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Research Interests: high-pressure crystallography, porous peptides, metal organic frameworks (MOFs).

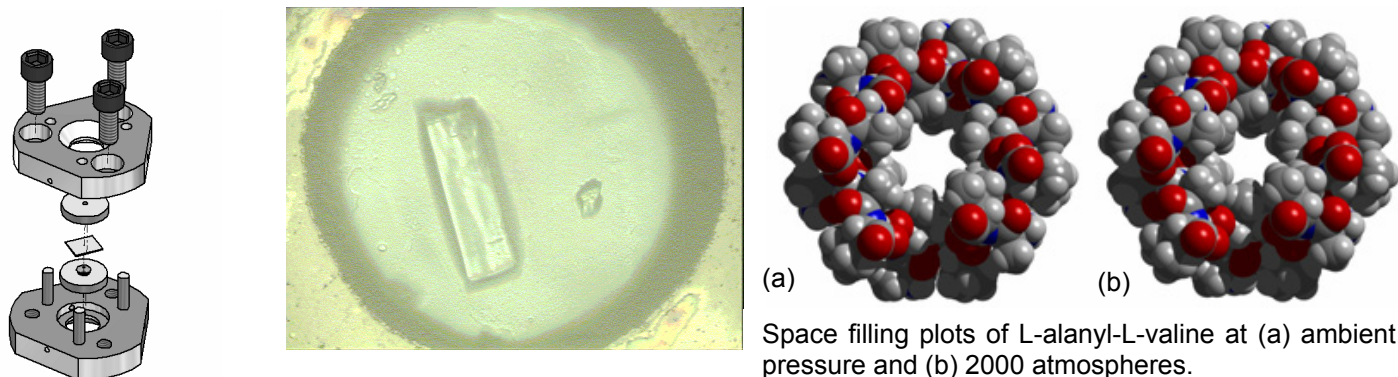


From the essential vacuum of space, to the pressures found at the centre of a neutron star, there are many more orders of magnitudes of pressure available to us in the Universe than there is temperature, and as a consequence we can induce far greater structural changes in materials by applying pressure. Application of pressure helps us understand the forces that hold molecules together to form solids, thereby enabling us to control and tune the properties of the solids themselves or the molecules they contain.

My current research is focussed on modifying the properties and selectivity of porous materials by applying pressure. Pore size determines the properties of these materials, and the aim of this research is to use pressure to modify properties through compression of pore size and shape.

The most familiar porous materials are zeolites, which have numerous applications including molecular sieves for selective absorption (e.g. for gas storage or water purification) and catalysis.

Although zeolites are well known, they form only one class of porous material. Molecular-based porous materials form an important growth area in crystal engineering, particularly for gas storage (e.g. H₂ storage materials) and for selective absorption; two classes of these materials are porous peptides and metal organic frameworks. These materials form large porous cavities, and are an attractive alternative to zeolites because they are not restricted to tetrahedral network topologies. For pressure modification, these materials are also ideal candidates as they are much softer than zeolites and therefore much more amenable to pressure modification (see Figure below).



The above left figure shows a schematic for a typical diamond anvil cell (DAC) which we use to apply pressure to our samples. The middle figure shows a single crystal sample of the amino acid L-serine at 40,000 times atmospheric pressure in the DAC. The figure on the right hand side shows the effect of pressure on the pore size in the crystal structure of the dipeptide L-alanyl-L-valine at 2000 times atmospheric pressure (note the large compression of the pore).

SELECTED RECENT PUBLICATIONS

1. Moggach, S. A.; Allan, D. R.; Parsons, S.; Warren, J. E. *J. Appl. Cryst.* **2008**, *41*, 249-251.
2. Moggach, S. A.; Parsons, S.; Wood, P. A. *Crystallogr. Rev.* **2008**, *14*, 143-184.
3. Prescimone, A.; Milios, C. J.; Moggach, S.; Warren, J. E.; Lennie, A. R.; Sanchez-Benitez, J.; Kamenev, K.; Bircher, R.; Murrie, M.; Parsons, S.; Brechin, E. K. *Angew. Chem., Int. Ed.* **2008**, *47*, 2828-2831.
4. Wood, P. A.; Francis, D.; Marshall, W. G.; Moggach, S. A.; Parsons, S.; Pidcock, E.; Rohl, A. L. *CrystEngComm.* **2008**, *10*, 1154-1166.