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A Theoretical Study of the Interactions of In^{+} and In^{+3} with a Stone-Wales Defect Single-Walled Carbon Nanotubes.

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Experimental techniques [1] have demonstrated the controllable, reversible and mass transport exchange of indium nanocrystals along surfaces of multi-walled carbon nanotubes (MWCNTs). In particular, at certain sites robust nucleation occurs suggesting preferred locations for controlled manipulation. We believe these site locations represent structural defects, like rehybridization, incomplete bonding and topological defects within the carbon network. Although minute, these defects can drastically modify the electrical, chemical and mechanical properties of CNTs.

This study was devoted to understand the role of structural defects, specifically a Stone-Wales (SW) defect in the surface transport and interaction properties of the In^{+1} and In^{+3} for both the singlet and triplet state. The effects of CNT surface curvature on In^{+1} and In^{+3} is also studied and compared to graphite. Geometries of complexes were optimized at the B3LYP level. The standard 6-31G(d) basis set was used for carbon and hydrogen atoms while an effective core potential (ECP) was used for indium. All calculations were performed using the Gaussian 03 suite of programs. The computed Mulliken charges and HOMO-LUMO gap energies, interactions and interaction energy (corrected by the basis set superposition error) of the systems have been studied and will be discussed. Figure 1 represents the comparison of the molecular electrostatic potential maps for a) In^{+} and b) In^{+3} with a SW defect CNT.

Reference:

1. A. Zettl, B. C. Regan, S. Aloni, R. O. Ritchie, U. Dahmen, *Nature*, **428**, 924, (2004).

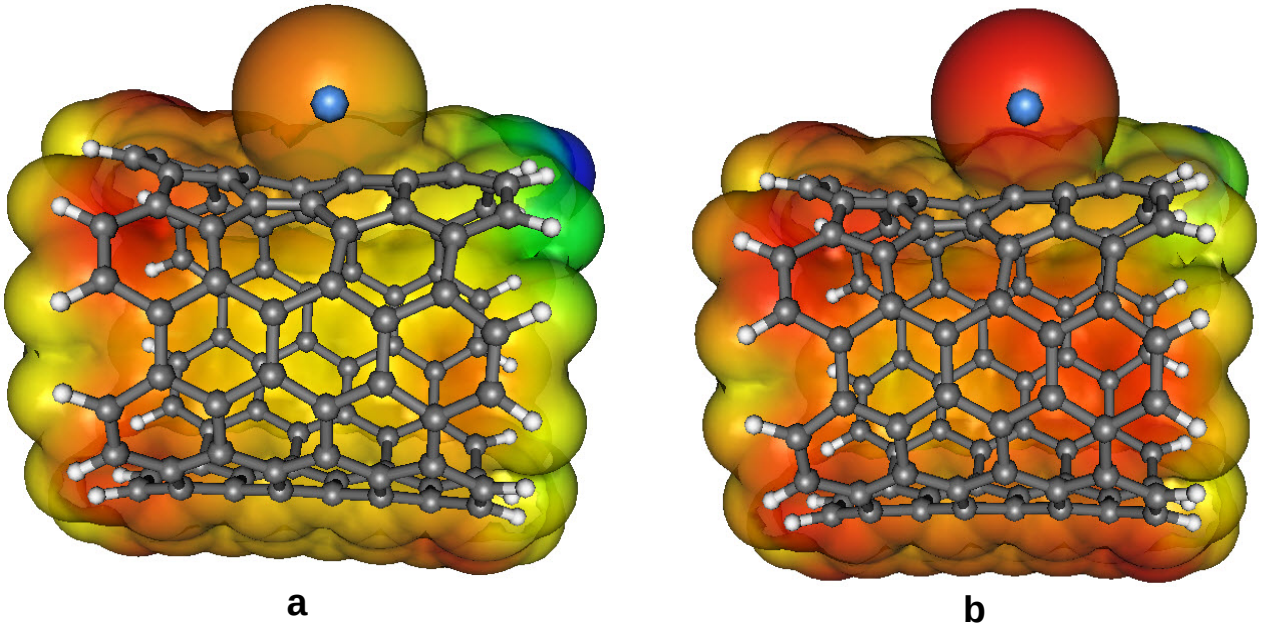

Figure 1. Comparison of the molecular electrostatic potential surfaces for the ground state configurations of a) In^{+1} and b) In^{+3} interacting with a SW-defect CNT.

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