Poster Presentation

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Compressibility Studies of Zirconium Based Metal-Organic Frameworks

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Metal-organic frameworks (MOFs) are a well-studied class of porous materials with the potential to be used in many applications such as gas storage and catalysis.[1] UiO-67 (UiO = University of Oslo), a MOF built from zirconium oxide units connected with 4,4-biphenyldicarboxylate (BDC) linkers, forms a face centred cubic structure. Zirconium has a high affinity towards oxygen ligands making these bridges very strong, resulting in UiO-based MOFs having high chemical and thermal stability compared to other MOF structures. Moreover, UiO-67 has become popular in engineering studies due to its high mechanical stability.[2] Using high pressure x-ray crystallography we can exert MOFs to GPa pressures, experimentally exploring the mechanical stability of MOFs to external pressure. By immersing the crystal in a hydrostatic medium, pressure is applied evenly to the crystal. On surrounding a porous MOF with a hydrostatic medium composed of small molecules (e.g. methanol), the medium can penetrate the MOF, resulting in medium-dependant compression. On compressing MOF-5 (Zn4O(BDC)3) using diethylformamide as a penetrating medium, the framework was shown to have an increased resistance to compression, becoming amorphous several orders of magnitude higher in pressure than observed on grinding the sample.[3] Here we present a high-pressure x-ray diffraction study on the UiO-based MOF UiO-67, and several new synthesised derivatives built from same metal node but with altered organic linkers, allowing us to study in a systematic way, the mechanical stability of the MOF, and its pressure dependence on both the linker, and pressure medium.

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