π–π Interactions between Single-walled Carbon Nanotubes and Aniline: a Photophysical Study

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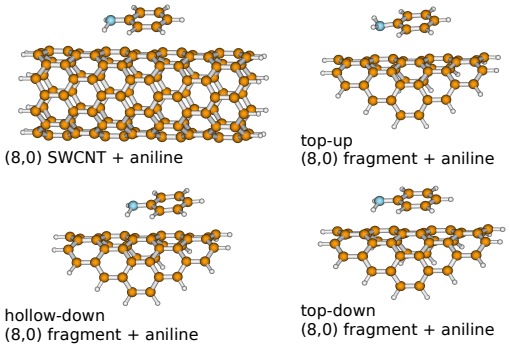
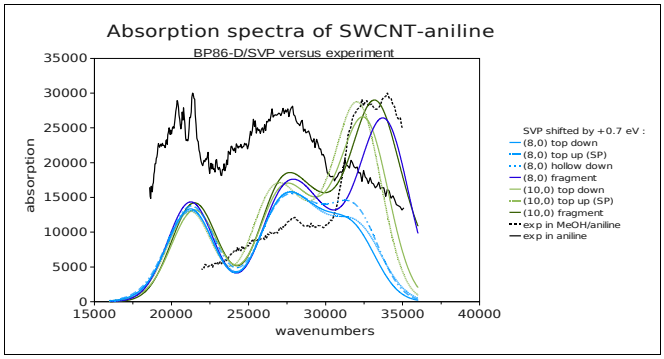
Non-covalent interactions, especially π–π stacking, between carbon nanotubes and aromatic molecules, provide an important mechanism for the solubilization of carbon nanotubes. To gain insight into this key feature in their solubilization process, photoluminescence and UV/Vis absorption spectra of single-walled carbon nanotubes (SWCNT) in pure aniline as well as in the aniline solutions diluted tenfold by several alcoholic solvents were measured [1].
To obtain a microscopic picture on the aniline-nanotube interaction the experimental data were evaluated on the basis of quantum-chemical calculations. Density functional calculations with different functionals (MPWB1K, PW91 and dispersion corrected BP86-D) are used to obtain geometries of the SWCNT interacting with aniline. Different initial orientations of the aromatic molecule with respect to the nanotube, namely top, near-bridge, and hollow [2], were considered. A fragment of the SWCNT has been used for the theoretical investigations.
Adsorption energies between aniline and SWCTNs for zig-zag (n,0) nanotubes with different diameters (n = 8, 10, 30) and graphene have been computed. Adsorption energies increase with increasing the diameter.
Electronic transition energies have been calculated by time-dependent density functional theory. The excitation process is interpreted on the basis of MO theory, and the interaction of aniline and the SWCNT is discussed in the presence of methanol and without. Absorption spectra were convoluted for the different nanotube diameters and compared to experimental absorption spectra [3].





[1] B. Peles-Lemli, P. Ács, L. Kollár, S. Kunsági-Máte, Full. Nanotubes Carb. Nanostruct 2008, 16, 247-257.
[2] L.M. Woods, S.C. Badescu, T.L. Reinecke, Phys. Rev. B 2007, 75, 155415.
[3] Excitation spectra were measured in solutions on a Fluorolog TAU3 spectrofluorimeter at the University of Pécs.

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