



Effects of carbon chain on hole-transport properties in naphtho[2,1-b:6,5-b']difuran derivatives: Remarkable anisotropic mobilities



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ABSTRACT

Theoretical investigations of hole-transport properties in two naphtho[2,1-b:6,5-b']difuran derivatives as novel p-type organic semiconductor based on the Marcus–Hush theory combining quantum mechanics are carried out. This work focuses on the effects of carbon chain on molecular orbitals, partial charge difference, ionization potential, internal energy relaxation, and hole-transport behaviors. Through computational modeling, we are shedding light on the favorable function of C8-DPNDF single crystal as p-type organic material. With the introduction of octyl group, C8-DPNDF single crystal possesses high hole-transfer mobilities ($1.589 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$) and remarkable anisotropic behavior. The simulated anisotropic mobility curve of C8-DPNDF demonstrates the maximum value of the mobility appears when the measuring conducting channel is along the *b*-axis of the single crystal. The adiabatic ionization potential (AIP) and vertical ionization potential (VIP) of C8-DPNDF are about 6.312 and 6.399 eV, that is, slightly smaller than those of DPNDF. The relatively small IP values can ensure effective hole injection from the source electrode. The data obtained from the present work can be used to prove that C8-DPNDF molecule has the potential to develop into high-efficient p-type organic semiconductor materials, whose hole-transport mobility can be further improved when the measuring transistor channel is controlled carefully.

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1. Introduction

Compared with inorganic semiconductor materials, the low cost and excellent performance of organic semiconductors have increased enormous interest for intrinsic scientific challenges and potential application in organic electronic devices to date, such as organic photovoltaic cells (OPVCs) [1–3], organic field-effect transistors (OFETs) [4–7], organic light-emitting diodes (OLEDs) [8–10], and so on. Organic field-effect transistors (OFETs), as a significant

type of electronic devices, have attracted more attention during recent years due to the advantages of mechanical flexibility and large-area fabrication [11–13]. Several research groups have done a great quantity of work and reported the significant progress in p-type organic semiconductors [14–23]. Recent studies show that the charge-transport properties of some p-type semiconductors such as pentacene and rubrene are comparable to amorphous silicon-based field-effect transistors (FETs) [24,25]. Although the development of p-type organic semiconductor materials is superior to that of n-type semiconductor materials, it is still very important for the progress in this

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field to develop new p-type organic semiconductors. Improving carrier mobility and environmental stability has become one of basic work for current research on organic semiconductors [26–30]. The most common method to improve the performance of electronic devices is of extending the π -conjugated systems. As is well-known, the mobilities of p-type semiconductors (holes) or n-type semiconductors (electrons) in solid-state organic materials are increased, which is the result of the increase in the intermolecular π orbital overlap [31].

Furan, as a ubiquitous organic frame, has been less studied than thiophene in the research of organic electronic [32–35]. The lack of interest may be attributed to the chemical instability of furan and its derivatives [36]. In fact, relatively lower aromaticity of furan than thiophene may lead to different electronic properties. It is more important that such small difference in the molecular properties will reflect distinct device characteristics. Recently, the synthesis of naphtho[2,1-b:6,5-b']difuran (NDF) used as a novel and effective single-crystal OFETs has been reported, which show hole mobilities of up to $3.6 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ as new p-type organic semiconductors [37]. In Mitsui et al. experiment, DPNDF and its octyl-substituted derivative C8-DPNDF were found to have the optimum structures for control of the solubility and device processability. A detailed understanding of the charge-transport mechanism in these two materials is of interest from both fundamental and practical points of views, since the charge mobility is the most significant parameter in the performance of electronic devices [38,39]. Among intrinsic properties of organic semiconductors, the electrical anisotropy has gained wide attention [40–46]. The strong anisotropic effects of rubrene crystals in the a–b plane were observed by Sundar et al. for the first time in 2004 [40]. To explain how chemical composition, geometric structure, and packing affect the transport properties, Han and coworkers developed a theoretical method to investigate the relationship between angular resolution anisotropic mobilities and molecular packing architecture parameters (r , θ , and γ) as well as underlying electronic properties (reorganization energy λ and intermolecular electronic coupling V) by first-principle quantum mechanics (QM) calculations based on Marcus–Hush theory [47,48]. They have investigated systematically the anisotropic mobilities in a series of organic semiconductors such

as acene, acene derivatives and rubrene, which coincide with experimental observations very well [49–55].

In this work, we make a comparative study on the charge mobilities of a class of naphtho[2,1-b:6,5-b']difuran (DPNDF and C8-DPNDF) through the first-principle calculations, in order to gain insight in the influence of carbon chain to the angular resolution anisotropic mobility. Using the simulation model proposed by Han et al., a full and accurate theoretical study on the influence of carbon chain to the charge transport properties is carried out. The molecular structures are presented in Fig. 1, and the crystal structures can be found in Ref. [37]. Based on the calculation results, the introduction of octyl group makes DPNDF and C8-DPNDF exhibit very different intrinsic transport properties. The theoretical analysis of charge transport mechanism is helpful to understand the quantitative structure–activity relationship between the charge mobility and the structures of organic semiconductor materials, and provide guidance for designing the high-performance organic semiconductor materials.

2. Theory and calculation

Our theoretical study is based on first-principles quantum mechanics (QM) calculations combined with Marcus–Hush theory [47,48], and the simulation model is proposed by Han et al. There are two kinds of mechanism to describe the charge transport behavior: one is the coherent band model; the other is the thermally activated hopping model. At room temperature, the transport of hole/electron for an organic semiconductor can be described appropriately by a hopping mechanism owing to the thermal disorder and scattering [56–58]. In this case, the hole/electron transport in organic semiconductors take place through the charge carrier hopping from one molecule to the adjacent molecule. That is to say, the charge carriers are localized on a single molecule. Using the hopping mechanism for an organic crystal at room temperature, the hopping rate (W) can be written as:

$$W = \frac{V^2}{\hbar} \left(\frac{\pi}{\lambda k_B T} \right)^{1/2} \exp \left(-\frac{\lambda}{4k_B T} \right) \quad (1)$$

where V is the intermolecular effective electronic coupling between neighboring molecules, λ is the reorganization

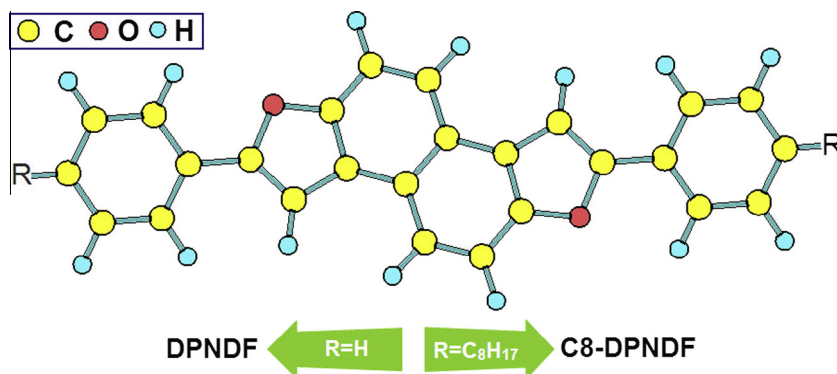


Fig. 1. The molecular structures of DPNDF ($R=H$) and C8-DPNDF ($R=C_8H_{17}$).

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