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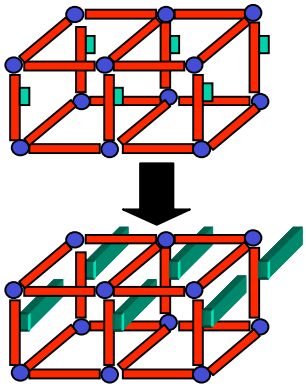
Controlled Modification of Metal-Organic Materials (Doing Reactions inside Crystals)

My groups work is centred in producing useful materials and molecules. We use principles of supramolecular chemistry and crystal engineering. The work interfaces organic and inorganic chemistry and deals with molecular recognition, host-guest chemistry, sensing, catalysis and bionanotechnology.

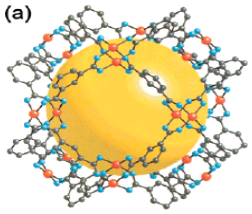


Metal-organic frameworks (MOFs)

MOFs are promising materials in areas as seemingly diverse as gas storage and drug delivery. The frameworks are composed of metal ions or clusters as vertices (blue dots) and divergent bridging ligands as linking struts (red rods). Within these crystalline solids the key property to many applications is porosity. My interests are directed toward preparing new porous materials and using the spaces created inside crystals to do chemistry in.

Tagging is a strategy to post-synthetically engender porous MOFs with more functionality. Schematically this is turning the small green rectangles into the blocks of the second structure in single-crystal-to-single-crystal transformations. I want to explore the limits of tagging methodology we have founded, answering the questions: What can be used as a tag? What reactions are possible to post-synthetically functionalise porous MOFs? There are multiple projects available in this area. See ref. 1 for an example of our work.

Metal-organic polyhedra (MOPs)



MOPs are not infinite networks but are discrete molecular entities and can be considered as being constructed from the self-assembly of edge sharing molecular polygons or the connection of molecular vertices. When built up from bridging ligands and metal-carboxylate clusters these structures are neutral, soluble in organic solvents and robust. Most importantly for my work they have internal spaces (the yellow sphere) suitable for doing chemistry inside. MOPs could conceivably be used as molecular containers for transporting or separating molecules and I'd like to look at applications of this, particularly toward catalysis and medicinal bionanotechnology. Several projects are available.

If you enjoy variety in synthetic work or want to choose a summer project that exposes you to a range of techniques then these projects should interest you. Most ligands require several steps of preparation. This will give you skills in organic synthesis and characterisation techniques. The preparation of MOFs and MOPs are solvothermal reactions, are very easy to carry out and will provide a different set of synthetic skills. The frameworks are solid crystals and will be examined by X-ray diffraction and, for viewing the materials at high resolution, a scanning electron microscope. Techniques such as NMR, IR, UV-Vis and Thermal Gravimetric Analysis (TGA) and electron dispersive X-ray measurements (EDX) will all be used in most projects. Many projects are potentially tailorable toward student interests.

[1] C. Richardson *et al. Angew. Chemie Int. Ed.* **2008**, *47*, 8482-8486.

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