Molecular modeling of aromatic interactions between pyrene derivatives and carbon nanotubes

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Abstract

Magnetic Resonance Imaging (MRI) is the most useful method for clinical diagnosis. Effectiveness of diagnosis by MRI is joined to the design of new MR sequences as well as the development of new Contrast Agents (CAs) increasing the quality, resolution and specificity of the MR images.[1] In a previous work we have used paramagnetic carbon nanotubes and diffusion weighted MR imaging methods to investigate the preferred direction of blood flow.[2] To increase solubility and paramagnetic character of MWNTs we have designed and synthesized a new generation of CAs based on labeled Gd(III) MWNTs through π−π stacking interactions with pyrene derivatives. Here, we present the results obtained from a theoretical study of the interactions between (6, 6) armchair nanotubes and several pyrene derivatives. We have placed pyrene, aminopyrene and nitropyrene molecules in different orientations over a (6, 6) CNT surface (see figure 1) and performed DFT[3] calculations to get a good understanding of the noncovalent functionalization of the outer surface of carbon nanotubes by these molecules. The analysis of the calculated binding energies, electrostatic potential surfaces (figure 2) and Mulliken charges can help us to shed some light on the way these aromatic systems interact.

References

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Figure 1. Parallel and perpendicular orientations of aminopyrene and nitropyrene relative to a (6, 6) CNT surface.

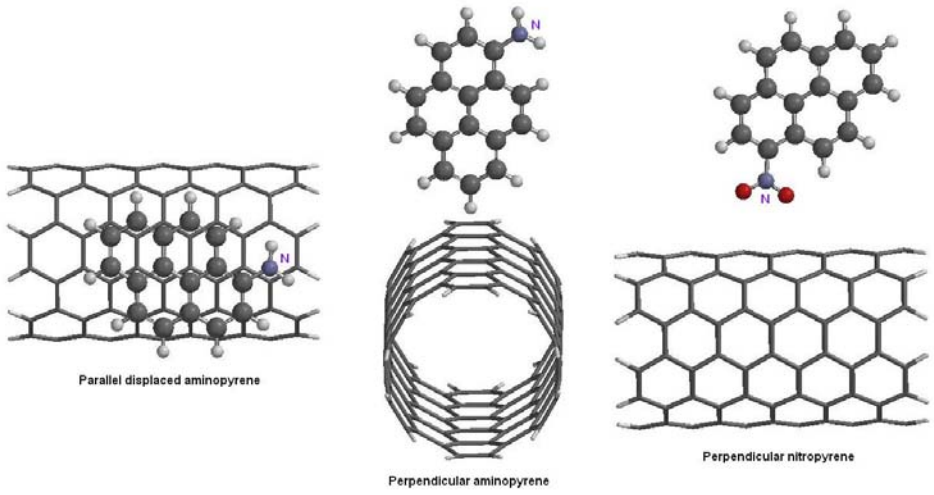

Figure 2. Electrostatic potential surfaces of isolated (a) and interacting (b) molecules. Blue colour indicates positive charge regions. Red colour indicates negative charge regions. Level contour: 0.009 kJ/mol.