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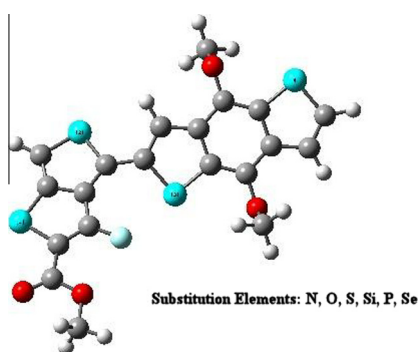
Density functional theory investigation of opto-electronic properties of thieno[3,4-b]thiophene and benzodithiophene polymer and derivatives and their applications in solar cell

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HIGHLIGHTS

- Two different approaches are applied to carry out the theoretical investigations: Oligomer extrapolation technique and periodic boundary condition (PBC) method.
- Substitution of nitrogen and oxygen atoms in the benzodithiophene (BDT) unit of pristine PTB7 while silicon, phosphorous, and selenium atoms are substituted in thieno thiophene (TT) unit can improve the maximum theoretical efficiencies (MTE) in donor/PC₇₁BM performances.
- Substitution of sulfur by nitrogen and oxygen atoms in the benzodithiophene (BDT) unit lead to a significant improvement in difference between the ground and excited states in local dipole moment of one monomer of PTB7 derivatives.

GRAPHICAL ABSTRACT



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ABSTRACT

PTBs polymers with thieno[3,4-b]thiophene [TT] and benzodithiophene [BDT] units have particular properties, which demonstrate it as one of the best group of donor materials in organic solar cells. In the present work, density functional theory (DFT) is applied to investigate the optimized structure, the highest occupied molecular orbital (HOMO), the lowest unoccupied molecular orbital (LUMO), band gap and dihedral angle of PTB7 at B3LYP/6-31G(d). Two different approaches are applied to carry out these investigations: Oligomer extrapolation technique and periodic boundary condition (PBC) method. The results obtained from PBC-DFT method are in fair agreement with experiments. Based on these reliable outcomes; the investigations continued to perform some derivatives of PTB7. In this study, sulfur is substituted by nitrogen, oxygen, silicon, phosphor or selenium atoms in pristine PTB7. Due to the shift of HOMO and LUMO levels, smaller band gaps are predicted to appear in some derivatives in comparison with PTB7. Maximum theoretical efficiencies, η , of the mentioned derivatives as well as local difference of dipole moments between the ground and excited states ($\Delta\mu_{ge}$) are computed. The results indicate that substitution of sulfur by nitrogen or oxygen in BDT unit, and silicon or phosphor in TT unit of pristine PTB7 leads to a higher η as well as $\Delta\mu_{ge}$.

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Introduction

Recently, a good number of experiments show that organic-based photovoltaic devices are interestingly low-cost and easily processed in comparison with their costly inorganic counterparts. The most successful organic solar cells (OSCs), so far manufactured, are bulk heterojunction (BHJ). The best-reported power conversion efficiency (PCE) of OSCs is still below 10% [1], and the theoretical studies have a long way to assist experts in manufacturing highly efficient solar panels.

BHJ OSCs are produced by mixing donors and acceptors in nano-scale phase separation [2]. With their high electron affinity and electron mobility, fullerene derivatives, such as [6,6]-phenyl C71 butyric acid methyl ester (PC₇₁BM), become the most appropriate candidates for the acceptor parts of the blend BHJ OSCs.

On the other side, the investigations show that poly(3-hexylthiophene) (P3HT) and PTB7 are two successful donors in a BHJ OSCs in combination with PC₇₁BM (Fig. 1). PTB7 with thieno[3,4-b]thiophene [TT] and benzodithiophene [BDT] units based on alternating ester units illustrates an improved efficiency up to 7.4% [3]. This research aimed at modifying the electronic properties of PTB7 using density functional theory (DFT) and predicting new organic donors for BHJ PC₇₁BM-based OSCs. Two theoretical approaches within DFT frame work are utilized: PBC-DFT method and oligomer extrapolation technique [4–7]. DFT calculations are performed to predict the optimized atomic geometries, electronic structures, band gaps, dihedral angles and dipole moments of the aforementioned structures. First, by means of DFT the structures of P3HT and PTB7 are studied. Second, the optimized geometries and electronic properties of different PTB7 derivatives are investigated.

Results show the possibility of synthesis of new polymers with such properties that may eventually lead to fabricate solar cells of better performance. To the best of our knowledge, no theoretical or experimental works have been yet reported on the most of the above-mentioned derivatives. Recently one of our predicted polymers has been synthesized successfully, and has shown a good performance in preliminary tests [8]. The proposed polymers are designed with the substitution of two sulfurs by nitrogen or oxygen atoms in benzodithiophene group and substitution of another two sulfurs by silicon or phosphor atoms in thieno [3,4-b] thiophene group of PTB7. For each substitution, a proper valence bond is maintained by hydrogen atoms. The calculated band gaps of these new structures are smaller than that of the pristine PTB7

with about 0.35–0.4 eV, which can preferably capture a broader range of solar spectrum. The theoretical investigation predicts a better planar feature of dihedral-angles for these structures in comparison with PTB7. This planar feature enables the π -conjugated electrons delocalize over the structure and therefore enhances the charge carriers mobility [9]. Also significant improvements of local difference dipole moments between the ground and excited states ($\Delta\mu_{ge}$) are predicted. This latter property is especially very important, as it may contribute to decrease electron-hole recombination rate [10,11]. All these features can lead to increase the short circuit current density (J_{sc}), and therefore to improve the PCE of the solar cell. In brief, according to these calculations, substituting nitrogen and oxygen with sulfur atoms in BDT unit decreases the band gap and enlarges the local difference dipole moment. On the other hand, the addition of silicon and phosphor atoms to special points of these polymers can improve their electronic characterization.

After the introduction in 'Introduction', this article continues in five main sections. 'Theoretical back ground' contains the essential descriptions of the theory. The computational methods are presented in 'Computational details'. Results and discussions are divided into different parts in 'Results and discussion'. First optoelectronic properties of P3HT and PTB7 are analyzed to validate this study, and then opto-electronic properties of PTB7 derivatives are investigated in detail. Explanations on $\Delta\mu_{ge}$ and charge density distributions associated with the HOMO and LUMO levels of these compounds are presented at the end of this section. Finally, a brief summary and the relevant conclusion is offered in the last section.

Theoretical back ground

It is well-known that the efficiency of an OSC is affected by three parameters: fill factor (FF), open circuit voltage (V_{oc}) and J_{sc} [12]. In contrast to inorganic semiconductors, photon absorption does not directly lead to the creation of a free electron and hole in organic semiconductors, but instead it results in an exciton generation. Excitons migrate to the donor-acceptor interface, where they should be dissociated into holes in the donor and electrons in the acceptor phase. Exciton binding energy is typically large in the order of 0.5 eV [13–15]. To achieve exciton dissociation, LUMO level of the donor must be above the LUMO level of the acceptor by at least 0.3 eV to supply a sufficient field for charge separation [16].

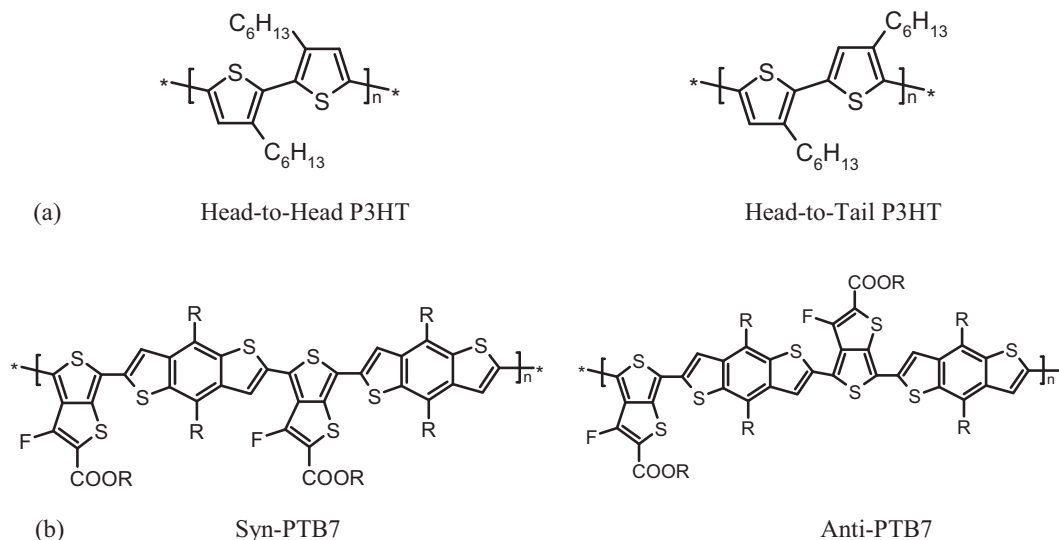


Fig. 1. Different configurations of (a): P3HT, (b): PTB7, with R = 2-ethylhexyl.

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