

Section V: Conclusion

The goal of this study was to explore MOFs that have demonstrated selectivity for CO₂ in prior papers and examine which perform the best and potentially why, which can be applied in the future towards designing a cost-efficient, energy-effective MOF for the direct air capture of carbon dioxide. RASPA 2 was used because of its special framework features, and Monte Carlo simulations were run to calculate adsorption. Although in all three MOFs, the CO₂ uptake was much smaller than the uptake of other components of air, caused by the low concentration of CO₂ in the air, CALF-20 and Cu-BTC performed similarly in CO₂ uptake from the air while CALF-20 has a smaller Helium void fraction, suggesting that maybe high CO₂ selectivity might be able to make up for factors that tend to decrease adsorption. The negative effects of global warming may seem distant and irrelevant, but they are already present and will only worsen if no changes are made to the large amount of carbon emissions released by human activity (NASA, n.d. a). Whether it be through the use of MOFs or clean energy or bioplastics, it is important to explore ways to slow down or even reverse global warming, for the Earth and all its inhabitants.