Solubility of single walled Carbon Nanotubes in Aniline

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The solvation of single walled Carbon Nanotubes in organic solvents is a well known problem. Y. Sun, R. Wilson and D. Schuster proposed in 2001 a high dissolution of Carbon Nanotubes(CNTs) in Aromatic Amine Solvents [(1)], due to a strong light emission, but their results where put into new perspectives a few years after that [(2)]. Thereby no appreciable dissolution of CNTs in Aniline and it's derivatives is expected.
On the basis of recent works, concerning the interaction of aromatic molecules with CNTs, calculated with density functional theory, investigations have been performed to study the collective adsorption behaviour of aniline molecules on a zig-zag(8,0) single walled CNT, as well as the interactions of CNTs within a bundle of Nanotubes. Equilibrium distances, maximum packing parameters of aniline on the CNT and adsorption energies have been obtained. The comparison between CNT-CNT interaction and aniline-CNT interaction yields a consistent picture of the solubilization, within the boundaries of a static theory.
All calculations have been performed with the self-consistent charges DFTB method, [(3)] augmented with an empirical dispersion term [(4)], as it has been found appropriate for predicting equilibrium structures of weak bound systems.
These calculations are preliminaries to dynamical studies, which will be performed to obtain insight into the solution mechanism at non-zero temperatures.

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