Structure of industrially relevant sp2 carbon using wide *Q*-range neutron total scattering: From bitumen to batteries via benzene

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Beyond crystalline graphite, planar sp2 hybridized carbon can make a wide array of different structures and therefore materials: From geologically formed asphaltenes, to new synthetic materials such as carbon nanotubes. Many of these materials are non-crystalline, making non-ambiguous structural determinations is therefore difficult. In this talk we will outline the combined use of wide *Q*-range total scattering, H/D isotopic substitution and classical molecular simulation to make progress in characterizing the structure in these industrially relevant materials.

We have studied the simplest sp2 carbon molecular liquids, the aromatics such as benzene, using Empirical Potential Structure Refinement (EPSR) methods. This reveals a complex mixture of local structures resulting from a delicate balance of different intermolecular interactions, rather than just archetypal pi-pi stacking [1]. We have pushed this approach to larger lengthscales using data from the NIMROD instrument at ISIS, with a simultaneous *Q*-range of 0.02-50Å^{-1}, allowing us to study the complex solvation structure of carbon nanotubes in amide solvents [2]. A molecular dynamics simulation-based approach has been extended to a considerably more complex set of aromatics, the asphaltenes, a heavy component of crude oil and bitumen, with a propensity to precipitate in oil recovery and refining. Simulations show a close match to the neutron scattering data, apart from at the lowest *Q*-range explored by NIMROD, due to the limited simulation size [3]. Finally, we will present recent *operando* studies of hard-carbon battery anodes on NIMROD. These promising materials comprise disordered nano-graphic domains allowing sodiation within the graphitic regions and nano-pores. The wide simultaneous *Q*-range of NIMROD affords a unique view of subtle changes at the atomistic and pore-scale during charge and discharge.

[1] T. F. Headen *et al*, *JACS*, **132**, 5735 (2010). T. F. Headen *et al*, *PCCP*, **20,** 2704 (2018)
[2] C. Di Mino *et al*, ChemArXiv 2023, doi:10.26434/chemrxiv-2023-pmkhn
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