

Dr. Stuart Batten

B.Sc.(Hons) PhD (Melb.) GCHE

Keywords: Inorganic Chemistry, Crystal Engineering, X-ray Crystallography, Coordination Polymers, Supramolecular Chemistry

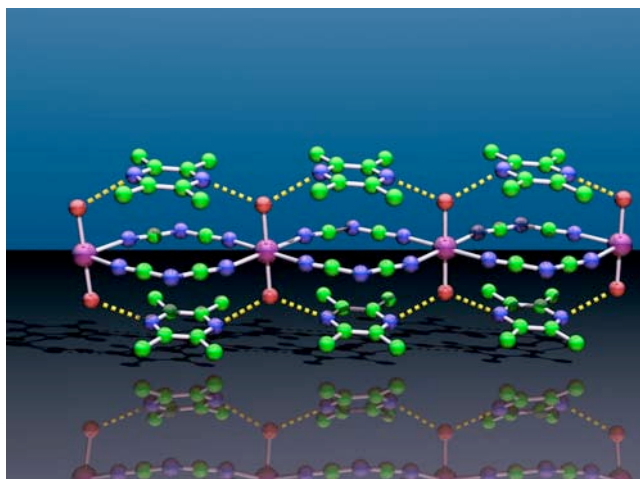
Web site:

<http://www.chem.monash.edu.au/staff/sbatten/>



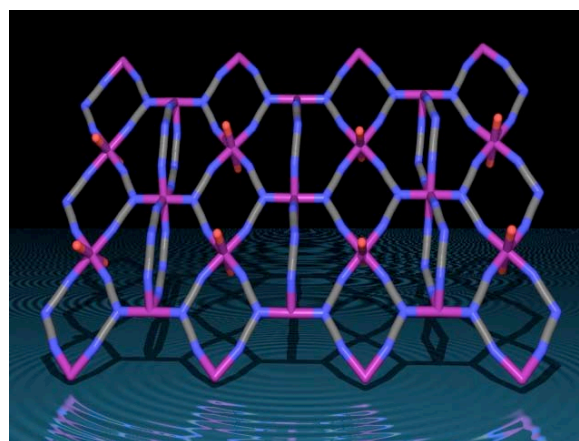
Crystal Engineering

The aim of crystal engineering is to control the way molecules assemble in the solid state. Since the properties of any material are largely due to its structure, control over the structure allows us to manipulate these properties. The crystal engineering of coordination polymers is of particular interest to our group. By judicious choice of preferred ligand and metal coordination geometries, control over the topology and geometry of the infinite networks can be gained. Such control allows the deliberate design of materials with a range of useful properties, including electronic properties, magnetic properties (long-range magnetic ordering, spin-crossover materials), microporosity (including the related properties of ion exchange and heterogeneous catalysis), non-linear optical effects and luminescent properties. We are currently developing a number of approaches to such materials.



Coordination Polymers of Pseudohalide Ligands

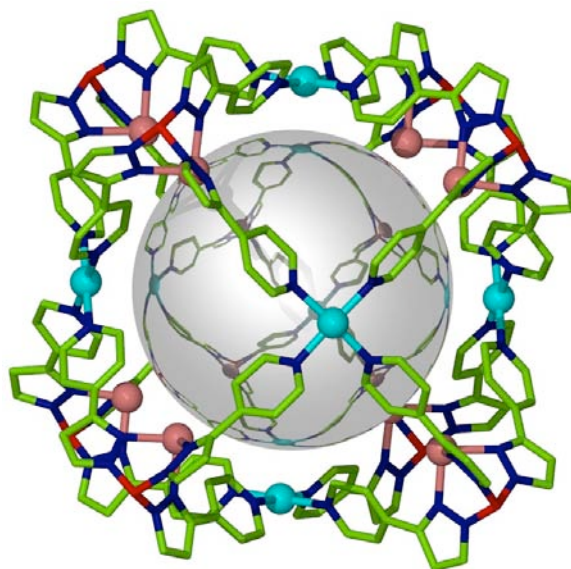
In particular, in conjunction with Prof. Keith Murray, we have been studying the structures and magnetism of coordination polymers of the less-common pseudohalide ligands, such as dicyanamide (dca , $\text{N}(\text{CN})_2^-$) and tricyanomethanide (tcm , $\text{C}(\text{CN})_3^-$). We have discovered a new class of magnetically ordering compounds that has sparked a surge in interest in dca coordination polymers. The α - $[\text{M}(\text{dca})_2]$ compounds all have rutile-like



structures in which octahedral metal centres are bridged by three-connecting dca ligands (which coordinate through all three nitrogen atoms). Despite their isomorphous structures, the magnetic properties vary widely: Cr, Mn and Fe are spin-canted antiferromagnets ($T_N = 47, 16, 19$ K), Co, Ni and Cu are ferromagnets ($T_c = 9, 21, 1.7$ K). We are now studying the effect that introduction of terminal or bridging coligands has on both the structure and magnetic properties. We have also found that anionic dca networks of $[M(dca)_n]^{(n-2)-}$, $n = 3, 4$ formulation have topologies dependant on cation choice – i.e. the networks are cation templated.

Chemically Active Coordination Polymers and Supramolecules

Despite the now extensive literature on coordination polymers and metallocupramolecules, there are few examples of these materials which show chemical activity after they are assembled. We are attempting to deliberately design ligands and complexes that will produce such higher assemblies which retain chemically active sites (e.g. coordination sites on metal atoms which are available for further chemical reactions; uncoordinated ligand donor atoms) after assembly. Such materials may be useful for homogeneous or heterogeneous catalysis, or as molecular sensors. One particularly interesting material is a self-assembled, nano-sized metallocupramolecule (2.9 nm external diameter) which contains 14 metal atoms and 8 ligands. The molecule has a hollow-ball shape like buckminsterfullerene (C_{60}), except it is large enough that it could potentially completely contain C_{60} in its internal cavity. The inner surface of the 'nanoballs' are decorated with potential coordination sites.



Selected Publications

1. "Structure and Magnetism of Coordination Polymers Containing Dicyanamide and Tricyanomethanide", S.R. Batten, K.S. Murray, *Coord. Chem. Rev.*, 2003, **246**, 103-130.
2. "Malleable Coordination Networks", S.R. Batten, K.S. Murray, *Aust. J. Chem.*, 2001, **54**, 605.
3. "Topology of Interpenetration", S.R. Batten, *CrystEngComm*, 2001, **3(18)**, 67.
35. "Coordination Polymers", S.R. Batten, *Curr. Opin. Solid State Mater. Sci.*, 2001, **5**, 107.
4. "Structure and Molecular Magnetism of the Rutile-Related Compounds $M(dca)_2$, $M = Co^{II}, Ni^{II}, Cu^{II}$, $dca = dicyanamide, N(CN)_2^-$ ", S.R. Batten, P. Jensen, B. Moubaraki, K.S. Murray, R. Robson, *Chem. Commun.*, 1998, 439.
5. "Interpenetrating Nets: Ordered, Periodic Entanglement", S.R. Batten, R. Robson, *Angew. Chem. Int. Ed.*, 1998, **37**, 1460.