**Optimal configurations of polycyclic aromatic hydrocarbons inside single-walled carbon nanotubes**

*Kyle StevensA, Ngamta ThamwattanaA*

ASchool of Mathematical and Physical Sciences, University of Newcastle, Callaghan, Australia

**Introduction**

Polycyclic aromatic hydrocarbons (PAHs) are compound of hydrogen and carbon atoms that are composed of aromatic rings. Examples include pyrene, naphthalene and anthracene. In Tran-Duc *et al.* (2011) benzene is modelled as concentric rings, namely inner carbon rings and outer hydrogen ring. This idea can be extended to larger circular shaped PAHs, such as coronene, corannulene, hexabenzocoronene. In this study, we assume a uniform distribution of atoms on PAHs, so we consider a circular shaped PAHs as a disk. We then compare our result with the concentric ring model.

Here, using a continuum approach, we present a mathematical model for the interaction between a nanotube and an encapsulated coronene. In particular the relationship between the radius of the nanotube and the minimum energy configuration of the PAH is explored.

**Methods**

The carbon nanotube is approximated as a hollow cylinder and the coronene molecule is assumed to comprise either four concentric rings (three carbon and one hydrogen rings) or a homogenous disk. The intermolecular potential is then derived using the Lennard-Jones potential, integrating over the surfaces of the molecules instead of summing the discrete atomic potentials. These integrals are solved analytically, resulting in explicit expressions relating the energy to the radius of the nanotube, the radius of the coronene, the tilted angle of the coronene and the displacement of the coronene from the tube’s central axis. These expressions are then analysed using a software package Maple where parameters of interest, such as minimum energy configurations, can be easily computed.

**Results**

For coronene with its centre fixed on a nanotube’s central axis, the ring approximation predicts that for all tubes with radii between 6.84 Å and 7.65 Å the lowest energy configuration occurs when the molecule is tilted between 0 and π/2 radians. For radii smaller than 6.84 Å, the coronene lies flat while for radii larger than 7.65 Å, the coronene orients perpendicularly to the tube’s axis. The disk approximation predicts the tilting to occur in the tubes with radii between 7.06 Å and 7.96 Å.

For the off-axis case, the disk approximation predicts that the coronene will move off axis in a tube with radius larger than 7.48 Å. Beyond 8 Å, the off-axis configurations start having equivalent energies to the standing on-axis configuration. The same off-axis behavior is found in the ring approximation.

**Discussion/Conclusion**

The range of tube radii that give the tilting regime in the ring approximation are in good agreement with DFT simulations performed by Anoshkin *et al*. (2014). The disk approximation gives ranges that are slightly different, though it is expected that the accuracy will increase as the size of PAHs increases.

The major results obtained here are the equivalent lowest energy configurations between lying off-axis and standing on axis at certain tube radii. This result may be useful for designing memory devices as outlined in Cox *et al.* (2008) where orientations of spheroidal fullerenes both on and off-axis are considered.

**References**

- Anoshkin, Ilya V., et al. "Coronene Encapsulation in Single‐Walled Carbon Nanotubes: Stacked Columns, Peapods, and Nanoribbons." *ChemPhysChem* 15.8 (2014): 1660-1665.

- Cox, Barry J., et al. "Orientation of spheroidal fullerenes inside carbon nanotubes with potential applications as memory devices in nano-computing." *Journal of Physics A: Mathematical and Theoretical* 41.23 (2008): 235209.

- Tran-Duc, Thien, et al. "Orientation of a benzene molecule inside a carbon nanotube." *Journal of Mathematical Chemistry* 49.6 (2011): 1115-1127.