Disorder-property relationships in strongly-correlated materials

A. R. Overy[1,2], C. Romao[1], A. Simonov[1], E. H. Wolpert[1], M. G. Tucker[3], P. A. Chater[2] and A. L. Goodwin[1]

[1]*Department of Chemistry, University of Oxford, South Parks Road, Oxford, OX1 3QR, UK*

[2]*Diamond Light Source, Chilton, Oxfordshire, OX11 0DE, UK*

[3]*Oak Ridge National Laboratory, 1 Bethel Valley Road, Oak Ridge, TN, 37830, USA*

alistair.overy@chem.ox.ac.uk

The link between structural order and physical characteristics of materials is well-established—many physical properties (e.g. piezoelectricity) can be targeted through specific ordered arrangements of atoms. By contrast the disorder-property relationship is relatively poorly-understood. It is anticipated that structural disorder will have an effect on collective properties such as lattice vibrations, electronic states and photonic properties. However, the exact role of disorder is notoriously difficult to ascertain both computationally and experimentally, chiefly because of the inherent structural complexity when periodicity is lost. Nevertheless, this is an important area of study as disorder is known to be a key factor in the physics of exotic functional materials including displacive disorder in high temperature superconductors [1] and dipolar disorder in ferroelectrics [2] and thermoelectrics [3].

This talk will explore the way in which different disorder correlations alter the collective physical properties of materials in meaningfully different ways. We calculate the vibrational, electronic and photonic band structure of a series of related systems, chosen in such a way as their average (long-range) structures are identical, but with different models reflecting meaningfully different types of disorder.

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