Self-assembly and properties of carbon nanoparticles containing fullerene-like molecules

Kimberly Bowal[1], Laura Pascazio[1], Jacob W. Martin[1,2], Markus Kraft[1,2,3]

[1]Department of Chemical Engineering and Biotechnology, University of Cambridge, UK
[2]Cambridge Centre for Advanced Research and Education in Singapore (CARES), Singapore
[3]School of Chemical and Biomedical Engineering, Nanyang Technological University, Singapore

The structure and properties of self-assembled nanoparticles containing curved polycyclic aromatic hydrocarbons (cPAHs) are investigated using molecular modelling. Due to the inclusion of one or more five-membered rings within their hexagonal lattice, these polar fullerene-like molecules possess unique steric and electronic properties that make them good candidates for many applications including microporous materials for gas storage, organic electronic devices such as imaging probes and batteries, sensors, and micelles for targeted nanomedicine. Development of these applications requires an understanding of the self-assembly and dynamic nanostructure of cPAH nanoparticles, which has not yet been well explored.

This work uses replica exchange molecular dynamics to determine the energy-dependent nanostructure of cPAH particles. The interactions between cPAH molecules is described using the new curPAHIP potential. A range of cPAH sizes and ratios are investigated, along with systems containing planar PAHs and ions, to explore the homogeneous and heterogeneous particle internal arrangements and properties.

Homogeneous cPAH particles are found to be tightly packed and less stacked than their planar PAH counterparts. The constituent cPAH size plays a role in the molecular arrangement, with larger cPAHs displaying long-range order absent in the small cPAH nanoparticles. Binary particles containing cPAHs of different sizes, such as those shown in Figure 1, display a core-shell structure in which the larger molecules make up the core and the smaller molecules comprise the shell, as seen with planar PAH nanoparticles. This trend is not strongly influenced by the molecule ratio. In addition, the presence of planar PAHs and ions within cPAH nanoparticles promotes arrangements likely to be indicative of mixed systems.

These results provide new information on structures and properties of nanoparticles containing cPAHs, including density, molecular structure, surface composition, and melting point estimation. This provides valuable understanding of the self-assembly and growth of nanoparticles with great potential in many applications.

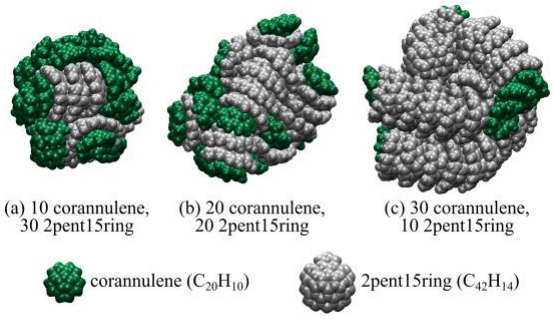

Figure 1: Stable configurations of heterogeneous cPAH clusters containing 40 molecules of corannulene and 2pent15ring molecules in different molecular ratios. Smaller corannulene molecules are coloured green and larger 2pent15ring molecules are coloured grey.

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