Section III: Results

CO_2 Uptake with Pure CO_2

The CO_2 uptakes of the MOFs were graphed against pressure when exposed to only CO_2. As seen in Figure 1, Cu-BTC performed the best and MUF-16 adsorbed the least amount of CO_2.

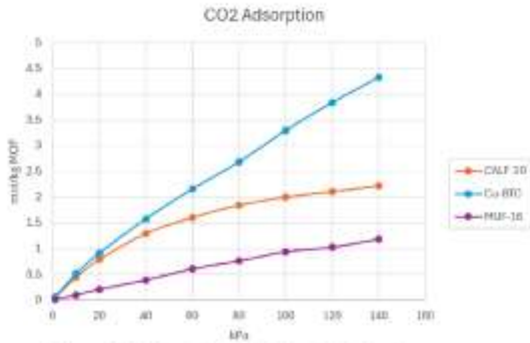

Figure 1: CO2 uptake of CALF-20, Cu-BTC, and MUF-16 at different pressures

CO_2 Uptake from Simulated Air

The gas uptakes of the MOFs were graphed against relative humidity. In Figure 2, it is shown that CALF-20 and Cu-BTC have similar CO_2 uptakes from air and MUF-16 has a significantly smaller one.

Figure 2: CO2 uptake of CALF-20, Cu-BTC, and MUF-16 from air with varied relative humidities

Gas Uptake from Simulated Air

The gas uptakes of the MOFs were graphed against relative humidity. In Figure 3, the gas uptakes of each individual MOF are graphed and all show higher uptake for N_2 and O_2 compared to CO_2 and H_2O, and these uptakes stay relatively constant over all relative humidities. When CO_2 and H_2O are graphed, the uptake of CO_2 stays relatively constant in all three MOFs, and the water uptake increases as the relative humidity increases. One reason why graphs 3E and 3F might appear “wavier” is because MUF-16

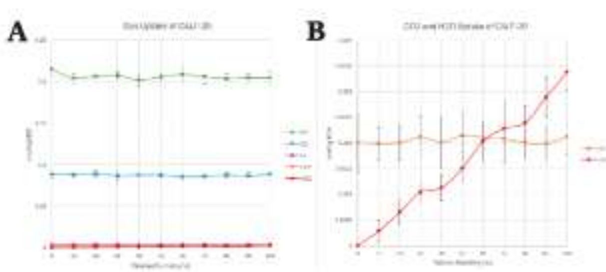

Figure 3: (A) Gas adsorption of CALF-20 at different relative humidities. (B) CO2 and water vapor adsorption of CALF-20 at different relative humidities. Error bars calculated by RASPA 2.

adsorbed the least amount and therefore has a smaller scale, allowing small differences have a larger impact on the graph.

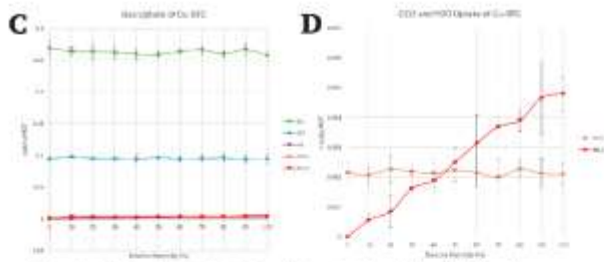

Figure 3: (C) Gas adsorption of Cu-BTC at different relative humidities. (D) CO2 and water vapor adsorption of Cu-BTC at different relative humidities. Error bars calculated by RASPA 2.

Figure 3: (E) Gas adsorption of MUF-16 at different relative humidities. (F) CO2 and water vapor adsorption of MUF-16 at different relative humidities. Error bars calculated by RASPA 2.

Section IV: Discussion

In terms of CO_2 uptake when exposed to solely CO_2, Cu-BTC performed the best, which could be due to the fact that it has the greatest Helium void fraction, meaning it is essentially the most "empty."

Although CALF-20 may have had a smaller void volume than Cu-BTC, its selectivity for CO_2 made it perform similarly to Cu-BTC. Cu-BTC had more volume to begin with, but when exposed to air, more of the volume was occupied by other components of air. MUF-16, however, has the lowest Helium void fraction of the three and also had the lowest CO_2 uptake from air as well.

Due to the low concentration of air in the atmosphere,

The original goal of this project was to design a MOF, but due to difficulty working with the software, along with an underestimation of the time needed to learn all the parameters associated with the simulations and how to fine-tune them, this study was more focused on taking pre-existing MOFs and applying them to simulated air rather than flue gas or other mixtures made up of a higher percentage of CO_2. However, this data still has the potential to be used in future studies regarding how to optimize a MOF to have a high selectivity for CO_2.

Please identify potential limitations, confounding variables, and how you addressed them. Highlight relevant failures and the challenges that you overcame. Explain the statistical tests and why those tests were used? Is there a statistical significance?

This project was a lot of trial and error

How does your work fit into past studies? How does your research differ? How might your research improve upon/forward the understanding in the field? Please include in-text citations for properly formatted references.