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Guest exchange and guest influence in dynamic frameworks

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Dynamic materials, capable of responding to their environment, require flexibility which may be achieved using weak interactions such as hydrogen bonding or through the use of suitable metals and ligands in coordination compounds. Thermochromic and mechanochromic coordination networks have recently received a great deal of attention. Materials of this type are particularly of interest if they are able to revert to their original state on application of another external perturbation signal.

The process of guest exchange within porous solids is of interest in a range of applications, such as selective absorption or separation of gases and heterogeneous catalysis. Frameworks may be made up of relatively strongly bound entities such as those that make up metal-organic frameworks (MOFs) or may be more loosely bound such as host-guest systems where the host molecules crystallise as independent entities but leave spaces which can accommodate guest molecules. In all cases the topology and dynamism of the framework, as well as its capacity to include and to exchange guests, is determined by the nonbonded interactions occurring in the system under defined conditions of temperature and pressure [1-3]. Nonbonding interactions include hydrogen and halogen bonding as well as other disperse interactions. All play an important role in the properties of porous crystalline solid materials. Rational design of such systems remains a challenge however, and is thus an exciting area for application of crystal engineering principles.

In this presentation, examples from recent work in our laboratory will be presented, including MOFs and 3D hydrogen bonded frameworks constructed from the same flexible ditopic ligands, 4-(4-pyridyl)benzoate and 3-(4-pyridyl)benzoate. The influence of halogen versus hydrogen bonding on a molecular host-guest system will also be described. Their ability to exchange guest molecules selectively as well as their chromic behaviour on application of external stimuli such as heat, grinding or exposure to solvent vapours will be described.

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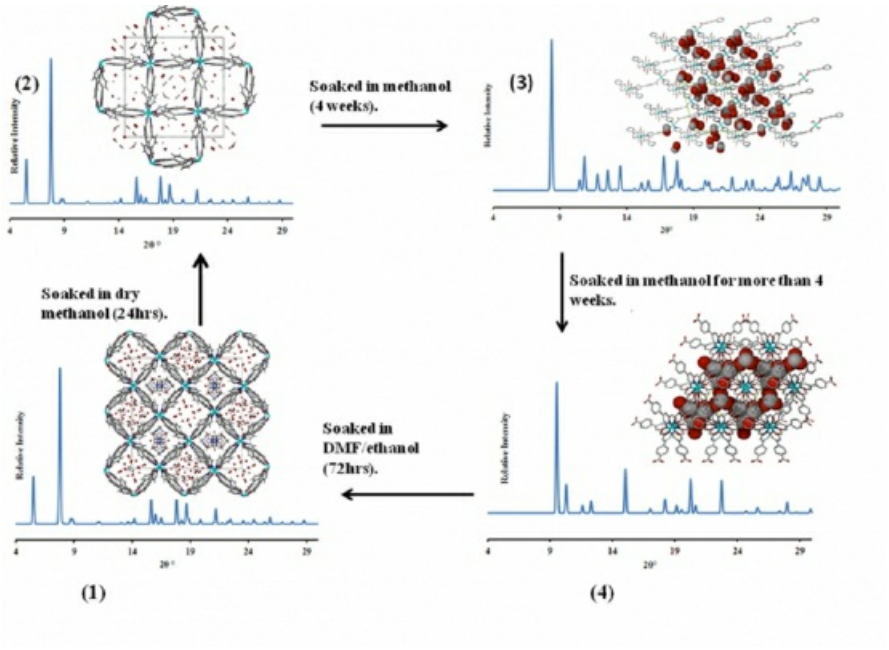
[3] Mehlana, et al. (2015) Polyhedron, 98, 224-229.



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