Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Reveal the mechanism of contrasting charge transport properties for phenyl and thienyl substituent organic semiconductors

Yanan Zhu[a], Xianzhe Zeng[a], Tianchen Fu[a], Yang Cao*[b] and Hong Meng*[a]

a. School of Advanced Materials, Peking University Shenzhen Graduate School, Shenzhen 518055, China.

b. Institute of Future Industrial Technologies, Peking University Shenzhen Graduate School, Shenzhen 518055, China.

*Email: menghong@pku.edu.cn and yangcao@pkusz.edu.cn

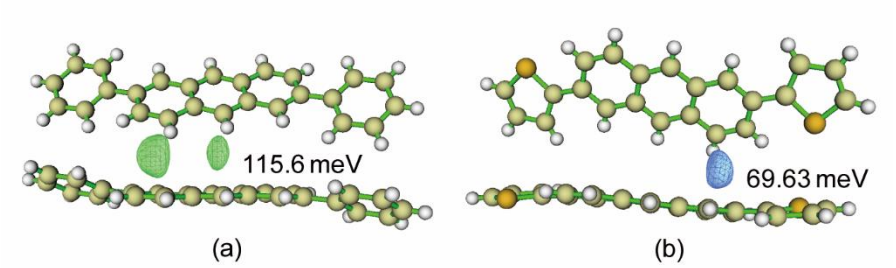

Figure S1. The HOMOs overlap of DPAnt and DTAnt. (a) and (b) are T-dimers of DPAnt and DTAnt separately. (Calculated by Multiwfn)

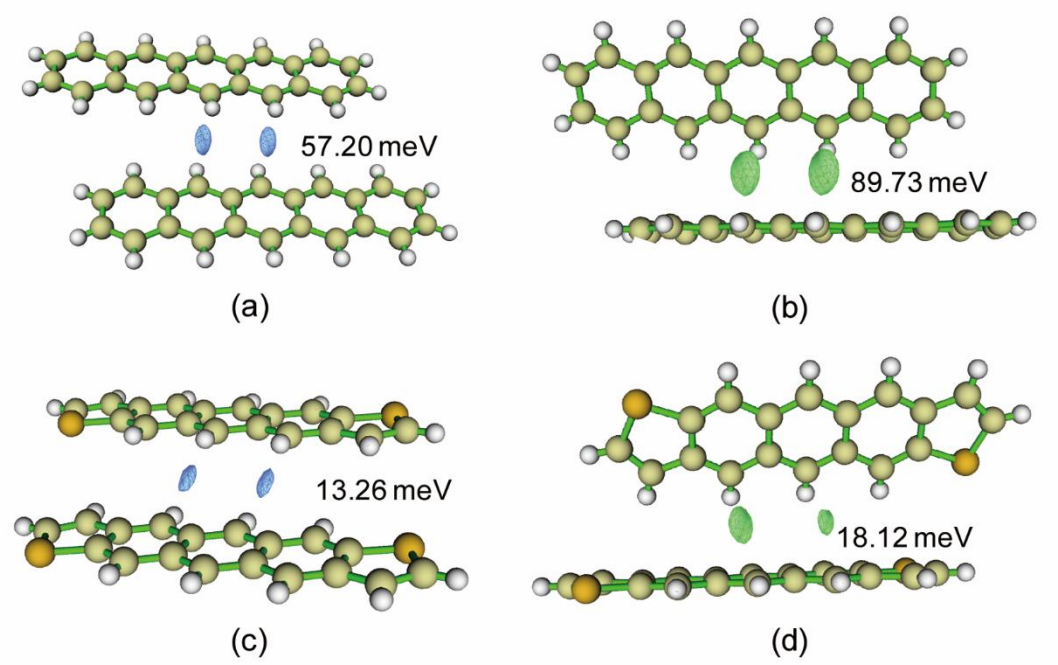

Figure S2. The HOMOs overlap of pentacene and ADT. (a) and (c) are the P-direction dimers of pentacene and ADT, respectively. In a similar way, (b) and (d) are the T-direction dimers of pentacene and ADT separately. (Calculated by Multiwfn)

Table S1 The intermolecular distance in crystal structure [Å].

Material	P-direction	T1-direction	T2-direction
DPAnt	6.24	4.82	4.82
DTAnt	6.09	4.84	4.84
Pentacene	6.27	5.21	4.76
ADT	5.92	5.03	4.73

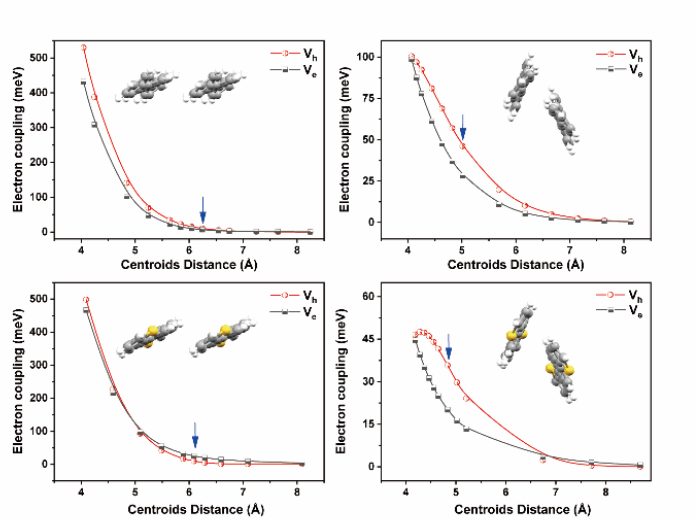

Figure S3 The electron coupling values with different intermolecular distances. The upper two are DPAnt's P-direction (left) and T-direction (right) dimer, and the lower two are DTAnt's P-direction (left) and T-direction (right) dimer, as shown in the ball-and-stick models. The blue arrows in the figures point to the experimental distances of each dimer. According to the Table S1, it indicates the value difference in the parameter of distance is small enough to ignore the little influence on the mobility for both the two series of materials. Furthermore, based on the Figure S3, there is no significant improvement for the contasting difference of two materials' electron coupling even though providing them with the same distance. In conclusion, the influence of intermolecular distance on the mobility here can be ignored.

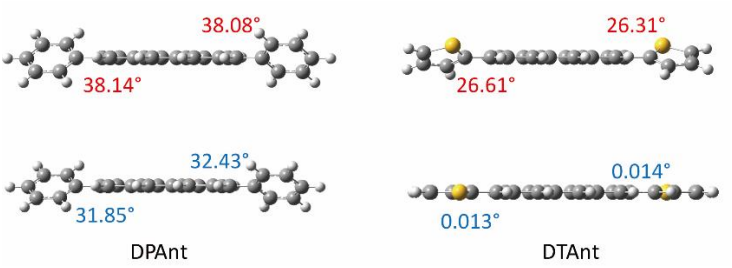

Figure S4 The geometric structures and torsion angles of DPAnt and DTAnt in the neutral and charged states. The left and right two molecules are DPAnt and DTAnt, respectively. The angles in red and blue represent separately the molecules in neutral and charged states. All the geometric structures are performed in B3LYP/6-311G** with Gaussian 09 package.