Self-assembly of curved aromatic molecules in soot particles
Kimberly Bowal, Jacob Martin, Markus Kraft
Computational Modelling Group, Department of Chemical Engineering and Biotechnology, University of Cambridge

1. Introduction
Curved polycyclic aromatic hydrocarbons (cPAHs) make up a significant portion of young soot particles. The flexoelectric effect gives cPAHs increased steric and electrostatic properties. Most molecular soot models include only flat aromatics (fPAHs), so little is known about the structure of nanoparticles containing cPAHs.

Detailed molecular dynamics simulations provide insight into the structure of clusters containing curved polycyclic aromatic hydrocarbons.

2. Methods
Employed replica exchange molecular dynamics with new curPAHIP potential for cPAHs.

Have a question? Or just want to chat? Please send me a message!
kib83@cam.ac.uk

3. Do cPAHs self-assemble into an ordered phase?
Molecular arrangement is primarily dependent on molecule size.

Large cPAHs form ordered stacks
Small cPAHs form disordered arrangements

Alignment angles within nanoparticles are similar to crystal structures (dashed lines)

4. What is the internal nanostructure of cPAH particles?
Mixing small and large cPAHs disrupts mesophase formation.

Molecules partition into a core-shell arrangement

Particle energy is highly dependent on cPAH sizes

5. How do complex cPAH particles self-assemble?
Effect of cations depends on constituent cPAH size.

Cations disrupt large cPAH stacking
Cations promote small cPAH ordering

Curved and flat molecules self-assemble into janus particles

References