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Investigation of the interaction between the single walled carbon nanotube and conjugated oligomers using various dispersion correction DFT methods

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The area of carbon nanotubes (CNT)-polymer composites has been progressing rapidly in recent years. Pure CNT and CNT-polymer composites have many useful (industry related) properties ranging from good electrical conductivity to superior strength. However the full potential of using pure CNTs has been severely limited because of complications associated with the dispersion of CNTs. CNTs tend to entangle with each other forming materials that have properties that fall short of the expectations. The goal of this work is to enhance the understanding as to which type of conjugated oligomers is best suited for the dispersion of single walled CNTs (SWCNTs). For this purpose, various methods of dispersion corrected density functional theory (DFT-D/ B97D, /WB97XD, /CAM-B3LYP) have been used to investigate the interaction between the SWCNT and the fluorene based oligomers with different end groups (aldehyde (ALD) and dithiafulvenyl (DTF)). We investigate the effect of intermolecular interactions on the structure, polarity and energetics of the oligomers. Our results indicate that DTF ended oligomers tend to stretch along the nanotube (i.e. they lie parallel to it). On the other hand, ALD ended oligomers tend to lie across the nanotube. As a result of this structural difference, our results also indicate that, DTF ended conjugated oligomers become somewhat more polarized than ALD ended oligomers in the presence of the SWCNT and the binding energy is higher for DFT ended than ALD ended oligomers without side chain.

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