

Department of Physics & Astronomy

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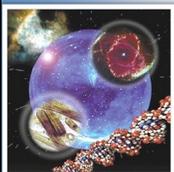
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Metal-Organic Frameworks with Functional Pores for Recognition of Small Molecules

Molecular recognition-- an important process in biological and chemical systems-- governs the diverse functions of a variety of enzymes and unique properties of some synthetic receptors. Because molecular recognition is based on weak interactions between receptors and substrates, the design and assembly of synthetic receptors to mimic biological systems and the development of novel materials to discriminate different substrates for selective recognition of specific molecules has proved challenging. The extensive research on synthetic receptors for molecular recognition— particularly on non-covalent complexes self-assembled by hydrogen bonding and metal-organic coordination— has revealed some underlying principles. In particular, these studies have demonstrated that the shapes of the supramolecular receptors play significant roles in their specific and selective recognition of substrates: receptors can offer concave surfaces that complement their convex targets.

This Seminar describes our research to develop a synthetic molecular recognition platform using porous metal-organic frameworks (MOFs). These materials contain functional pores to direct their specific and unique recognition of small molecules through several types of interactions: van der Waals interactions of the framework surface with the substrate, metal-substrate interactions and hydrogen bonding of the framework surface with the substrate. These materials have potential applications for gas storage, separation and sensing. We demonstrate a simple strategy to construct a primitive cubic net of interpenetrated microporous MOFs from the self-assembly of the paddle-wheel clusters, $M_2(\text{CO}_2)_4$ ($M = \text{Cu}^{2+}, \text{Zn}^{2+}$ and Co^{2+}), with two types of organic dicarboxylic acid and pillar bidentate linkers. This efficient method allows us to rationally tune the micropores to size-exclusively include different small gas molecules, leading to the highly selective separation and purification of gases. By optimizing the strong interactions between open metal sites within porous MOFs and gas molecules such as hydrogen and acetylene, we have developed several MOF materials with extraordinary acetylene storage capacity at room temperature. We have also immobilized Lewis acidic and basic sites into luminescent porous MOFs to recognize and sense neutral and ionic species. Using the strategy to systematically immobilize different open metal sites within porous MOFs from the metallo-ligand precursors, we have developed the first microporous mixed-metal-organic framework (M'MOF) with enhanced affinity for hydrogen molecules, which successfully separated D_2 from H_2 using kinetic isotope quantum molecular sieving.

Because we can functionalize the pores to direct their specific recognition of small molecules, the emerging porous MOFs serve as novel functional materials for gas storage, separation, heterogeneous catalysis, and sensing.



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