Using data driven methods and industrial scale process simulations to design materials at the atomic level for CO_2 capture.

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Metal organic frameworks (MOFs) are crystalline, nanoporous inorganic-organic materials that have attracted significant attention as enabling materials for various clean energy applications such as CO_2 capture.[1] These materials present an almost infinite design space with innumerable combinations of inorganic and organic building units that can combine to form a permanently porous material. In this talk, we will describe how high throughput screening and data driven methods have aided in the development of experimentally realized, high-performance materials for CO_2 capture. These tools developed include the creation of a diverse materials database of hundreds of thousands of MOFs, machine learning of important simulation parameters for high throughput screening, and data-mining methods to identify key chemical features for our experimental collaborators to target. The work presented stands out as the first study in which a MOF was designed from computational high throughput screening that was successfully synthesized in the lab. [2] More recently, we have developed a multi-scale technique that combines atomic scale simulation of gas adsorption in MOFs with process models of the CO_2 capture systems at the industrial scale. The goal of this work is to design materials at the atomic level, that will be high performing based on industrial scale metrics such as how much energy the process will use or how pure the CO_2 that is extracted will be.

[1] Lin et al. "A scalable metal-organic framework as a durable physisorbant for Carbon Dioxide Capture" *Science*, **2021**, *374*, 6574.
[2] Boyd et al. "Data driven design and synthesis of metal-organic frameworks for wet flue gas CO_2 capture", *Nature*, **2019**, *576*, 253.