Exploring Soft Porous Crystals: Discoveries and Future Perspectives in Chemistry

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Metal-organic frameworks (MOFs) or porous coordination polymers (PCPs) possess inherent voids that allow storing, delivering, and separating substances, particularly gases. Among them, 3rd generation MOFs called flexible MOFs or soft porous crystals (SPCs),1 -3 exhibit a structural change from crystal to crystal in response to physical and crystalline stimuli. This feature distinguishes them from other porous materials, reminiscent of the induced fit mechanism of enzymes and the cooperative phenomenon of hemoglobin. In contrast to rigid materials showing a Langmuir type I isotherm, SPCs possess a sigmoidal isotherm, higher usable capacity, and efficient recognition of guest species. The flexibility depends on the binding ability and mobility of unit ligands and metal ions, as well as other factors, including the deformation of the entire framework due to the guest molecules in the pores. We predicted the existence of SPC[4] at an early stage and have been leading the way in the chemistry of diverse flexible MOFs with dynamic chemical functions such as adsorption. Recently, it has become clear that MOF[5], for which we first demonstrated gas adsorption in 1997, is indeed SPC.[6] This means that the first example of PCP/MOF is SPC.

Strategies using framework motif functionalization have been developed to investigate the properties, but have mainly focused on discovering and understanding dynamic phenomena in SPCs. This trend has now shifted towards controlling the adsorption properties for practical applications. This talk provides an essential and accessible overview of the historical background of the chemistry of SPCs, their features, and outlook as 4th generation MOFs,[7,8] in particular, design and synthesis, dynamic structure analysis, flexibility and function, and theoretical treatment and interpretation of the mechanism, as well as their applications.8.9

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