Investigating the self-assembly and structure of nanoparticles containing fullerene-like molecules

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Outline

- Fullerene-like molecules
- Nucleation
- Nanostructure

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Fullerene-like molecules

Curvature is caused by the presence of pentagonal ring(s) within a hexagonal structure

**CORONENE**

Coronene

**CORANNULENE**

Corannulene

Curvature causes a dipole moment due to the polarisation of $\pi$ electrons from the concave to convex surface

Interact with ions?

Motivation

• Expect a significant impact on systems containing curved aromatics such as:
  – Microporous materials: gas storage, separation
  – Organic electronic devices: imaging probes, batteries
  – Nanoparticle formation: soot, carbon blacks, atmosphere
  – Nanomedicine: sensors, targeted micelles

• Development requires understanding of self-assembly and dynamic nanostructure of curved aromatics
Nucleation: System description

- New curPAHIP potential
- 500 - 1500 K
- 1000 molecules
- 4 cases:
  1. Planar aromatics
  2. Curved aromatics
  3. Planar aromatics with $K^+$
  4. Curved aromatics with $K^+$
Molecular dynamics simulation videos

Curved aromatics without $K^+$

Curved aromatics with $K^+$

Bowel, K., Martin, J. W., Misquitta, A. J., & Kraft, M. *Comb Sci & Tech* (2019)
Curved aromatics and K$^+$ show greatest ability to form clusters

Molecular arrangement maximises electrostatic interactions
SLIDES 8 – 13 OMITTED
(UNPUBLISHED WORK)
Curved aromatic molecules have a significant dipole moment due to the shift of electrons between curved surfaces.

Enhanced interactions promote nucleation of curved aromatics around ion.
Thank you

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