**Dispersion Modelling of Polyaromatic Compounds**

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Polyaromatic compounds are encountered in a range of industries from pharmaceuticals to fuels. Unlike ultrapure organic compounds synthesized for pharmaceuticals, fuel-based polyaromatic compounds have been shown to exhibit > 20,000 distinct structures, making any prediction of solution behavior extremely challenging. Our recent work has shown the stability of fuel-based polyaromatic species is strongly influenced by the chemical architecture of the molecule, with certain molecule features appearing to promote the formation of nanoaggregates which deteriorates the fluid performance. In the current project we will combine modelling and experiments to better understand the different aggregation routes when the chemical architecture of the molecule is systematically transformed. To provide clarity on these aggregation routes, a big-data approach will be adopted combining grid-based molecular modelling and high-fidelity experiments (FT-ICR-MS, XPS, NMR, and SANS) to study model compound structures and native species present in fuels. A successful outcome of the project will provide clarity on the dominant aggregation routes such that preventative measures can be designed to achieve long-term fluid performance.