Computational Analysis of Nano-Porous Gas Adsorption Materials for Mobile Carbon Capture

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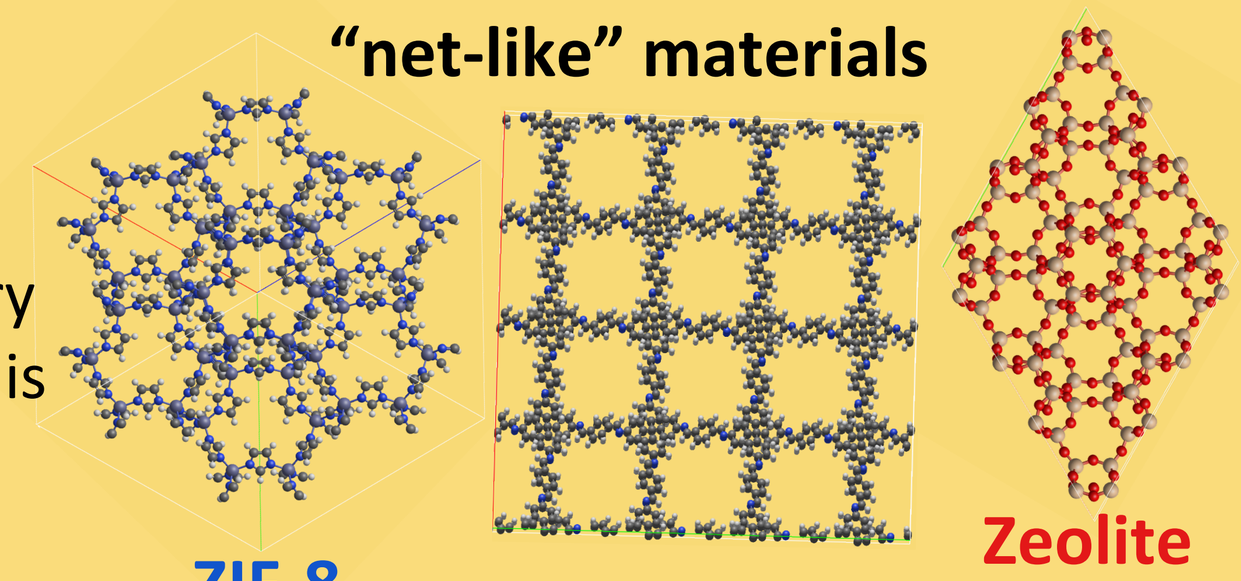
Background: Nano-porous materials have applications in water purification, gas separation, and carbon capture. This project seeks to use computational methods to accelerate materials discovery and characterization. Eventually the goal is to find a material suitable for Mobile Carbon Capture.

Nano-Porous "net-like" materials



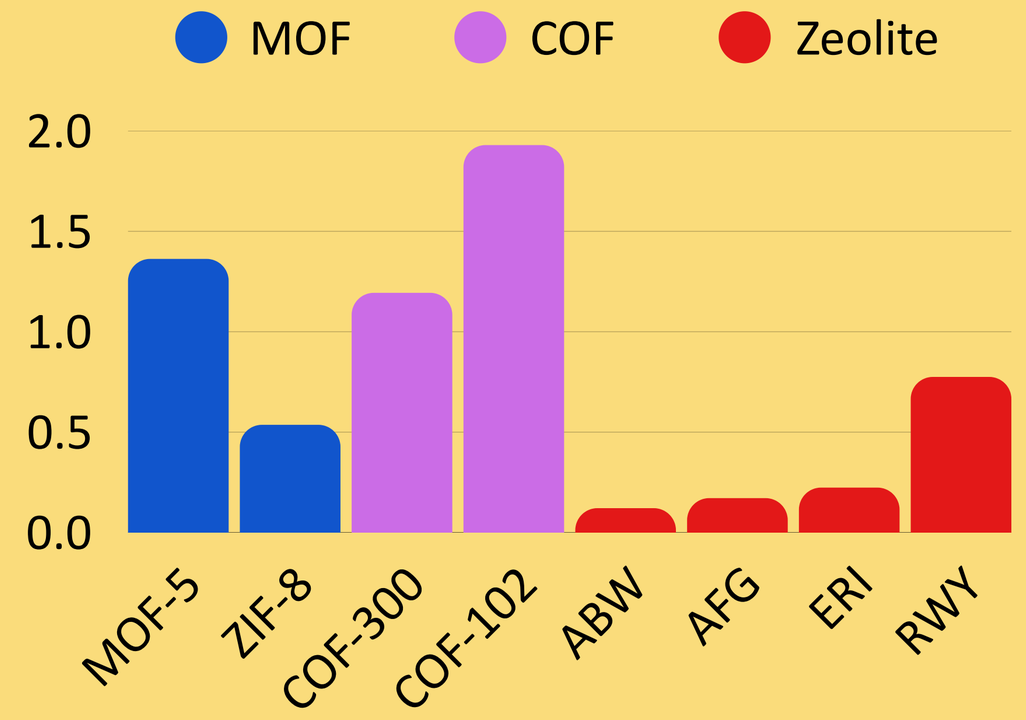
Experimental Methods: A lot of this project was spent exploring various methods from quantum mechanical(DFT) to semi-empirical(xTB) to force field based calculations(RASPA). Although I don't have much data for every method, I learned a lot which will help to prepare me for future research.

Conclusions: Structural properties such as density and pore size can easily be calculated given known crystal structures. DFT can be used to optimize crystal structures and calculate CO_2 adsorption energy, although there are other adsorbing effects at play.

Future Research: There was a lot more I wanted to do for this project! Moving forward I want to find comparable experimental data. Furthermore, I want to test thermal properties with phonon analysis and ion-exchange affects in X-zeolites**.** Finally, I am interested in investigating piezoelectric properties for electrically induced desorption and carbon upcycling through piezo-catalysis.

Results

CO_2 Accessible Pore Volume [cm^3/g] (iRASPA)



CO_2 Adsorption Energy [kCal/mol](CP2K)