Rigid metal organic framework capable of showing guest induced phase transition

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Abstract:
Metal-organic frameworks (MOFs) have been explored widely for decades for their profuse applications, most importantly for gas adsorption and separation. Microporous MOFs (MMOFs) are especially known for such applications owing to their large surface areas and specific window aperture which facilitates selective gas separation via host-guest interaction[1, 2]. The pore openings of these materials depend on the type of linker, their respective orientation and binding mode to the metal center. Generally, MMOFs with smaller struts have a rigid structure, which provides them sufficient stability and recyclability up to more adsorption-desorption cycles. However very rarely apart from being constructed of rigid linkers there comes an overall inherent flexibility to the structure which can be further tuned by external stimuli like temperature, pressure, solvent etc.[2] In recent past, we have reported a flexible ultra-microporous MOF in which gas driven framework flexibility resulted in shooting up the CO_2 adsorption capacity by 42% as compared to its non-flexible polymorph [3]. However, it is still a challenge to obtain a direct crystallographic evidence for this type of flexibility taking place in such small pore systems. In the current work, I will be discussing how a different binding mode of ligand provides flexibility to a MMOF irrespective of being constructed from rigid linkers. Further, the direct structural evidence for solvent depending flexibility of the framework will be provided in details and how this framework flexibility affects the overall porosity of the framework will also be emphasized in the presentation.

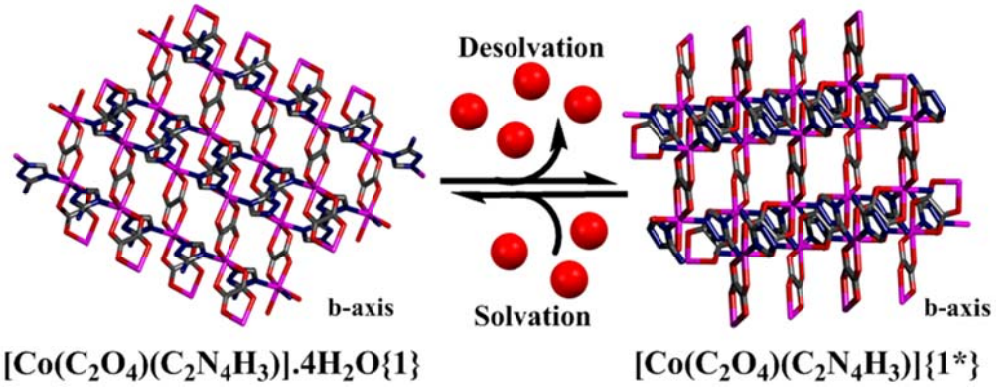

Figure: View along crystallographic b-axis showing the guest dependent framework flexibility of the MOF. (Colour code: Pink: Cobalt, Blue: Nitrogen, Red: Oxygen, Grey: Carbon. Hydrogens have been omitted for clarity of the picture)

References and Notes:

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