

Synthesis of a Novel Metal Organic Framework with a PCU Topology for CO₂ Separation in CCS

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The atmospheric release of CO₂ is strongly correlated with climate change. Metal organic frameworks (MOFs), porous, uniform, and crystalline structures, have demonstrated high promises for CO₂ separation in Carbon Capture and Storage. MOF X synthesized in 2013 demonstrated limited gas uptake abilities due to interpenetrated pore structure. To overcome the limitation, various solvents were utilized to control the degree of interpenetration. Therefore, this present study reports a novel MOF with a pcu topology, C₂₀H₁₆N₄F₆SiCu (Z), synthesized utilizing the layering technique. An ASAP 2020 determined gas sorption behaviors. The Zur Loye group processed Z via single crystal XRD, powder diffraction, and TGA. TGA revealed that Z was thermally stable up to 225°C while powder diffraction demonstrated Z remained chemically stable in the presence of CO₂ and N₂. Z's 77K N₂ adsorption revealed a BET surface area 1057m²/g. Gas sorption analyses indicate that Z adsorbed 33cm³/g of CO₂, significantly higher than that of MOF X and other published adsorbents such as Mg-MOF-1, MOF-2, and ZIF-8. Z's binding energy to CO₂ was 28kJ/mol, highly optimum for CO₂ separation, as Z's regenerative costs will be considerably lower than current chemisorbent's. Z's IAST selectivity of CO₂ over N₂ at 15% and 85% flue gas composition, respectively, was calculated at approximately 20.2, primarily attributed to the electrostatic interaction between CO₂ and the SiF₆ anion. Z provides a new platform for post-synthetic modification to potentially develop more effective adsorbents for gas separation technology.

Awards Won:

Second Award of \$2,000

United States Steel Corporation: First Place Award of \$1,500