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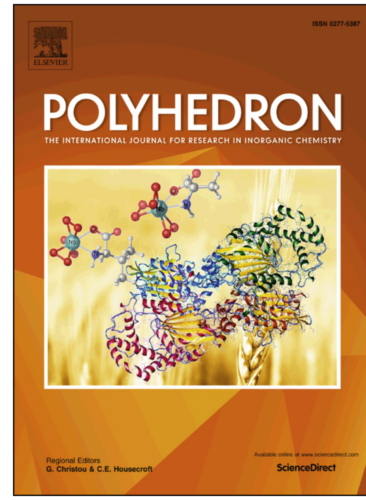

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Carbon Dioxide Capture in MOFs: The Effect of Ligand Functionalization

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Abstract:

The carbon dioxide challenge is one of the most pressing problems facing our planet. Physisorption between certain adsorbents and CO_2 molecules could allow conveniently reversible processes to capture CO_2 gas. Metal-organic frameworks (MOFs) have recently attracted intense research interest because of their permanent porous structures, large surface areas, and potential applications as novel adsorbents. Tuning the interior pores of MOFs to improve their adsorption characteristics is considered an effective approach to enhance gas adsorption/separation performance. Recently, there is a growing interest to explore the impact of grafting functional groups with variable polarities (-NH_2, -OH, -CO_2H, -CF_3, -SO_3H, -NO_2,. . .) onto the surfaces of MOFs through their organic ligands or directly coordinated to open metal centers on the CO_2 capture/separation performance. Ligand functionalization in MOFs has been demonstrated to enhance gas adsorption and while ligand functionalization does not change the overall structure of the frameworks, it can influence the gas uptake behavior. In this review, we show how ligand functionalization influences the CO_2 affinity and adsorption capacity of MOFs. The comparisons drawn in this review have sought to provide a roadmap for the future development of functionalized MOFs.

Keywords: Metal-Organic Frameworks; Ligand Design; Functionalization; CO_2 Capture;

1. Introduction

The global warming caused by emission of greenhouse gases is by far the most serious environmental problem such as glaciers melting, sea levels rising, frequent extreme weather and ozone depletion. Among them, carbon dioxide is the major contributor [1]. Indeed, CO_2 emissions account for ca. 70% of the gaseous irradiative force causing the greenhouse effect, followed by CH_4 and N_2O. Since preindustrial times, the CO_2 concentration in the troposphere has increased from 280 ppmv in 1750 to > 380 ppmv at present, with an annual increase of about 1 ppm [2]. A drastic reduction of these CO_2 emissions is indispensable in order to limit the increase in global average temperature. In this spirit the EU, through the European Strategic Energy Technology Plan (SET-Plan) and the Carbon Capture and Storage (CCS) Technology Roadmap, has agreed to enable the cost competitive deployment of CCS after 2020 and to further