A Novel Approach to Capturing CO2 Directly from the Air Using Metal-Organic Frameworks

Global warming has many negative effects on the planet, including worsening droughts, stronger storms, and rising sea levels. In fact, by the end of this century, the sea level is projected to rise at least one foot, though it could rise by more than six feet if nothing is done to reduce these effects (NASA, n.d.). The main cause of global warming is the abundance of heat-absorbing greenhouse gases in the atmosphere that causes heat to remain in the atmosphere (NASA, n.d.). This effect, the greenhouse effect, is crucial to maintaining a temperature that supports life on Earth, but due to the excessive amount of greenhouse gases in the atmosphere, the earth is retaining a lot more heat than it should be, causing an increase in temperature. For this reason, if the amount of greenhouse gases in the atmosphere decreased, global warming could slow down or reverse (Herring, D. & Lindsey, R., 2022).

Reducing Carbon Dioxide

There are many different greenhouse gases including carbon dioxide, water vapor, methane, and nitrous oxide, but carbon dioxide is especially notable because it is the most abundant greenhouse gas released by human activity (NASA, n.d.). The most straightforward approach to reaching "net-zero" carbon emissions, where there is no overall addition of carbon dioxide into the atmosphere, is to decrease carbon emissions in general, but with the dependency of many industries on processes that emit carbon dioxide, simply reducing emissions may prove difficult. Additionally, in the long run, the overall concentration of carbon dioxide needs to be not only restricted from further increase but reduced to reverse the effects of global warming (Sanz-Pérez, E. S. et al, 2016). As a result, many hope to develop efficient technology that can help remove carbon dioxide from the atmosphere, offsetting any carbon emissions, to reach net-zero or net-negative carbon emissions (Brazzola, N. et al, 2024).

Metal-Organic Frameworks

Many methods of carbon capture already exist, including the use of amine-based solvent systems and liquid sorbents, but more recently, there has been a less established method of carbon capture that is potentially more energy efficient and cost effective: metal-organic frameworks (MOFs) (Lin, J. et al., 2021). MOFs are a porous nanomaterial formed by metal ions or clusters connected by organic ligands. They are very versatile, and their pore size and porosity can vary a lot. By changing the metal ions or organic ligands used to form the framework, the physical and chemical properties can be manipulated, which can change a MOF's ability to absorb, almost like a sponge, certain substances. The ability to absorb a certain molecule over another molecule when the MOF is presented with a mixture of the two is described as having a higher selectivity for the specific molecule (Safael, M. et al., 2019). When applied to carbon capture, one might test a MOF's selectivity for carbon dioxide over other molecules present in air, such as nitrogen or water vapor.

MOFs in Carbon Capture

Pre-existing MOFs optimized for carbon capture tend to be designed for point-source capture rather than direct air capture (DAC) (Lin, J. et al., 2021). Point-source capture, also known as post-combustion capture, refers to the capture of carbon dioxide directly from flue gas, power plant emissions that are a mixture of carbon dioxide and other gases such as water vapor and nitrogen (Lin, J. et al., 2021). Direct air capture refers to the capture of CO2 directly from air rather than from flue gas released from a power plant (Myers, J., 2020). DAC tends to be more difficult and costly since the concentration of CO2 in the atmosphere is so much lower than the concentration of CO2 in flue gas. Thus far, few MOFs have been optimized for DAC, posing the question of what type of MOF would be the most efficient at capturing CO2 directly from the atmosphere.

Simulations

To determine which MOFs have the highest selectivity for CO2 over other molecules typically found in air, Monte Carlo simulations and Molecular Dynamics simulations were performed using RASPA 2, a simulation software commonly used when working with frameworks (Dubbeldam et al., 2015). Three MOFs were tested (CALF-20, Cu-BTC, and MUF-16), chosen because their potential in CO2 capture has been demonstrated in previous studies.