DFT Study of the Interaction between Single-walled Carbon Nanotubes and Organic Conjugated Oligomers

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ABSTRACT: Using dispersion corrected density functional theory (DFT) methods, we study the interaction between oligo(phyenylene ethynylene)s (OPEs) with different end groups: aldehyde (ALD) and dithiafulvene (DTF), with single-wall carbon nanotube (SWCNT). We investigate the structure and electronic properties of isolated OPEs and OPE/SWCNT molecular combinations. This research is important for greater understanding of dispersion of nanotubes with the use of linear conjugated oligomers. In particular, we focus on understanding of the role of the end groups in the dispersion of nanotubes.

We consider a number of DFT methods: B3LYP, B97D, wB97XD, and CAM-B3LYP and employ the 6-31G* basis set in all of our calculations. We obtain geometries, dipole moments, binding energies, and intermolecular distances for the oligomer and nanotube combinations. The comparison of results obtained using different DFT methods is also made. Our results show that OPE-DTF interact more strongly with the nanotube than OPE-ALD.

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