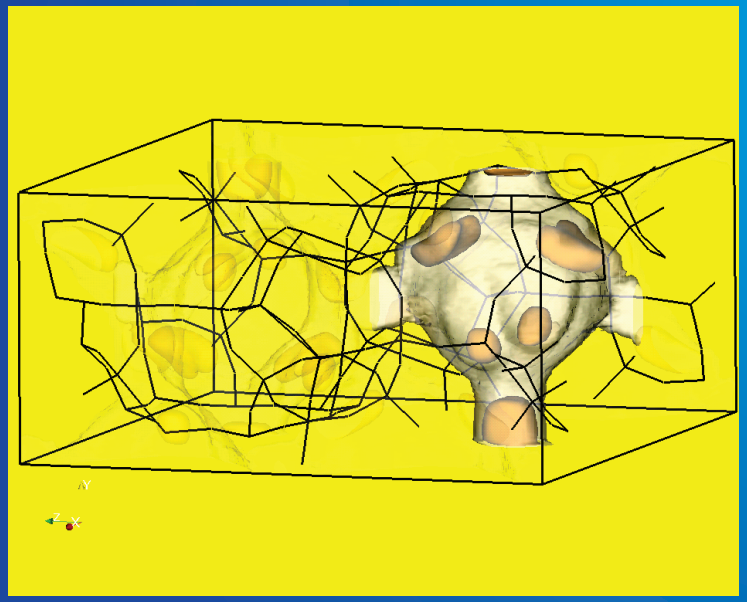
# Studying the behavior of $CO_2$ within Zeolites: Atomistic Simulations

Daniela Kohen Chemistry Department, Carleton College, Northfield, MN 55057

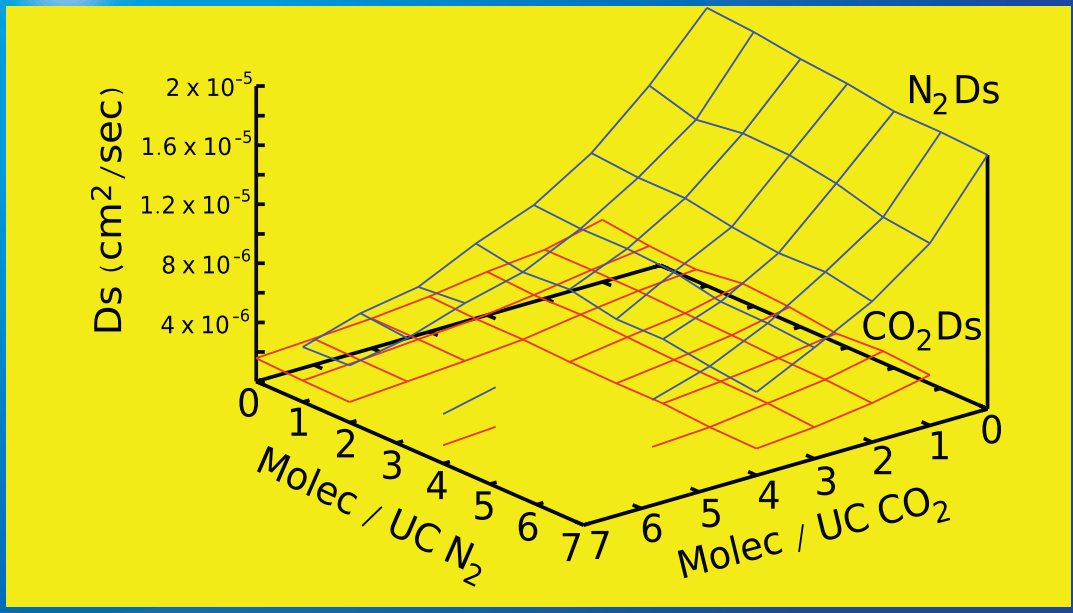
To efficiently separate $CO_2$ from multi-species gas streams, sorbents must have high $CO_2$ selectivity. Zeolites are one attractive option as sorbents due to their variety of structures, availability, and thermal and chemical stability. We aim to understand and characterize at the molecular level how carbon dioxide and other small gas molecules behave in pores of a variety of zeolites. Using atomistic modeling techniques we study the adsorption and diffusion processes within zeolites to aid in the identification of adsorbents selective for $CO_2$.

ITQ-3 is a zeolite that very selectivly adsorbs $CO_2$ over $N_2$. We have been able to show that within this zeolite the adsorption sites for these two gases are the same.



The wire frame above shows the zeolite's atoms framework within one unit cell. One of its pores is highlighted. In white are the locations within the zeolite's s pore that are available to the gas molecules, while the preferred sites are in orange.

We have been able to demonstrate that within some siliceous zeolites that are highly selective for carbon dioxide, diffusion is fast enough to enable the use of these materials in practical separations. Interestingly, we have also shown that within ITQ-3 the presence of $CO_2$ affects the diffusion of $N_2$ but that the reverse is not true.




The 3D plot below shows Self Diffusion for $CO_2$ and $N_2$ mixtures within ITQ-3. Note how $CO_2$ (in red) diffuses more slowly than $N_2$, and its concentration greatly affects the behavior of the faster $N_2$ molecules.