

Metal-organic frameworks for carbon capture

They present a database of **324,426 hypothetical Metal-Organic Frameworks (MOFs)** screened for potential carbon dioxide scrubbers. Using a method to assemble these materials with topological blueprints, we only selected materials that could be accurately represented with the MEPO-QEq charge generation method. By ensuring that the electrostatic potential is accurately represented in these materials, screening for CO₂ adsorption properties should result in very few false positives/negatives.

Post-combustion flue gas was simulated at a temperature of both 298K and 0.15 bar CO₂, and 313K and 0.15 bar CO₂. Mixture adsorption was simulated with the conditions 298K and 0.15:0.85 CO₂/N₂ with a total pressure of 1 bar. We report working capacities, i.e. the difference of adsorption of CO₂ between two thermodynamic state points. The adsorption state point(s) are mentioned above, and two desorption values were simulated; 0.1 bar CO₂ at 363K (vacuum swing adsorption) and 0.7 bar CO₂ at 413K (temperature swing adsorption).

Over **8,000 materials were selected for more refined simulations**, including re-defining partial atomic charges with the REPEAT method, and more detailed simulations to obtain common chemical patterns surrounding CO₂ binding sites (adsorbaphores).

The interactive figure allows to explore the full database of assembled structures, together with their properties. All structures and properties can be downloaded in bulk from the Materials Cloud archive entry linked above.