

# Synthesis of a Novel Metal Organic Framework with a PCU Topology for CO<sub>2</sub> Separation in CCS

Zheng, Steve

The atmospheric release of CO<sub>2</sub> is strongly correlated with climate change. Metal organic frameworks (MOFs), porous, uniform, and crystalline structures, have demonstrated high promises for CO<sub>2</sub> 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, C<sub>20</sub>H<sub>16</sub>N<sub>4</sub>F<sub>6</sub>SiCu (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 CO<sub>2</sub> and N<sub>2</sub>. Z's 77K N<sub>2</sub> adsorption revealed a BET surface area 1057m<sup>2</sup>/g. Gas sorption analyses indicate that Z adsorbed 33cm<sup>3</sup>/g of CO<sub>2</sub>, 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 CO<sub>2</sub> was 28kJ/mol, highly optimum for CO<sub>2</sub> separation, as Z's regenerative costs will be considerably lower than current chemisorbent's. Z's IAST selectivity of CO<sub>2</sub> over N<sub>2</sub> at 15% and 85% flue gas composition, respectively, was calculated at approximately 20.2, primarily attributed to the electrostatic interaction between CO<sub>2</sub> and the SiF<sub>6</sub> anion. Z provides a new platform for post-synthetic modification to potentially develop more effective adsorbents for gas separation technology.

## Awards Won:

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

Second Award of \$2,000