MONASH University
Centre for Electron Microscopy

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Local structure and disorder in coordination frameworks

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Tuesday 26th July
1.30am – 2.30pm
MCEM Meeting Rm, Building 81
10 Innovation Walk, Monash University

Abstract and Bio

Coordination frameworks often mimic purely inorganic materials in both topology and functionality, and these links often extend beyond the realm of perfect crystalline order. Like the silicates, the zeolitic imidazolate frameworks form glasses; like the oxide perovskites, cyanide- and formate-linked perovskites exhibit dielectric phase transitions involving cooperativity between disordered cations within the framework. Understanding these materials' structure and functionality – and the ways in which these might be predictable from our knowledge of their inorganic analogues – will require us to understand their local as well as their average structure. An ideal experimental probe of disorder in both crystalline and amorphous framework materials is total neutron scattering, where both the Bragg peaks from the crystalline component of a sample and the diffuse scattering from the disordered component are measured. Reverse Monte Carlo analysis of the resulting data allows us to construct atomistic models that reproduce both the diffraction profile and the pair distribution function: in other words, both the material's average and its local structure. I will present total neutron scattering experiments illustrating the local structure of metal-organic silicate, perovskite, and elpasolite analogues. These results demonstrate the importance of considering local structure in attempts to design and engineer functional framework materials.

Anthony was born and grew up in Perth and studied at the Universities of Sydney (BSc 2006) and Cambridge (PhD 2011) before moving to Queen Mary, University of London, where he is currently Lecturer in Condensed Matter and Materials Physics. His research focuses on neutron scattering from functional materials, with a particular interest in disorder, phase transitions, low-dimensional magnetism, and other unusual behaviour in coordination frameworks.

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