

Peripheral and Structural Effects on the Band Gap of Acceptor-Donor Type Conducting Polymers Containing Pendant Bisfulleroid Groups

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Abstract

In this computational study, the band gap energy of an acceptor-donor type conducting polymer consisting of terthiophene repeating units with fused bisfulleroid group was estimated by extrapolating excitation energies approximated by the HOMO-LUMO energy differences as well as the TDDFT method with respect to the inverse number of monomer units. Optimizations were performed both in vacuum and in *o*-dichloro benzene (as solvent) using the B3LYP and MPW1B95 functionals. The calculated optical band gap was found to be in good agreement with experimentally reported band gap in the literature. However, different band gaps with different experimental techniques were reported in the referred experimental study for the same system. In order to understand the reasons behind this behavior, effects of the structural (inter- and intra-molecular stacking) and environmental (explicit and implicit solvation and acidic doping) factors on the absorption of the terthiophene monomer with fused bisfulleroid were investigated. Acid-doping was found to be very important in terms of the present system.

