Selective Adsorption of CO_2 in Mg-MOF-74 under Humid Conditions

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Research question: How does moisture affect the selective adsorption of CO_2 in Mg-MOF-74?

Introduction

- Metal-organic framework, also known as MOFs, can be artificially synthesized[1]. The central atoms are the metal cation with positive charges linking by the organic ligands[2].
- The structure of Mg-MOF-74 is honeycomb topology, which the porous structure provides the basis for a large capacity of carbon dioxide adsorption[4].

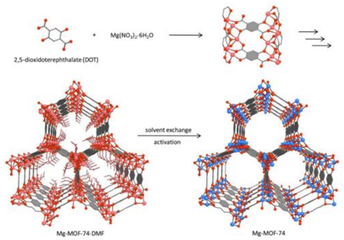

Figure 1: The process of how the Mg-MOFs-74 formed.[3]

- Key concepts involved are physical adsorption, open metal sites (OMS) and Lewis's acid and base interactions.
- The process of metal-organic framework uptakes carbon dioxide is mainly the physical adsorption process[6].
- OMS defines as how many coordinates can be linked with a central metal cation[1,3].

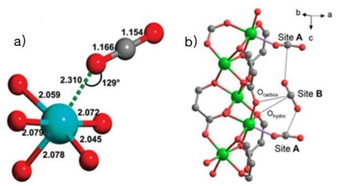

Figure 2: Configuration on the left a) shows the angle of the Mg^{2+} and carbon b) shows the single-crystal X-ray structure of CO_2-adsorbed.[7,9]

- The Lewis acid and base interactions occur between oxygen in carbon dioxide and metal ion as well as carbon in carbon dioxide and carboxylate oxygen on plane[1,7,8].

Result

In order to examine the selectivity of CO_2, new concept will be involved. Isosteric heat, Q_{st}, is the parameter to determine the adsorption ability. With higher Q_{st} means better adsorption amount.

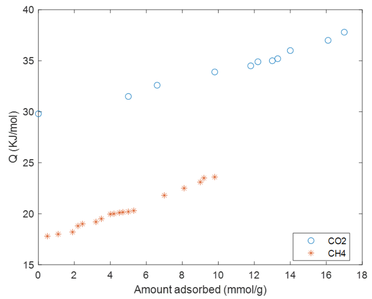

Figure 3: The amount adsorbed (mmol/g) vs. isosteric heat Q (KJ/mol) between CH_4 *and* CO_2.[5]

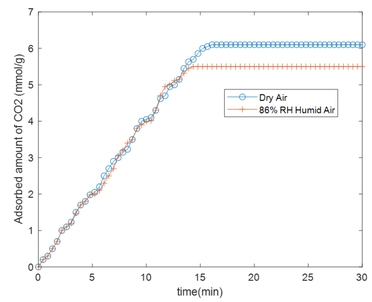

Figure 4: The adsorbed amount of CO_2 (mmol/g) vs. time (min). The data is gain at constant pressure under 101.35kP and temperature at 300K. [8]

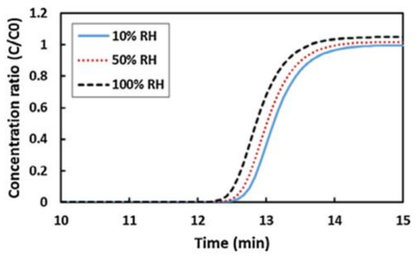

Figure 5: The concentration ratio and time (min) has been analyzed under different relative humidity. [5]

Impact

The humid environment ruins the adsorption of Mg-MOF-74 which has a strong affinity toward water[2,3]. Water molecules occupy the primary sites on metal sites and significantly reduce the adsorption of carbon dioxide. This research can greatly help us to mitigate the Also, excessive carbon dioxide emission causes a worse and worse greenhouse effect. Increasing the adsorption of Mg-MOF-74 can effectively control the greenhouse effect.

Further Work

- Adding a water adsorption layer to the packed bed to reduce the humidity and protect MOFs.
- Improving the structure of Mg-MOF-74 to increase the affinity toward carbon dioxide instead of other gas to boost its selectivity toward CO_2 capture.
- Controlling the temperature and pressure of the operation at a certain range to maximize the amount of CO_2 adsorption.

Reference

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