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A theoretical study about three organic semiconductor based on oligothiophenes

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Abstract. Three derivatives based on oligothiophenes were theoretically investigated about the electronic and charge transport properties using density functional (DFT) theory based on the Marcus-Hush theory. The predicted highest hole mobility is 0.218 $cm^2V^{-1}s^{-1}$, and the highest electron mobility is 0.373 at 300 K. The calculated data demonstrated that the compound 1 should be a high-performance n-type organic material candidate and compound 3 may well be potential p-type materials with high mobility values. Our work also indicates that the face-to-face π-π interaction and S-S interactions is favorable for the molecular stacking and charge transport behaviors. The calculated results provide an additional possibility to be able to improve the origin semiconductor performance and design new electronic devices.

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Key words: Organic semiconductor, charge transport, Oligothiophene.

1 Introduction

Organic semiconductor materials are promising materials for organic field effect transistors (OFETs), organic light emitting diodes (OLEDs), and organic photovoltaic cells(OPVCs) because of their potential applications in low-cost, flexibility, and mass chemical synthesis during the past decades. [1-7] Many efforts have been exclusively conducted to improving the performances of the organic semiconductor, such as designing new organic semiconductors and optimizing device configurations. As we all know, the performance of the semiconductors depends largely on the charge transport. [8-10] It is crucial to understand the principles of charge transport and the relationship between the performance and the electronic structure for the material structure design.

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Thiophenes-based materials are an important class of organic semiconductors because they exhibit many different intra- and intermolecular interactions from the high polarizability of S electrons in the thiophene rings. [11-15] Oligothiophenes are among the most effective molecular for organic materials with significantly electronic properties. Furthermore, the organic device shows remarkable charge carrier mobility in OFETs, as high as 2.0 $cm^2V^{-1}s^{-1}$ based on annelated β-oligothiophenes. [16] S-S and S-π intermolecular interaction can provide different charge transport pathways.It is very necessary to a further study of the relationship between the interactions and the performance.Recently, organic semiconductors have been widely investigated based on β-oligothiophenes. To further investigate the relationship of electron property and structure for the thiophene-based materials, discussions of the charge transport properties are studied based on three single crystal structures.

In this work, we investigate Charge transport behavior is of great interest in organic materials. The performance of the devices strongly depends on their charge transport, quantified by the charge-carrier mobility. Room-temperature mobility for many different single-organic molecules have been reported. We need to gain a complete theoretical fundamental understanding of the mobility in organic materials to understand the structure-transport relationships and transport mechanisms, and the theoretical method

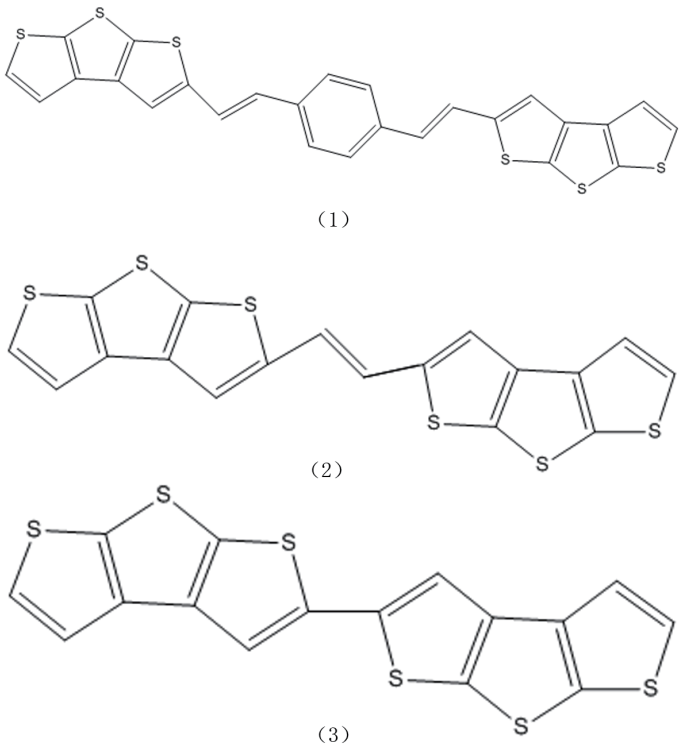

Figure 1: Molecular structure of compounds 1-3.