1 Solid-State Molecular OrganoMetallic Catalysis: Crystalline Molecular Factories

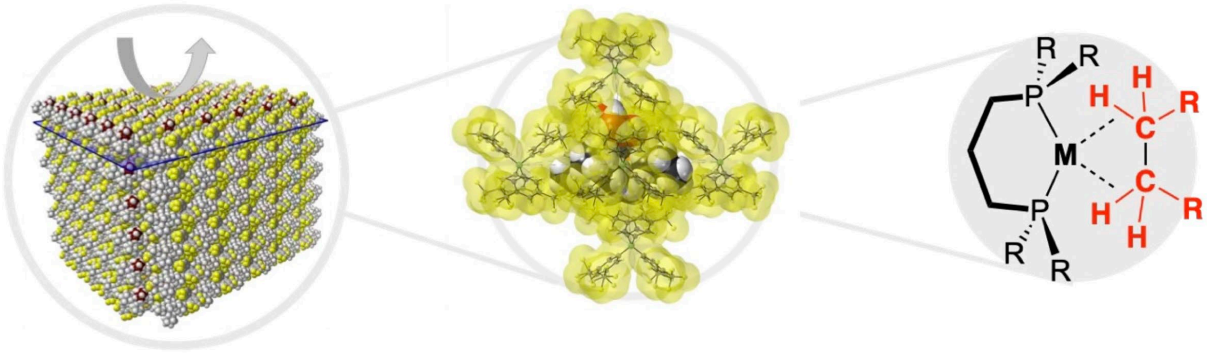
Andrew Weller

University of York, York, United Kingdom

Abstract

Organometallic synthesis and catalysis are normally performed in the homogeneous solution state, where the advantages of metal/ligand catalyst design provide exquisite control over fundamental mechanistic steps. Such control, through precise atomic placement, is more challenging for heterogeneous systems. Bridging the gaps between the two areas are supported molecular catalysts (surface organometallic catalysis) that lead to very active catalysts, but still present challenges in precise catalyst speciation and mechanistic elucidation. We have been developing an alternative approach to this challenge using, so-called, solid-state molecular organometallic chemistry (SMOM),[1] where synthesis and reactivity is studied *in crystallo* using well-defined organometallic complexes. These studies have focused on the synthesis and characterisation of highly reactive species that can be isolated using "crystalline matrix isolation methods". Consideration of the likely surfaces of such molecular organometallic crystals as single atom catalytic sites offers possibilities and opportunities for catalysis.

In this talk the SMOM approach to organometallic catalysis using 3D- and 2D- site-isolated reaction centres in single-crystals will be outlined by showcasing their use in three scenarios: The industrially-relevant ethene to propene (ETP) process, the catalytic generation of hyperpolarised gases for potential medical imaging applications, and the use of solution unstable Ir(II) open-shell complexes in catalysis.



Scheme Solid-state Molecular Organometallic Chemistry

[1] K. M. Altus, S. K. Furfari, J. C. Goodall, M. R. Gyton, J. H. Heaton, C. L. Johnson, A. I. McKay, M. Sondrup Møller, S. D. Pike and A. S. Weller *Dalton Trans.* 2026, **55**, 6649