

PAPER



Cite this: *J. Mater. Chem. C*, 2015, **3**, 10856

Isomers of organic semiconductors based on dithienothiophenes: the effect of sulphur atoms positions on the intermolecular interactions and field-effect performances†

Wenjing Yi,^a Shuai Zhao,^a Huiliang Sun,^a Yuhe Kan,^b Jianwu Shi,^{*a} Shisheng Wan,^a Chunli Li^a and Hua Wang^{*a}

2,5-Distyryl-dithieno[2,3-*b*:2',3'-*d*]thiophene (**DEP-*bt*-DTT**), an isomer of 2,5-distyryl-dithieno [2,3-*b*:3',2'-*d*]thiophene (**DEP-*bb*-DTT**) and 2,5-distyryl-dithieno[3,2-*b*:2',3'-*d*]thiophene (**DEP-*tt*-DTT**), was synthesized. Organic field-effect transistors (OFETs) based on these three isomers were fabricated. The structure cell parameters and the formation of intermolecular interactions in their single crystals show regular change when the positions of sulphur atoms vary from top–bottom–top in **DEP-*tt*-DTT** to bottom–bottom–top in **DEP-*bt*-DTT**, then to bottom–bottom–bottom in **DEP-*bb*-DTT**. Combining the results of theoretical calculations and OFET performances, it reveals that: (1) the positions of sulphur atoms determine the contribution extent of sulphur atoms to the molecular conjugation and the formation of intermolecular interactions; (2) the existence of the intermolecular interactions, especially for S– π , benefits for the charge transport; (3) the field-effect mobility (μ) increases with increasing of the sulphur atom contribution to the molecular conjugation.

Received 27th July 2015,
Accepted 14th September 2015

DOI: 10.1039/c5tc02287h

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Introduction

Over the past few decades, organic electronics have received much attentions due to their potential advantages of flexibility, light-weight, large-area processes and low cost.^{1–10} Organic field-effect transistors (OFETs) are one of the important components of modern organic electronics. Their performances have been improved by adopting new organic semiconductors or optimizing the device configurations.^{6–28} Based on these efforts, the field-effect mobilities (μ) of OFETs have reached and even exceeded their inorganic counterparts (conventional α -H: silicon-based transistors), especially for OFETs with small molecules as active layers.^{29–34} However, they are still lower than that of inorganic devices based on polysilicon and monocrystalline silicon. The major difference between inorganic and organic semiconductors is the combination mode. For organic semiconductors, they are coalesced *via* weak intermolecular

interactions, such as van der Waals interactions, S–S interactions, π – π interactions, and C–H interactions, instead of strong covalent bonds in inorganic semiconductors.^{35–39} So enhancing the intermolecular interactions may be an effective way to improve the performances of OFETs.

Dithienothiophene (DTT) derivatives, as analogues of acenes, have shown considerable mobility.^{35–48} For these fused thiophene structures, there may exist various intermolecular interactions including weak hydrogen bonding, π – π stacking, C–H interactions, and S–S interactions. In our previous studies, it was found that the introduction of the C=C double bond can lead to the formation of S– π intermolecular interaction and is responsible for a high μ of 2.2 cm² V^{−1} s^{−1} in 2,5-distyryl-dithieno[2,3-*b*:3',2'-*d*]thiophene (**DEP-*bb*-DTT**).³⁸ Furthermore, the intermolecular interactions can transform from S–S in 2,5-diphenyl-dithieno[2,3-*b*:3',2'-*d*]thiophene (**DP-*bb*-DTT**) with no field effect, to S–C in 2,5-dibiphenyl-dithieno[2,3-*b*:3',2'-*d*]thiophene (**DBP-*bb*-DTT**) with μ of 0.45 cm² V^{−1} s^{−1}, to S– π in **DEP-*bb*-DTT**, and to the coexisting of S–S and S– π in 1,4-di-[2-dithieno[2,3-*b*:3',2'-*d*]thiophen-2-yl-vinyl]-benzene (**D-*bb*-DTT-EP**) with μ of 0.15 cm² V^{−1} s^{−1} as the end-capping groups change. Combining the theoretical calculations, it can be concluded that the intermolecular interactions play an important role in the device performances.³⁹ But for 2,5-distyryl-dithieno[3,2-*b*:2',3'-*d*]thiophene (**DEP-*tt*-DTT**), there also exist S–S and S–C intermolecular interactions in the single crystal while μ of 0.17 cm² V^{−1} s^{−1} was

^a Key Lab for Special Functional Materials of Ministry of Education, Henan University, Kaifeng 475004, China. E-mail: jwshi@henu.edu.cn, hwang@henu.edu.cn

^b Jiangsu Province Key Laboratory for Chemistry of Low Dimensional Materials, School of Chemistry and Chemical Engineering, Huaiyin Normal University, Huanan 223300, China

† Electronic supplementary information (ESI) available. CCDC 1414571. For ESI and crystallographic data in CIF or other electronic format see DOI: 10.1039/c5tc02287h

obtained from OFETs.³⁷ It was obvious that the difference in sulphur atom positions between the isomers of **DEP-*bb*-DTT** and **DEP-*tt*-DTT** causes a dramatic change in the device performances. In this field, there was no report about the relationship between the device performances and the isomers of organic semiconductors, except the studies on the isomerization and the substituting position of alkyl chains.⁴⁹ As we all know, the isomers are different organic molecules that have the same numbers and kinds of atoms in different structural arrangements. The varying of atoms arrangements will lead to the changes in the physical and chemical properties. So it is necessary to study the relationship between the molecular structures of isomers and their OFET performances, which will benefit us to further understand the essence of the charge transport in organic semiconductors and to improve the device performances.

Herein, as another isomer of **DEP-*bb*-DTT** and **DEP-*tt*-DTT**, 2,5-distyryl-dithieno[2,3-*b*:2',3'-*d*]thiophene (**DEP-*bt*-DTT**) was synthesized. The single crystal structures and OFETs based on these three isomers were investigated. Combined with the theoretical calculations, it can be confirmed that the positions of sulphur atoms play a decisive role in the conjugation extent of sulphur participation and the forms of intermolecular interactions, which affect the charge transport and OFET performances.

Results and discussion

Synthesis and characterization

DEP-*bb*-DTT was synthesized according to our previous report.³⁸ The synthesis of **DEP-*tt*-DTT** and **DEP-*bt*-DTT** is described in Scheme 1. The total yield after sublimation is 35% for **DEP-*tt*-DTT** and 31% for **DEP-*bt*-DTT**, respectively. All the intermediates were validated by NMR and MS. The target compounds **DEP-*tt*-DTT** and **DEP-*bt*-DTT** were confirmed by HRMS. The single crystals of **DEP-*bt*-DTT** (CCDC number 1414571) were obtained in the sublimation process.

Single crystals and intermolecular interactions

X-ray diffraction studies of the single crystal structure are shown in Fig. 1. The **DEP-*bt*-DTT** molecule displays a quasi-bowed shape, which is similar to **DEP-*tt*-DTT** and **DEP-*bb*-DTT**.^{37,38} The twisted angles between the terminal phenyl groups and the DTT plane in **DEP-*bt*-DTT** single crystal structures are 9.3° and 11.7°, respectively. There exist S–C and S–S intermolecular interactions between the neighbouring molecules of **DEP-*bt*-DTT**. And the molecules adopt the herringbone arrangement in their packing with a herringbone

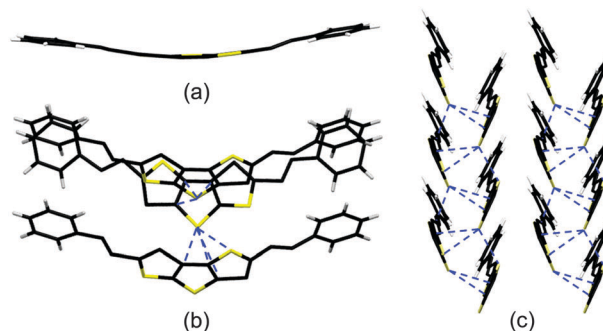


Fig. 1 Molecular shape and intermolecular interactions in the single crystals of **DEP-*bt*-DTT**. (a) Side view; (b) intermolecular interactions; (c) the packing pattern. The dashed line represents the close contact between atoms.

angle of 48.6°. Between the adjacent parallel molecules, the π - π spacing is about 2.448 Å.

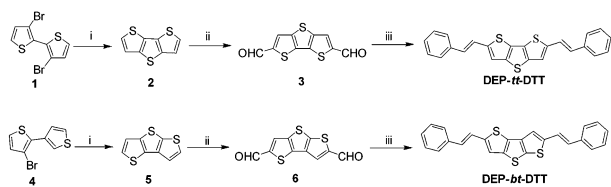
For detailed comparisons, Table 1 lists some structural parameters in the single crystals of these three isomers. It is obvious that the herringbone angle and the π - π spacing in **DEP-*bt*-DTT** single crystals are lower than that in **DEP-*bb*-DTT**, but higher than that in **DEP-*tt*-DTT**, while the twisted angles in **DEP-*bt*-DTT** are higher than that in **DEP-*bb*-DTT**, but lower than that in **DEP-*tt*-DTT**. Furthermore, it should also be noted that the intermolecular interactions in their single crystals of these three isomers are different. For **DEP-*tt*-DTT**, the intermolecular interactions consist of three S–C interactions between the sulphur atom on the middle thiophene unit (the bottom position) and the three carbon atoms on the middle thiophene unit in the neighbour molecule, and two S–S interactions between the sulphur atom at the bottom position and the sulphur atoms on the other two thiophene units (top positions) in the neighbour molecule. As the positions of sulphur atoms vary from top–bottom–top in **DEP-*tt*-DTT** to bottom–bottom–top in **DEP-*bt*-DTT**, the same three S–C intermolecular interactions remain unchanged while two S–S intermolecular interactions in **DEP-*tt*-DTT** turn into one S–S intermolecular interaction between the sulphur atom at the bottom position and the sulphur atom on the thiophene unit at the opposite position (top positions) in the neighbour molecule. However, the S–S interaction disappears with four S–C (or S- π) interactions forming between the sulphur atom at the bottom position and the whole four carbon atoms on the middle

Table 1 The structural information of **DEP-*bb*-DTT**, **DEP-*bt*-DTT** and **DEP-*tt*-DTT** in their single crystals

Materials	Twisted angle ^b (°)	Herringbone angle ^c (°)	Intermolecular interaction ^d	<i>d</i> ^e (Å)
DEP-<i>bb</i>-DTT ^a	8.2 10.0	52.0	4 S–C/(S- π)	2.575
DEP-<i>bt</i>-DTT	9.3 11.7	48.6	3 S–C/1 S–S	2.448
DEP-<i>tt</i>-DTT ^a	10.9 13.2	43.1	3 S–C/2 S–S	2.256

^a The crystal data were downloaded from Cambridge Crystallographic Data Centre (CCDC 836921 for **DEP-*bb*-DTT** and CCDC 7116820 for **DEP-*tt*-DTT**).

^b The twisted angle is the angle between the plane of the terminal phenyl group and the DTT unit. ^c The herringbone angle represents the angle between the neighbour molecules of the herringbone arrangement in their single crystal structures. ^d The information of intermolecular interactions among the packing molecules. ^e The distance of π - π spacing.



Scheme 1 Synthesis of **DEP-*tt*-DTT** and **DEP-*bt*-DTT**. (i) *n*-BuLi (2.2 equiv.), (PhSO₂)₂S (1.05 equiv.); (ii) LDA (2.2 equiv.), DMF (4.0 equiv.); (iii) PhCH₂PPh₃Br (2.2 equiv.), *t*-BuOK (3.0 equiv.).

thiophene unit of the neighbouring molecule. Thus, it can be deduced that the varying of sulphur atoms positions can lead to this disciplinary change not only for the molecular arrangements but also for the intermolecular interactions.

Topographical images and absorption properties of films

Topographical images of **DEP-*bt*-DTT** deposited at different substrate temperatures (T_s) were investigated as shown in Fig. 2. All the films possess high crystallinity and the growth habit of **DEP-*bt*-DTT** shows the layer-by-layer mode. The film at T_s of 60 °C (as shown in Fig. 2(b)) is composed of large lamellar crystals with an average layer spacing of around 2.0 nm, which is similar to that of **DEP-*bb*-DTT** and **DEP-*tt*-DTT**.^{37,38} (The topographical images of **DEP-*tt*-DTT** and **DEP-*bb*-DTT** are shown in Fig. S20 in the ESI.†) This result demonstrates that these three isomers have the same properties in the progress of their film growth.

X-ray diffraction patterns of **DEP-*bt*-DTT** films deposited at different T_s were also investigated. Fig. 2(d) shows the typical X-ray diffraction patterns of all films. All the films exhibit a series of peaks with multiple orders of reflection, which indicates that all these films are highly crystalline even if they were deposited at T_s of RT. This result is consistent with that of topographical images. According to the single crystal structure, the indices of the crystallographic plane (00 l) for **DEP-*bt*-DTT** were established. The interplanar spacing, calculated according to Bragg's equation, is about 2.0 nm, which is consistent with that obtained from AFM and the half length of the molecular long axis in the single crystals. Therefore, it can be concluded that the molecular long axis of **DEP-*bt*-DTT** is almost perpendicular to the substrate. In the process of film growth, the array of the

material molecules would adopt the same way as that in their single crystals due to the intermolecular interactions. So it states that the molecular arrangement in **DEP-*bt*-DTT** films should be consistent with that in their single crystals. For **DEP-*tt*-DTT** and **DEP-*bb*-DTT**, the X-ray diffraction patterns (as shown in Fig. S21 and S22, ESI†) also indicate that their molecular arrangements are consistent with that in their single crystals, as discussed in ref. 37 and 38.

Fig. 3(a) illustrates the UV-vis absorption properties of these three isomer films deposited on the quartz substrates with a thickness of 50 nm. The absorption peaks are 273 and 306 nm for **DEP-*bb*-DTT**, 291 and 364 nm for **DEP-*bt*-DTT**, 336 and 387 nm for **DEP-*tt*-DTT**, respectively. The onsets of the absorption spectra are about 418 nm, 443 nm and 550 nm for **DEP-*bb*-DTT**, **DEP-*bt*-DTT** and **DEP-*tt*-DTT**, respectively. From **DEP-*bb*-DTT** to **DEP-*bt*-DTT**, then to **DEP-*tt*-DTT**, a distinct bathochromic-shift is observed in the absorption spectra. Generally, the absorption properties are close to the molecular configuration and the conjugation extent. In these three isomers, all the molecules have a quasi-bowed shape. So the difference among the absorption properties can be attributed to the difference in the molecular conjugation extent. For **DEP-*tt*-DTT**, it shows the complete conjugation through the whole molecule with altering single and double bonds, while they are composed of two partial conjugations in **DEP-*bt*-DTT** and **DEP-*bb*-DTT** as shown in Fig. 3(b). The different way of conjugation may result in the different extent of conjugation in these three isomers, which accounts for the distinct bathochromic-shift in the absorption spectra. Furthermore, this change also matches the varying rule of structural parameters in their single crystals as discussed above.

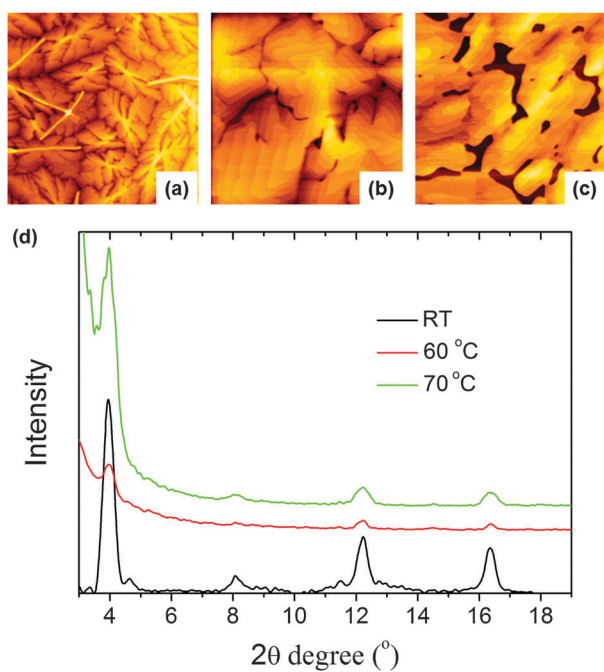


Fig. 2 The topographical images: (a) RT, (b) 60 °C, (c) 70 °C and the X-ray diffraction patterns (d) of **DEP-*bt*-DTT** films at different substrate temperature.

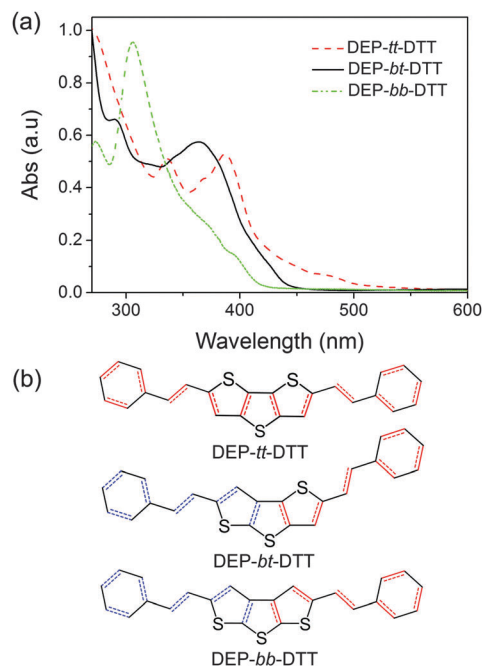


Fig. 3 (a) Normalized UV-vis absorption spectra of **DEP-*tt*-DTT** (dashed line), **DEP-*bt*-DTT** (solid line) and **DEP-*bb*-DTT** (dashed with dotted line) films deposited on the quartz with a thickness of 50 nm. (b) The conjugation way of these three isomers.

Field-effect characteristics

OFETs based on these three isomers were fabricated under the same conditions except the substrate temperatures (T_s). The characteristics of these OFETs at different T_s are listed in Table 2. Based on the films of **DEP-*bt*-DTT** with large lamellar crystals as shown in Fig. 2(b), the higher μ of $0.1 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ was obtained. For **DEP-*bb*-DTT**, the values of μ are nearly equivalent to those of previous reports, while the values of μ for **DEP-*tt*-DTT** are lower than those of previous reports.³⁷ This may be attributed to the OTS-modified SiO_2/Si substrate in ref. 37. With carefully comparing the field-effect characteristics among OFETs based on these three isomers, it can be found that the values of μ increase from 0.04 to 0.1, then to $2.0 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$, and the absolute values of threshold voltage (V_T) increase from 30 to 52, then to 60 V, when the positions of sulphur atoms vary from the top-bottom-top in **DEP-*tt*-DTT** to bottom-bottom-top in **DEP-*bt*-DTT**, then to bottom-bottom-bottom in **DEP-*bb*-DTT**. That is to say that the characteristics of OFETs based on these three isomers also present regular changes with the positions of sulphur atoms varying. For these changes including intermolecular interactions, structural parameters in

Table 2 The characteristics of OFETs based on **DEP-*bb*-DTT**, **DEP-*bt*-DTT** and **DEP-*tt*-DTT**

Materials	T_s ($^{\circ}\text{C}$)	μ^a ($\text{cm}^2 \text{ V}^{-1} \text{ s}^{-1}$)	V_T^a (V)	$I_{\text{on}}/I_{\text{off}}$
DEP-<i>tt</i>-DTT	RT	0.02	-25	10^4
	60	0.04	-30	10^4
	70	0.01	-35	10^4
DEP-<i>bt</i>-DTT	RT	0.04	-48	10^4
	60	0.1	-52	10^4
	70	0.03	-56	10^4
DEP-<i>bb</i>-DTT	RT	1.4	-66	10^5
	70	2.0	-60	10^5
	100	1.2	-66	10^5

^a The average values from more than five parallel devices.

molecular packing, absorption and OFET properties, they show regular variation on the macroscopic level, which is caused by a microscopic change in the positions of the sulphur atoms. A deep study is required for explaining these changes.

Theoretical calculations

As discussed above, the changes in intermolecular interactions, structural parameters in molecular packing, absorption and OFET properties are interrelated with the positions of the sulphur atoms. Normally, it is well known that the lone electron pair of sulphur atom combine with the $\text{C}=\text{C}$ double bonds of thiophene to form a large π conjugation system. For further understanding the role of sulphur atoms in these three isomers, the energy levels and the natural bond orbital charges (NBOs) were analyzed by the theoretical calculations.^{50–53} Fig. 4 shows the distribution of electron cloud at the highest occupied molecular orbital (HOMO) level, the lowest unoccupied molecular orbital (LUMO) level and NBO charges of sulphur atoms, $\text{C}=\text{C}$ double bonds, phenyl and styryl groups. As shown in Fig. 4, the distribution of electron cloud on the sulphur atoms in **DEP-*tt*-DTT** is very few, which maybe indicate that the sulphur atom rarely participate in the molecular conjugation. For **DEP-*bt*-DTT**, the two sulphur atoms at the bottom-bottom positions completely contribute to the molecular conjugation, while the other sulphur atom at the top position only partly contribute to the molecular conjugation. On the contrary, all the sulphur atoms almost completely participate in the molecular conjugation in **DEP-*bb*-DTT**. So it can be deduced that the contribution extents of the sulphur atoms to the molecular conjugation are different in these three isomers. In fact, the contribution extents of the sulphur atoms to the molecular conjugation can also be confirmed by the NBO charges. As marked in Fig. 4, the NBO charges of sulphur atoms are 0.466, 0.447 and 0.466, and the total value is 1.379 in **DEP-*tt*-DTT**. For **DEP-*bt*-DTT**, the NBO charges of sulphur atoms are 0.463, 0.471 and 0.465, and the total value is 1.399. The NBO charges of sulphur atoms in **DEP-*bb*-DTT** are 0.461, 0.495 and 0.461 with

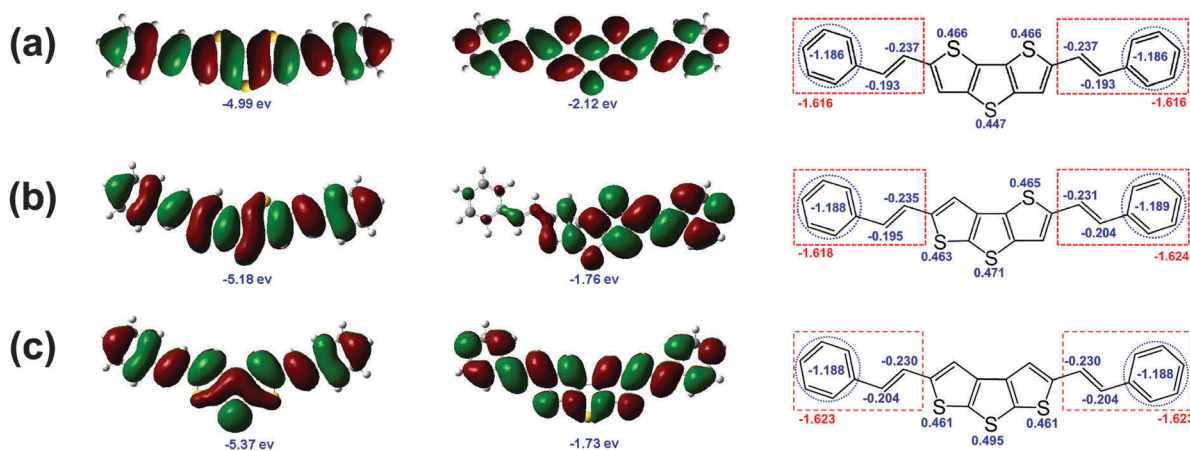


Fig. 4 The distribution of electron cloud at the highest occupied molecular orbital (HOMO) level (left column), the lowest unoccupied molecular orbital (LUMO) and the natural bond orbital charges (NBO) (right column) obtained from the theoretical calculations: (a) **DEP-*tt*-DTT**; (b) **DEP-*bt*-DTT** and (c) **DEP-*bb*-DTT**.

the total value of 1.417. It is very obvious that the contribution extents of the sulphur atoms are different among these three isomers.⁵² As a result, the phenyl and styryl groups also show different contribution to the molecular conjugation as shown in Fig. 4. Furthermore, the intermolecular interactions present in various forms because of these different contribution extents of sulphur atoms. For **DEP-*bb*-DTT**, it can form S- π intermolecular interaction between the neighbouring molecules due to the high NBO charge of the middle sulphur atom. In spite of the high NBO charge of the middle sulphur atom, S-S intermolecular interaction does not appear due to the large distance between the molecules in **DEP-*bb*-DTT**. However, S-C and S-S intermolecular interactions coexist under the coefficient effect of high NBO charges of the middle sulphur atoms and the short distances between the molecules in **DEP-*bt*-DTT** and **DEP-*tt*-DTT**.

In order to further understand the effect of the intermolecular interactions on the charge transport in OFETs, the charge transfer integrals^{54–57} were carried out in the directions of intermolecular interactions and π - π stacking as shown in Fig. 5. The higher values emerge in the directions of S-C (or S- π) intermolecular interactions in three isomers, which means that S-C (or S- π) intermolecular interactions are the most efficient way for the charge transport. Comparing the values of transfer integrals in the direction of π - π stacking in these three isomers, it is found that the values of transfer integrals are the highest in **DEP-*bb*-DTT** and the lowest in **DEP-*bt*-DTT**. As mentioned above, there also exist one S-S intermolecular interaction and two S-S intermolecular interactions in the direction of π - π stacking in **DEP-*bt*-DTT** and **DEP-*tt*-DTT**, respectively. So it may be inferred that: (1) the S-S intermolecular interaction also has a weak effect on improving the charge transport; (2) the S-S intermolecular interaction can

trenchantly reduce the effect of the π - π intermolecular interaction on the charge transport when they are in the same direction. On the other hand, the absolute values of V_T reduce gradually with the strengthening of the S-S intermolecular interaction from **DEP-*bb*-DTT** to **DEP-*bt*-DTT**, then to **DEP-*tt*-DTT**.

Conclusions

In summary, **DEP-*bt*-DTT**, as a new isomer of **DEP-*bb*-DTT** and **DEP-*tt*-DTT**, was synthesized. Combining the single crystal structures, the properties of OFETs and the theoretical calculations, it was found that the positions of sulphur atoms play an important role in the formation of intermolecular interactions and device performances in these three isomers. With the positions of the sulphur atoms varying from top-bottom-top in **DEP-*tt*-DTT** to bottom-bottom-top in **DEP-*bt*-DTT**, then to bottom-bottom-bottom in **DEP-*bb*-DTT**, the contribution of sulphur atoms to the molecular conjugation increases, together with the decreasing of twisted angles for phenyl groups contorting from the **DTT** plane and the increasing of and the increase of the herringbone angle and π - π spacing. Due to the changing of the contribution extent to the molecular conjugation, the sulphur atoms possess different NBO charges, which result in the various intermolecular interactions between the neighbouring molecules in these three isomers. All the intermolecular interactions including S-C (or S- π) and S-S benefit for the charge transport, but the S-S intermolecular interaction can sharply weaken the effect of the π - π intermolecular interaction on the charge transport when they are in the same direction. This will help us to design more new organic semiconductors with high μ by improving the contribution of the sulphur atoms to the molecular conjugation.

Acknowledgements

This work was financially supported by the National Natural Science Foundation of China (50803015 and 20972041) and Program for SRFDP (20124103110004). We also thank IFMC of NENU for providing ADF computational resources.

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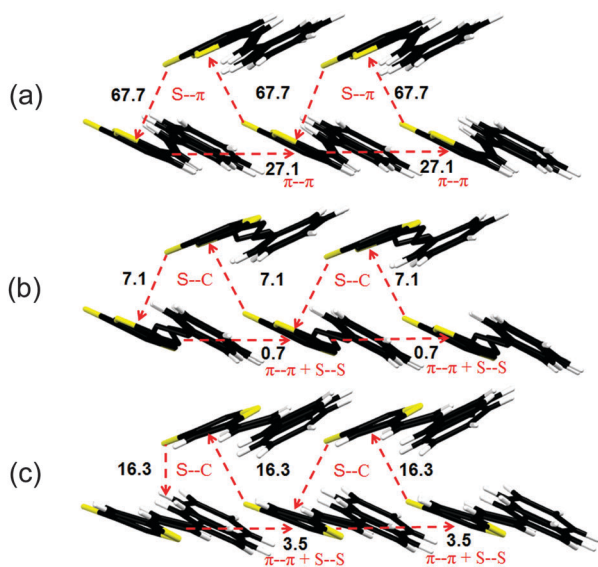


Fig. 5 The charge hopping pathway and the values of hole transfer integrals between the neighboring molecules of **DEP-*bb*-DTT** (a), **DEP-*bt*-DTT** (b) and **DEP-*tt*-DTT** (c) taken from the single crystal structure.

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