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Investigation of intermolecular interactions between single walled nanotubes and conjugated oligomers using the dispersion-corrected DFT methods[1] JOLANTA B LAGOWSKI, SUAD ALJOHANI, M. ZAHIDUL H. KHAN, YUMING ZHAO, Memorial University — 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 electronic electrical conductivity to superior strength. However the full potential of using CNTs as reinforcements (in say a polymer matrix) 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 identify the type of conjugated oligomers that are best suited for the dispersion of single walled CNT (SWCNT). 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 organic conjugated 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 and SWCNT combinations. The comparison of results obtained using different DFT approximations is made. Our results show that DFT-endcapped oligomer interact more strongly with CNT than ALD-endcapped oligomer.

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Jolanta B. Lagowki
Memorial University

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