

Nanoengineering of Metal-Organic Frameworks (MOFs) for Carbon Capture

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Abstract

The world energy consumption is expected to be rising over the next few decades and so is the atmospheric concentration of carbon dioxide, possibly contributing to global climate change. To mitigate climate change, CO₂ capture technologies from the post-combustion flue gas have been implemented. Adsorption processes onto porous solid media are one of the well known CO₂ capture technologies.

Metal organic frameworks (MOFs) are new class of nanoporous solids where metal clusters, or metal ions, are linked together by organic moieties forming three-dimensional highly crystalline frameworks. These materials were found to have well-defined porosity, high surface areas, and tunable chemical functionalities. At high-pressure ranges, MOFs report to have a superior CO₂ adsorption capacity over other physisorbents such as zeolites and activated carbons. Unfortunately, in the conditions of interest with low-pressure environment, most MOFs do not perform as well.

Among those that show promise, Mg/DOBDC reports the highest and competitive adsorption capacity of 0.38 g CO₂/g sorbent at low CO₂ partial pressures. Mg/DOBDC consists of Mg (II) ions connected by organic linkers of 2,5-dioxido-1,4-benzenedicarboxylate (DOBDC). After synthesis and activation of the material, one dimensional pore structures create coordinatively unsaturated metal sites that are able to adsorb CO₂ molecules. However, high energy input is required for a full regeneration of the Mg/DOBDC¹. Also, based on recent studies, the materials adsorption capacity decreases with multiple cycles of adsorption and desorption operations². The hydrophilic nature of MOFs additionally suggests that CO₂ adsorption capacity may drop under humid conditions. One of the proposed ways to deal with current issues of Mg/DOBDC is to functionalize the open metal sites with amine groups. Introduction of amine groups onto Mg/DOBDC may help to preserve the structure under dry and humid conditions by added compounds. Amine sites are also known to be very effective in CO₂ adsorption, especially under humid conditions (presence of water molecules enhances CO₂ uptake). In this project, functionalization of open metal sites with ethylene diamine (ED), as a grafting agent, is performed with hope of reducing the energy input for the full regeneration of the adsorbent (Mg/DOBDC), and better performance under both dry and humid conditions.

¹ Yazaydin, A. O.; Snurr, R. Q.; Park, T. H.; Koh, K.; Liu, J.; LeVan, M. D.; Benin, A. I.; Jakubczak, P.; Lanuza, M.; Galloway, D. B.; Low, J. J.; Willis, R. R. *J. Am. Chem. Soc.* **2009**, *131*, 18198

² Britt, D.; Furukawa, H.; Wang, B.; Glover, T. G.; Yaghi, O. M. *Proceedings of the National Academy of Sciences of the United States of America* **2009**, *106*, 20637