Donor-acceptor organic materials with low band-gap for photovoltaic applications: a theoretical investigation

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Résumé

In this paper, we report theoretical investigations on the structural, optoelectronic and photovoltaic properties of some conjugated oligomers containing thiophene and thiophene rings and acceptor moieties (e.g. 2,1,3-benzothiadiazole). This study is achieved by using the quantum chemical calculations based on density functional theory (DFT) at B3LYP functional with 6-31G(d) basis set for all atoms. The calculations were performed by Gaussian 09 program supporting by Gauss View 5.0. The results reveal that the geometrical parameters (dihedral angles, bond lengths) of all molecules possess nearly planar conformations.
Moreover, the optoelectronic properties (HOMO, LUMO, Egap...) were determined from the fully optimized structures obtained by B3LYP/6-31G(d). The absorption properties (λmax, Etr, OS) of these molecules are calculated using TD-B3LYP/6-31G(d) method.
The studied molecules (Mol i with i = 1-6) have the low band-gaps with appropriate energy levels of HOMO and LUMO which are desired in the photovoltaic applications, especially the Mol 6 molecule, leading us to suggest this candidate as active layer in organic solar cells.

Mots-Clés: Conjugated oligomers, thiophene, phenylene, optoelectronic properties, DFT, TD.

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