The design and discoveries of metal-organic frameworks (MOFs) or porous coordination polymers (PCPs) during the past two decades or so have inspired materials scientists to look MOFs/PCPs beyond the scope of traditional porous materials such as zeolites and porous carbon.[1] An intriguing property of the MOFs is flexibility,[2] the later combined with enormous opportunities to tune the nanospaces have made MOFs promising for applications in important areas such as gas technology, catalysis and biomedicines. The nanospaces can be tuned in terms of size, shape and chemical functionality in a desired manner for a targeted function. This presentation will try to focus on some of the design strategies and mechanistic aspects of some “flexible” and “not so flexible” MOFs/PCPs for efficient and selective capture of gases, in particular CO2.[3] Improving gas adsorption by utilizing weak interaction in porous compounds is highly attractive for the design of energy efficient storage materials. Inspired with this idea, here we present a rational design for such adsorption process using synergistic functions between dynamic motion in a local module and weak host-guest interaction, viz. halogen bond (XB) in MOFs. Some examples of interpenetrated MOF compounds will be provided that show promise for highly controlled adsorption of CO2 gas through chemical modulation.[3] Multi-stimuli structural response and associated crystal dynamics of the interpenetrated MOFs will also be discussed in detail.


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