Investigating the self-assembly and structure of nanoparticles containing curved carbons

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Curved carbon materials arise from the inclusion of non-hexagonal rings within a hexagonal lattice and exhibit unique steric and electronic properties. These fullerene-like molecules are candidates for many applications including gas storage, batteries, imaging probes, and targeted nanomedicine. Development of these technologies requires an understanding of the self-assembly and dynamic nanostructure of particles containing curved carbons, which has not yet been well explored.

This work uses advanced molecular dynamics simulations to explore the nucleation behaviour and properties of nanoparticles containing curved carbons. Intermolecular interactions were described using the recently developed curPAHIP potential able to capture the enhanced interactions of curved aromatics. Large timescales and temperature ranges were sampled to provide insight into the dynamic behaviour of curved aromatics in homogeneous systems as well as those containing planar molecules and cations. It was seen that heterogeneity has a significant effect on particle nucleation, with electrostatic interactions between polar components dominating. The size and ratio of constituent fullerene-like molecules have significant effects on the internal structure and surface properties of nanoparticles. These results provide information on the self-assembly of curved carbons, as well as insight into the energetic and structural properties of the resulting nanoparticles, useful for an accurate understanding of the dynamic nature of these systems.