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