Theoretical Investigation on thiophene-benzothiadiazole based polymers

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Abstract:

Theoretical investigation has been developed on the basis of density functional theory (DFT) quantum chemical calculations to predict the theoretical properties of polymer based on thiophene and benzothiadiazole units. We predict the properties of thiophene-benzothiadiazole polymer (PTBT); where we add a thiophene unit to the benzothiadiazole backbound. Our calculation show that PTBT polymer presents a moderate band gap (1.96 eV), HOMO and LUMO energy level -5.07 eV and -3.11 eV respectively and maximum of absorption at 677 nm. Which are a suitable properties to be used as an active layer in optoelectronic devices such as organic solar cells.

Keywords: Benzothiadiazole, Thiophene, Energy Band Gap.