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Investigations of the Intermolecular Interactions between Organic Conjugated Monomers, and Conjugated Oligomers and Nanotubes Using Dispersion-Corrected DFT

Tuesday 14 June 2016 13:15 (30 minutes)

This talk will focus on discussing and analyzing intermolecular interactions between organic conjugated polymers used in organic light-emitting diodes (OLEDs) and between conjugated oligomers and carbon nanotubes (CNTs) in CNT-oligomer composites. Dispersion-corrected density functional theory will be employed to study these systems. The construction of multilayered OLEDs typically involves extensive experimental searches for the combinations of polymers that give the optimum device performance. As an example, combinations of different fluorene-based conjugated polymers such as alternating triphenylamine-fluorene (TPAF)- and oxadiazole-fluorene (OxF)-based conjugated copolymers were considered as components of multilayered OLEDs. It was found that certain combination gave the best OLED performance. Our results illustrate that the best combination of polymers has monomers that have the closest intermolecular distance and the highest binding energy relative to all the other combinations. Pure CNT and CNT-oligomer/polymer composites have many useful (industry related) properties: ranging from 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). We investigate the effect of intermolecular interactions on the structure, polarity and energetics of the oligomers in presence of SWCNT.

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