Neutron Scattering and Quantum Chemistry Track Terahertz-Driven Phenomena

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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 quantum theory.

We used quantum chemical methods to design and guide a series of inelastic neutron experiments at the pulsed neutron and muon facility at the Rutherford Appleton Laboratory (RAL, Oxfordshire, UK). A widely-used bioactive composite was analysed towards understanding changes in material properties during setting on the VESUVIO neutron compton scattering experiment. 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

Results derived on VESUVIO allowed for quantitative tracking in real-time of kinetic energy for each atom in the composite cement. 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 uncovering THz-driven phenomena in catalysis and composites.