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First-Principles Studies on Photoinduced Charge Transfer in Functionalized Carbon Nanotubes[1] IEK-HENG CHU, DMITRI KILIN, HAI-PING CHENG, Department of Physics and the Quantum Theory Project, University of Florida, Gainesville, Florida
— We have studied the binding energy, electronic structure, optical excitation, and relaxation of dinitromethane molecules ($CH_2N_2O_4$) on semiconducting carbon nanotubes (CNTs) of chiral index (n, 0) (n=7,10,16,19). The electronic structures calculated from density functional theory (DFT) show that the dinitromethane introduces a localized state inside the band gap of CNT systems of n=10,16 and19, which indicates that the state can trap an electron when the CNT is photoexcited. The dynamics of intra-band relaxations in such systems has been investigated using reduced density matrix formalism combined with DFT. For pristine CNTs, we have found that the calculated charge relaxation time constants agree well with the experimental time scales. Upon adsorption, these constants are modified and there is not a clear trend for the direction and magnitude of the change. However, our calculations predict that electron relaxation in the conduction band is faster than hole relaxation in the valence band, for CNTs with and without molecular adsorbates.

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