

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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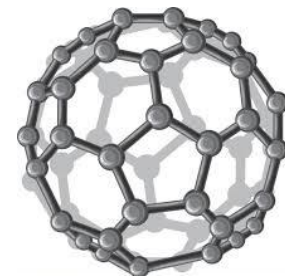
Laura
Pascazio



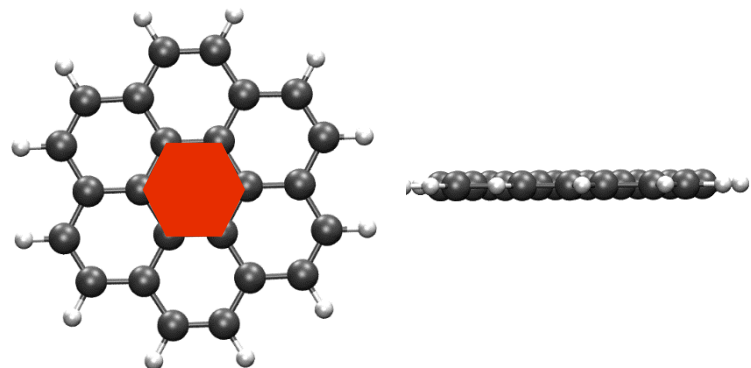
Markus
Kraft

Fullerene-like molecules

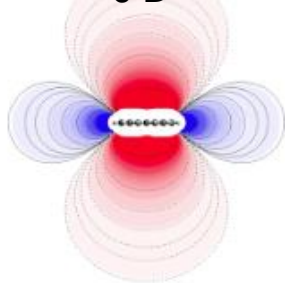
Curvature is caused by the presence of pentagonal ring(s) within a hexagonal structure



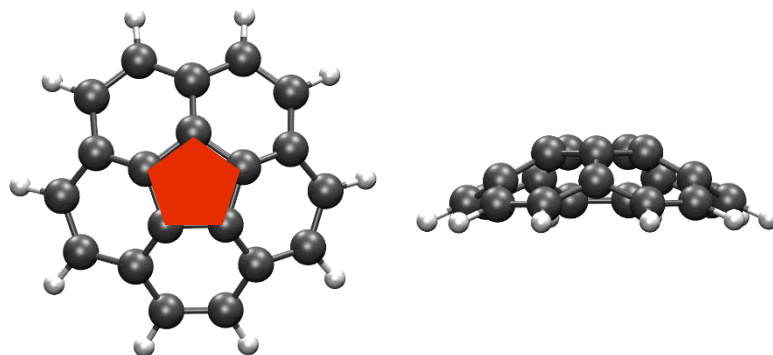
CORONENE



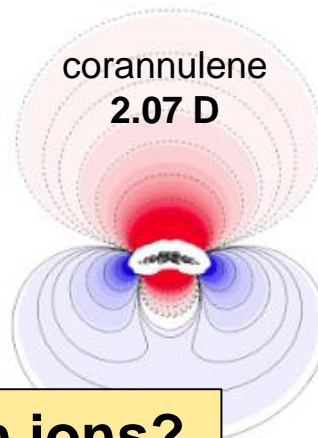
coronene
0 D



CORANNULENE



corannulene
2.07 D

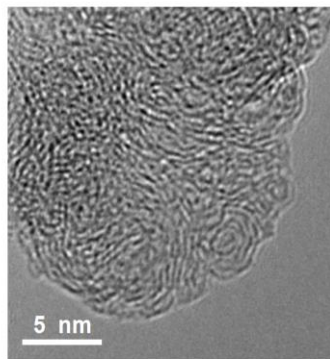


Interact with ions?

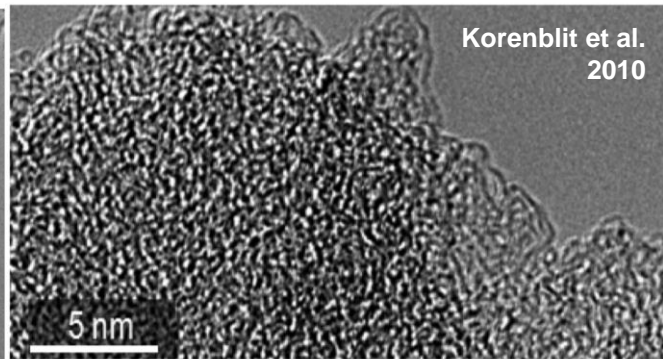
Curvature causes a dipole moment due to the polarisation of π electrons from the concave to convex surface

Motivation

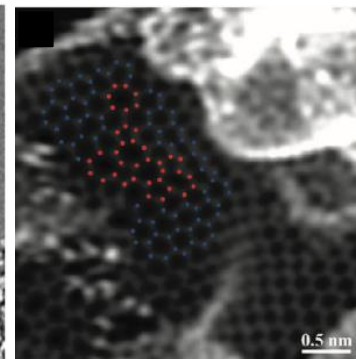
- Expect a significant impact on systems containing curved aromatics such as:
 - Microporous materials: gas storage, separation
 - Organic electronic devices: imaging probes, batteries
 - Nanoparticle formation: soot, carbon blacks, atmosphere
 - Nanomedicine: sensors, targeted micelles
- Development requires understanding of self-assembly and dynamic nanostructure of curved aromatics



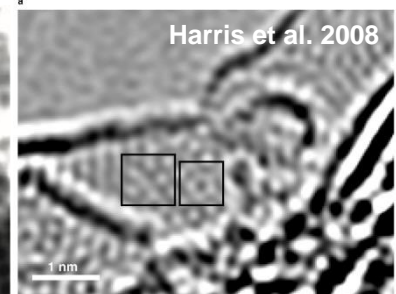
soot



battery electrode



charcoal

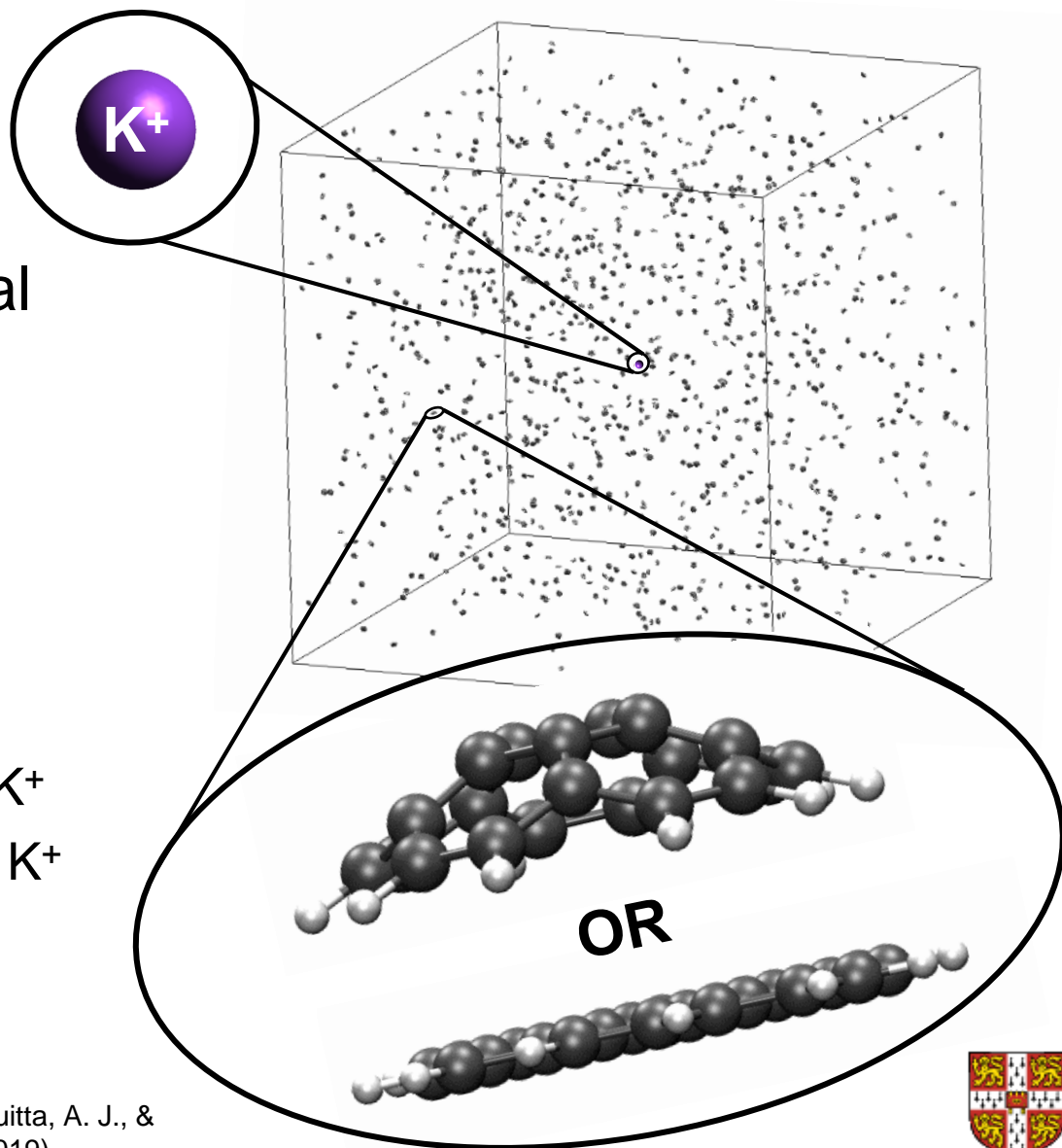


activated carbon

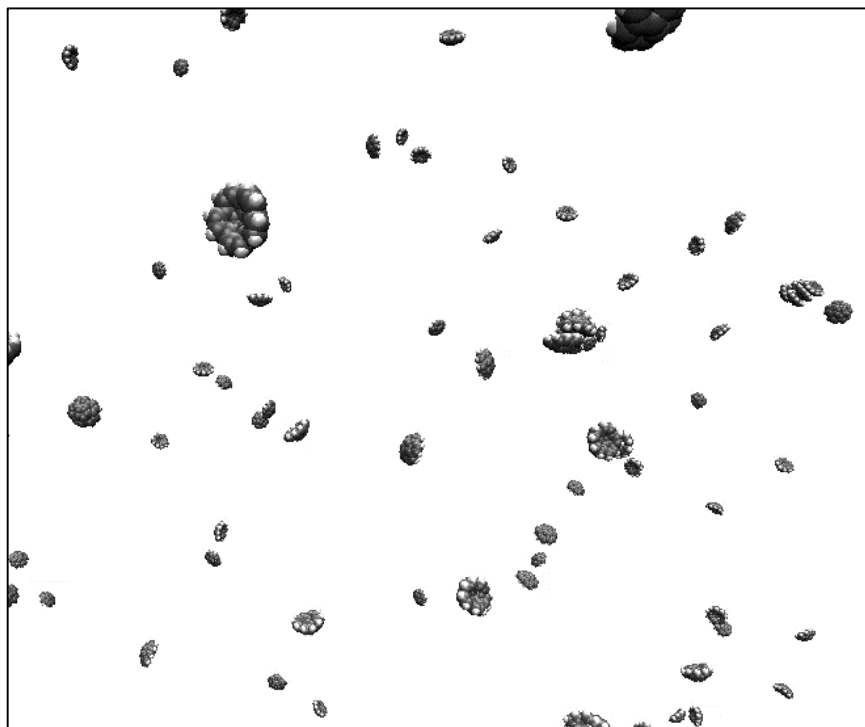


Nucleation: System description

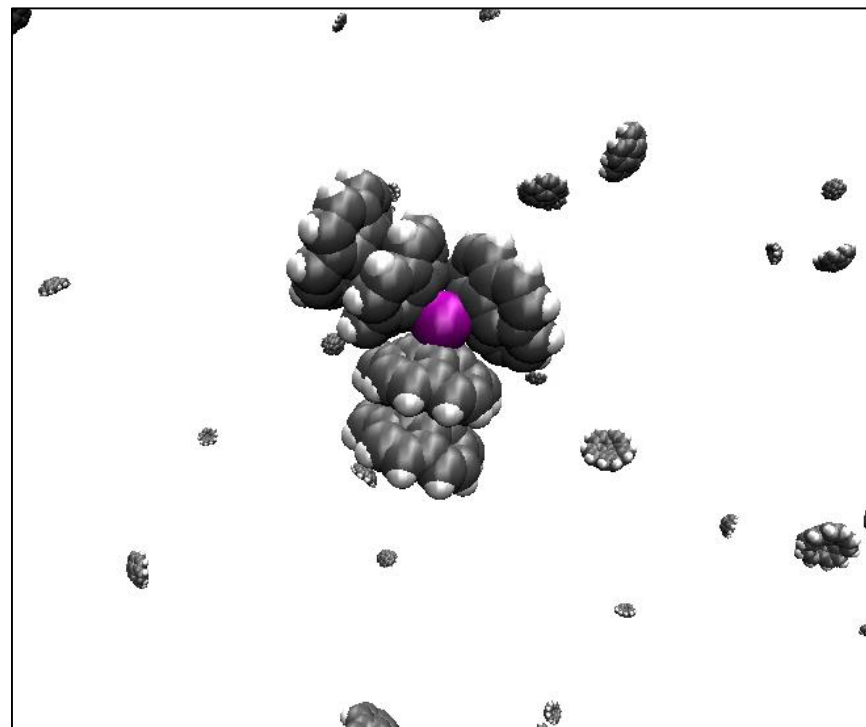
- New curPAHIP potential
- 500 - 1500 K
- 1000 molecules
- 4 cases:
 1. Planar aromatics
 2. Curved aromatics
 3. Planar aromatics with K^+
 4. Curved aromatics with K^+



Molecular dynamics simulation videos

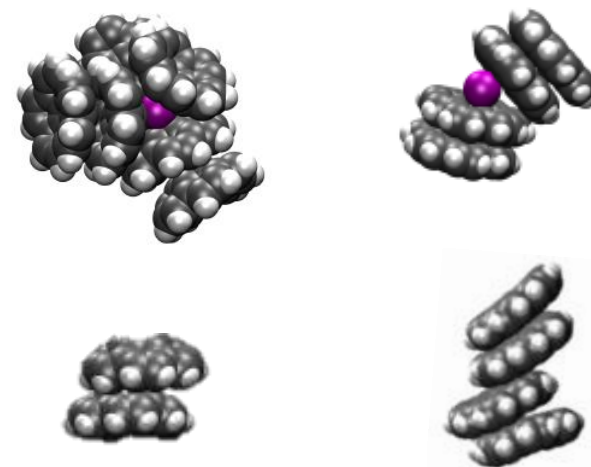
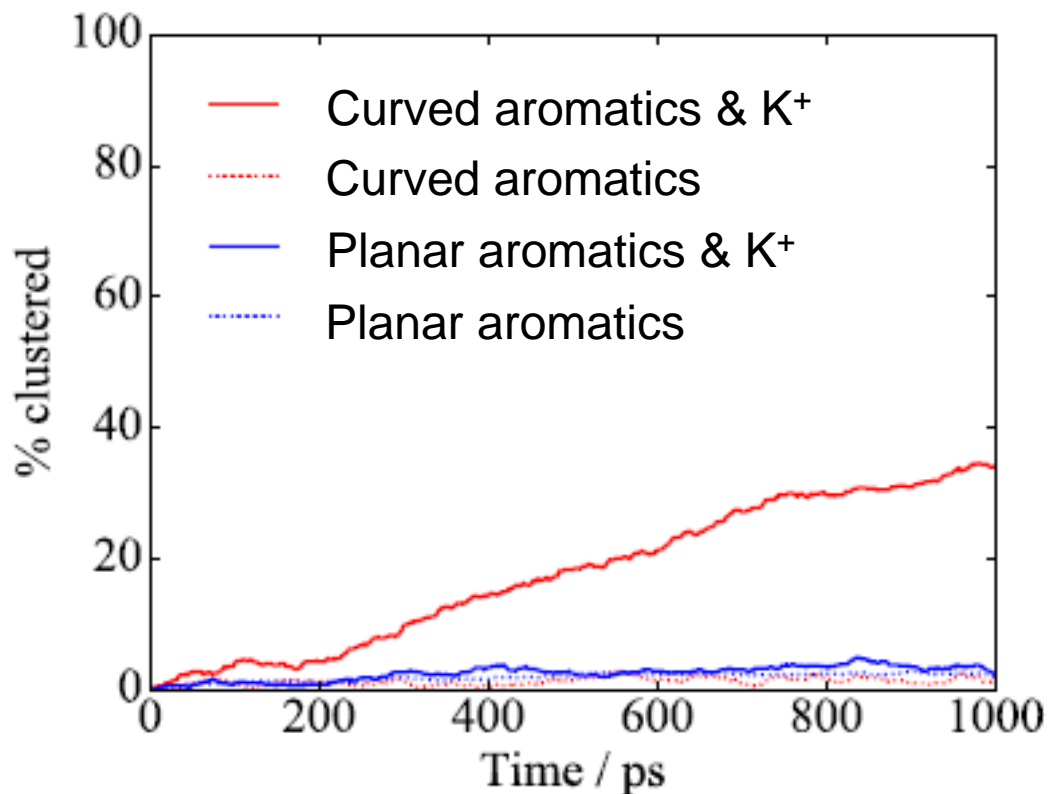


Curved aromatics
without K^+



Curved aromatics
with K^+

Clustering results

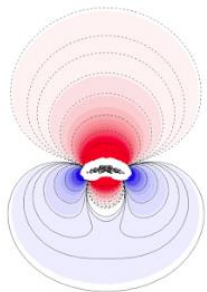


Molecular arrangement
maximises electrostatic
interactions

Curved aromatics and K⁺ show greatest ability to form clusters

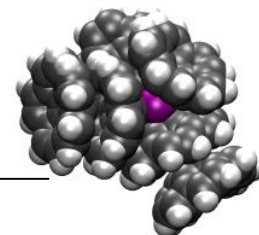
SLIDES 8 – 13 OMITTED
(UNPUBLISHED WORK)

Summary

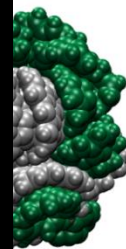


— Curved aromatic molecules have a significant dipole moment due to the shift of electrons between curved surfaces

Enhanced interactions promote nucleation of curved aromatics around ion —



OMITTED – UNPUBLISHED WORK



Thank you

Contact Kimberly Bowal at klb83@cam.ac.uk

