Poster

Gas sorption studies of mixed ligand metal-organic frameworks containing substituted diimide ligands

E. Batisai[1], L. Mbonzhe[1], R. Mahwasane[1], N. Chatterjee[2], C. Oliver[2]

[1]*Department of Chemistry, University of Venda, P Bag X5050, Thohoyandou 0950, South Africa* [2]*Department of Chemistry, University of Cape Town, Rondebosch 7701, South Africa eustina.batisai@univen.ac.za*

Metal-organic frameworks are porous compounds consisting of metal nodes and bridging organic ligands [1,2]. MOFs are potential candidates for application in gas storage, catalysis, and drug delivery due to their unique properties such as large surface areas, large pore volumes, tuneability, and flexibility [3,4]. Our research focuses on the synthesis and investigation of gas sorption properties of new porous MOFs containing substituted diimide ligands. These ligands have been used to synthesize metal-organic frameworks with various topologies, some of which have shown potential in gas sequestration and sensing. To this end we have synthesized three structurally related substituted diimide ligands namely; 2,2′-bis(pyridin-3-ylmethyl)-[5,5′-biisoindoline]-1,1′,3,3′-tetraone (L1), 5,5′- carbonylbis(2-(pyridin-3-ylmethyl)isoindoline-1,3-dione) (L2) and 2,2'-bis(pyridin-4-ylmethyl)-[5,5-biisoindoline]-1,1-3,3'-tetraone (L3). Reactions of these ligands with metal salts and carboxylate ligands (2,6-naphthalenedicarboxylic acid (2,6-NDC), 4,4′- oxybis(benzoic acid) (OBZ) and terephthalic acid (TER)) under solvothermal conditions yielded four new porous 3D MOFs namely $\{[Cu(2,6\text{-}NDC)(L1)_{0.5}]\cdot 3DMF\}_n$ (1), $\{[Zn(2,6\text{-}NDC)(L2)]\cdot 2DMF\}_n$ (2), $\{[Zn_2(OBZ)_2(L1)]\cdot 4DMF\}_n$ (3) and $\{[Co_3(TER)_3(L3)(DMF)]\cdot 5DMF\}_n$ (4). The MOFs were characterized using single-crystal X-ray diffraction (SCXRD), thermogravimetric analysis (TGA), and powder X-ray diffraction (PXRD). SCXRD revealed that the MOFs are 3D and possess 33%, 27%, 23%, and 33% of solvent-accessible volumes, respectively. CO_2 and N_2 sorption experiments were conducted on the activated phases of the MOFs. Activated phases of 1, 2, and 4 adsorb modest amounts of CO_2 and display a type-I sorption behavior at 195 K and 273 K while 3 displays a stepwise and hysteretic sorption of CO_2 at 195 K due to a structural transformation. The X-ray diffraction, thermal analysis and gas sorption results are discussed.

[1] Yaghi, O.M. & Hailian, L. (1995), *J. Am. Chem. Soc.*, **70**, 10401.

[2] Yaghi, O.M., Guangming, L. & Hailian, L. (1995), *Nature*, **378**, 703.

[3] Furukawa, H., Ko, N., Go, Y.B., Aratani, N., Choi, S.B., Choi, E., Yazaydin, A.Ö., Snurr, R.Q.; O'Keeffe, M.; Kim, J. & Yaghi, O.M., (2010), *Science,* **329**, 424.

[4] Farha, O.K., Yazaydin, A.Ö., Eryazici, I., Malliakas, C.D., Hauser, B.G., Kanatzidis, M.G., Nguyen, S.T., Snurr, R.Q., Hupp, J.T., (2010), *Nat. Chem.*, **2**, 944.