

Boosting crystallinity in metal-organic polyhedra

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Internship Description:

Metal-organic polyhedra (MOPs) are discrete molecules that can show permanent porosity. Packing in the solid state of MOPs is often dominated by weak dispersion forces, meaning that they have a tendency to collapse into amorphous phases when any solvent molecules present in their crystal structure are removed. These amorphous phases then show very slow gas diffusion and limited gas uptake.

We want to study whether high degrees of crystallinity in bulk powders of MOPs can lead to increased uptake of gas molecules. To direct the packing of the MOPs, we will use synthetic chemistry to append hydrogen bonding groups to the skeleton of the molecules. The objectives of the project are to: (i) Synthesise novel ligands and MOPs; (ii) Characterise them using a variety of physical techniques; and (iii) Use gas sorption measurements to show how the crystal packing affects gas uptake.

Prospective tasks: The majority of the internship will be used to synthesise new ligands and metal-organic polyhedra, and perform their characterisation. In the first instance, this will include IR and NMR spectroscopy, and single crystal and powder X-ray diffraction. There may also be opportunities for gas sorption measurement, depending on the project progress, and possibly magnetic measurements using a SQUID magnetometer.

Qualifications:

The student should have some experience of practical chemistry - having done an undergraduate lab course ought to be enough. For example, they should be able to set up a reflux without requiring supervision.