Section II: Methodology

Role of Student vs. Mentor

I completed the majority of the work of this project; I ran the simulations and analyzed the results. However, I sought assistance from a few mentors to help with the installation and compilation of RASPA 2, the simulation I used.

Equipment and Materials

RASPA 2, a simulation software that is particularly useful when simulating frameworks, was used. In addition, a free version of Mercury was used to help with the visualization the MOFs and the Cambridge Crystallographic Data Centre (CCDC) was used for their directory of CIF files of existing MOFs. VMD was used to generate the movie of the adsorption of H2O and CO2 into CALF-20.

Technique 1

Monte Carlo simulations built into RASPA 2 were run in order to find the Helium void fraction of the MOFs, both to use as a parameter for more complicated simulations and to gain a better understanding of the void volume inside the MOFs. The CIF files used to define the MOFs were from the CCDC and run through the program FINDSYM (Stokes and Hatch, 2005) for greater compatibility with RASPA.

Technique 2

Monte Carlo simulations built into RASPA 2 were run to find the CO2 adsorption of the MOFs at various pressures, which can be helpful to compare against CO2 uptake when exposed to air instead of pure CO2. The definition files of the forcefields and molecules were from the RASPA example definitions.

Technique 3

Monte Carlo simulations were run to find the gas adsorption of the MOFs at various relative humidities in order to understand how water vapor and the other components of air might affect CO2 adsorption and examine the CO2 selectivities of the MOFs. Originally, partial pressures were used to simulate the air at different RHs, but it was unsuccessful, and mole fractions were instead used as a parameter. A chart of partial pressures and mole fractions for each component of air at each relative humidity measured will be provided in supplemental files, along with the formulas used. The Tip5p water model was used.

Technique 4

Molecular Dynamics simulations were run and imported into VMD to study CALF-20's selectivity of CO2/H2O described in paper by Lin J., et al. in 2021.