Exploring chemical function in structurally disordered systems

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Over the past decade, the inexorable trends in the exploitation of structurally disordered systems for chemical synthesis and action, have highlighted an increasing need for analytical methods that can provide a holistic view of atomic and molecular structure. Atomistic models driven for consistency with diffraction data [1] have proven to be a powerful window into this world, and particularly when enhanced via reference to complementary information drawn from other experimental probes such as X-ray absorption spectroscopy or small angle scattering. In this presentation I will outline the basis of these methods and illustrate their application to questions in chemical science on length scales ranging from the atomic and molecular, to the chemically engineered nanoscale. Examples will include investigations of chemical speciation and interactions [2], molecular liquid nanostructure [3], nanoparticle growth and templating [4], and molecular adsorption [5], as well as addressing questions such as "How much disorder is too much disorder?" or "What kind of influence can a support matrix have on chemical or physico-chemical outcomes?". The presentation will conclude with a few thoughts and remarks on the new directions these techniques are taking, and the challenges that are driving their evolution.

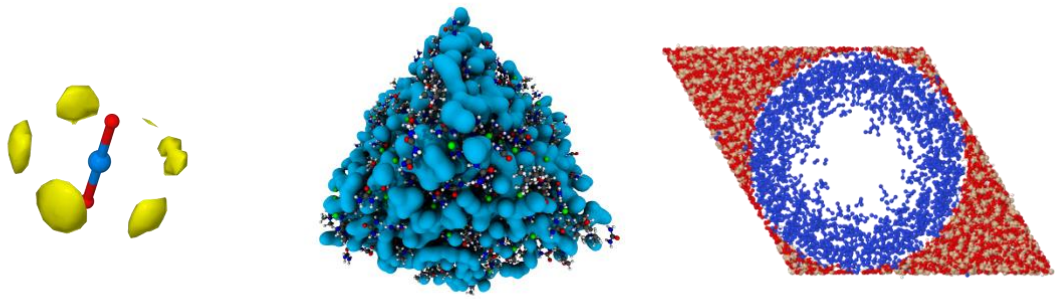

Figure 1. Examples of structurally disordered systems characterised by refinement against diffraction data, from left to right (i) the structure of the UO_2^{2+} aqua-ion [2], (ii) the structure of a hydrated deep eutectic solvent [3], and (iii) the structure of liquid nitrogen confined with MCM-41 silica [5].

[1] *Experimentally consistent atomistic modelling of bulk and local structure in liquids and disordered materials by empirical potential structure refinement.* Daniel T. Bowron, *Pure Appl. Chem.* **80** 1211 (2008)

[2] *Insights into the solution structure of the hydrated uranyl ion from neutron scattering and EXAFS experiments.* Samuel J. Edwards, Daniel T. Bowron and Robert J. Baker, *Dalton Trans.* **51**, 13631 (2022)

[3] *The effect of water upon Deep Eutectic Solvent nanostructure: An unusual transition from ionic mixture to aqueous solution*. Oliver S. Hammond, Daniel T. Bowron, and Karen J. Edler, *Angewandte Chemie Int. Ed.***56** 9782-9785 (2017)

[3] *Structural evolution of iron forming iron-oxide in a deep eutectic-solvothermal reaction*. Oliver S. Hammond, Ria S. Atri, Daniel T. Bowron, Liliana de Campo, Sofia Diaz-Moreno, Luke L. Keenan, James Doutch, Salvador Eslava and Karen J. Edler, *Nanoscale* **13** 1723 (2021)

[4] *Adsorption of simple gases into the porous glass MCM-41*. Alan K. Soper and Daniel T. Bowron, *J. Chem. Phys.* **154** 184503 (2021)