Department of Chemistry: Part III Project 2017/18

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Metal Oxide Clusters: Materials at the Molecular Scale

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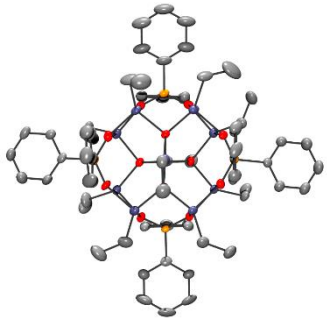
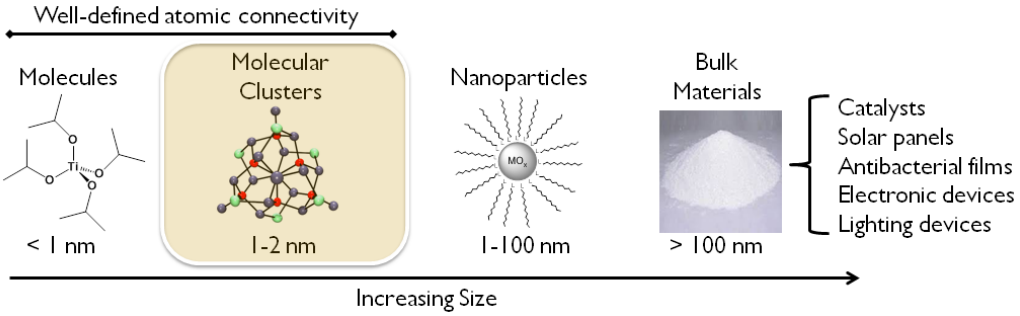
When does a molecular cluster start behaving like a bulk material? How does size effect a material's properties? A part III project student will investigate these ideas by building metal-oxide clusters from organometallic precursors.[1] Metal-oxide materials find applications in photovoltaic devices, heterogeneous catalysts, antibacterial surfaces, and even self-cleaning windows. By studying well defined molecular analogues we aim to examine some of these processes at the atomic level. Molecular clusters can be identified and studied by NMR spectroscopy and X-ray crystallography. We also use UV light to excite clusters into high energy states for use in photocatalysis or as photoluminescent materials - this can be thought of as analogous to promoting valence electrons into the conduction band in a semiconducting metal-oxide material.

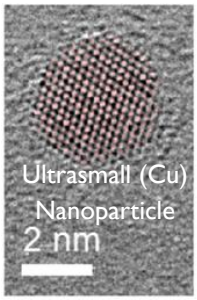


Zn-O cluster formed during the synthesis of ZnO nanoparticles



Potential projects:

Photoluminescent Copper Clusters. Cu is a cheap and available metal and shows promise in photoluminescent materials which may be developed into next generation LEDs.[2] You will use reactive organocopper reagents to build Cu oxide clusters ligated by phosphines, and test for luminescent properties. The growth and reactivity of these clusters can be followed by ^{31}P NMR spectroscopy.



Silver Oxide Nanoparticles. Ag_2O is a narrow band gap material that can absorb visible light, and is therefore of interest in photoelectronic devices. You will investigate forming clusters and ultrasmall (1-3 nm, 50-1000 atoms) nanoparticles (NPs) from organo-silver precursors,[3] and then determine how quantum confinement changes the properties of such small particles in comparison to bulk Ag_2O.

Seb is a Herchel-Smith Research Fellow with a newly formed research group. In joining the group you will be a crucial member of the research team and will work closely with Seb. We join the Wright group for group meetings and social events.

1. S. D. Pike, E. R. White, M. S. P. Shaffer and C. K. Williams, *Nat. Commun.*, 2016, **7**, 13008.
2. D. Di, A. S. Romanov, L. Yang, J. M. Richter, J. P. H. Rivett, S. Jones, T. H. Thomas, M. Abdi Jalebi, R. H. Friend, M. Linnolahti, M. Bochmann and D. Credgington, *Science*, 2017, **356**, 159-163.
3. S. D. Pike, E. R. White, A. Regoutz, N. Sammy, D. J. Payne, C. K. Williams and M. S. P. Shaffer, *ACS Nano*, 2017, **11**, 2714-2723.