Using Neutron Scattering and Quantum Chemistry to Optimise Composites and Tune Catalyst Selectivity

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Librational and low-energy vibrational (i.e. far-infrared) phenomena have long been associated with functional properties of material and molecular systems. However, accessing this 'fingerprint' region by standard spectroscopic methods is hindered by selection rules, sensitivity and energy resolution. Neutron scattering methods provide a solution, with associated phenomena now spatially, energetically and temporally intelligible in conjunction with chemical modeling.

To these ends, we computationally designed and carried out a series of inelastic neutron experiments. Of which, a widely used bio-cement, in addition to Portland construction were analysed towards understanding changes in material properties during setting on the VESUVIO neutron compton and NIMROD small-angle neutron scattering experimental setups. Likewise, the TOSCA indirect-geometry experimental setup was used to characterise low energy dynamics of cross-coupling catalysts employed in the production of functional materials

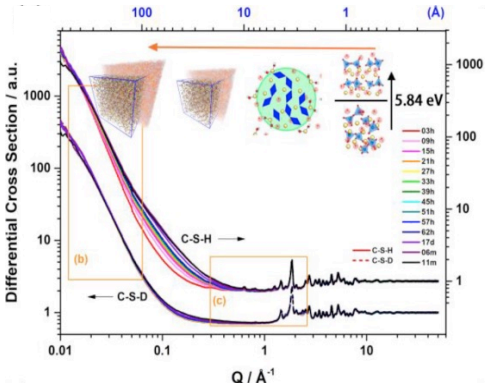

Fig.1: Our results*: SANS/WANS tracking particle growth (0-12 month) over setting of H_2O vs. D_2O cements. complementary models of atomistic 0.1 - 2 nm) through mesoscopic scales (1 - 30 nm).*

Results derived on VESUVIO and NIMROD allowed for quantitative tracking in real-time of kinetic energy for each atom, and atomistic to mesocscopic interfacial structures in the composite cement (**Fig.1**). Atom-specific bonding strengths were subsequently derived and tracked over the course of the setting reaction, showing the polymer component's C-C and C-O bonds as the major contributors 'providing toughness' to the composite bulk.

TOSCA results showed catalyst performance to be a function of cooperative dynamics. Quantification of each molecular component's contribution to the overall systemic properties of 3 cross-coupling catalyst families revealed low-energy vibrational modes (terahertz) to be intimately coupled to reaction pathway preference in each family.

The talk provides an overview of the successful application of quantum theory in the design of effective neutron beam experiments in catalysis and composites.