Investigating the effect of the metal ion in carbon dioxide sorption in flexible isostructural metal–organic frameworks.

L. Mbonzhe, E. Batisai

University of Venda, P Bag X5050, Thohoyandou, South Africa.

Eustina.Batisai@univen.ac.za

Metal-organic frameworks (MOFs) are 2-D or 3-D porous crystalline materials composed of metal ions or clusters coordinated to organic ligands.[1] Their high surface areas and tunable structures make them potential candidates for various applications such as gas storage and sequestration, separation, drug delivery, and catalysis.[2-5] One of the widely studied areas of MOFs research is carbon dioxide capture due to the potential for selective adsorption and high uptake capacities.[6] Flexible MOFs, often called soft porous crystals, exhibit dynamic structural changes in response to external stimuli. Unlike rigid MOFs, their flexibility enables reversible transformations, enhancing their performance in applications such as selective gas adsorption and sensing.[7] Herein, we report the synthesis, characterization, and carbon dioxide sorption studies of a series of isostructural flexible MOFs, with general formula $[M(OBZ)(L1)_{0.5}]\cdot 2DMF$ where M is Co, Zn, Ni, Cu or V; L1 is 2,7-bis(pyridin-3-ylmethyl)benzo[lmn][3,8]phenanthroline-1,3,6,8(2H,7H)-tetraone; and OBZ is 4,4′-oxybis(benzoic acid). The Zn and Co MOFs were synthesized directly via solvothermal methods, while the Ni, Cu, and V analogs were obtained via post-synthetic metal exchange of the Zn-based framework. The MOFs were characterized using powder X-ray diffraction (PXRD), variable temperature PXRD, single crystal X-ray diffraction (SCXRD), thermogravimetric analysis (TGA), and Energy Dispersive X-ray Spectroscopy (EDS). CO_2 sorption studies were conducted up to 20 bar at 298 K. Despite having the same overall framework, the MOFs exhibit distinct sorption behaviors and uptake capacities. Studying isostructural MOFs, which share the same framework but differ only in the metal ion, provides valuable insight into the role of the metal ion in shaping CO_2 sorption behavior. These comparisons advance our understanding of structure–property relationships, which are critical for rationally designing efficient CO_2 capture materials.

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