Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C

Electronic Supplementary Information:

Crystal structure versus charge transport in organic single crystals of [1]benzothieno[3,2-*b*][1]benzothiophene derivatives from a multiscale theoretical study

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Table S1. The total intramolecular reorganization energies (in meV) for C_n-BTBT (n=8, 10, 12) from the NM analysis approach and the AP approach, respectively.

	C_8-BTBT	C_{10}-BTBT	C_{12}-BTBT
NM	248.3	245.7	245.0
AP	236.3	253.6	241.8

Table S2. The transfer integrals (in meV) for all the nearest-neighboring dimers of each system in Fig. 1 from the experimental crystal structures.

Dimers	C_8-BTBT	C_{10}-BTBT	C_{12}-BTBT
A1	38.37	45.02	53.55
A2	38.37	45.02	53.56
B1	-7.26	-21.58	-36.91
B2	-7.25	-21.59	-36.92
C1	-7.25	-21.57	-36.91
C2	-7.26	-21.55	-36.91

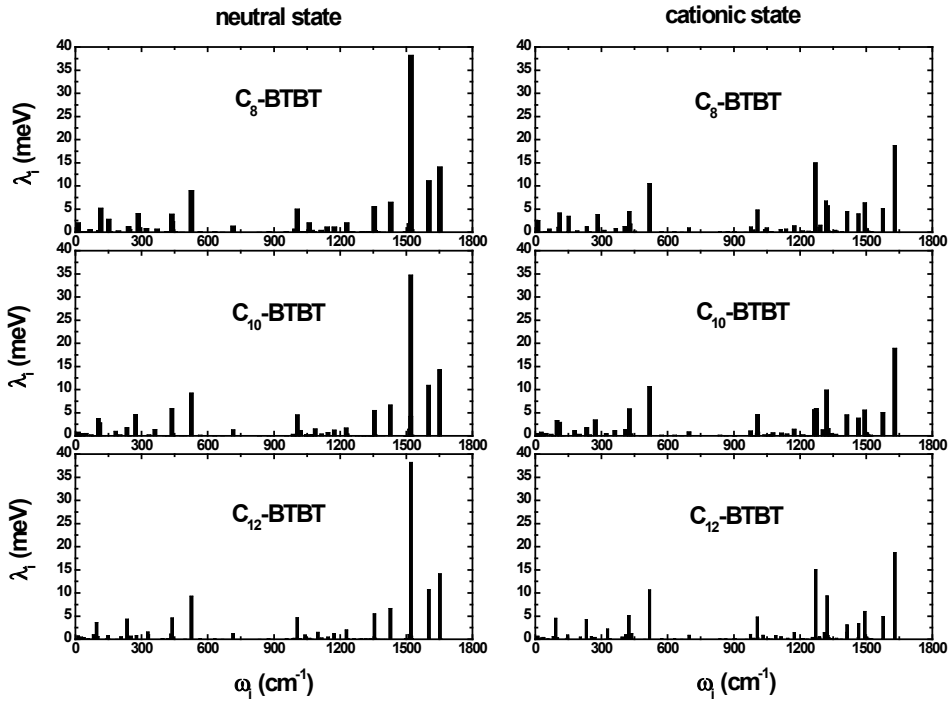

Figure S1. The vibrational frequency ω_i and reorganization energy λ_i of each normal mode in C_n-BTBT (n=8, 10, 12) for neutral and cationic states, respectively.

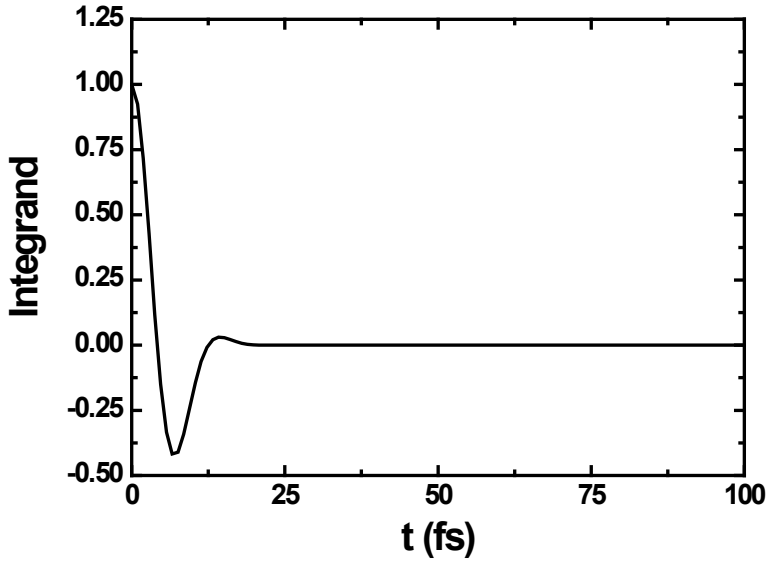

Figure S2. The relationship between integrand and time (t) in Eq. (3) are shown for C_8-BTBT at 300 K. The case is much similar for C_{10}-BTBT and C_{12}-BTBT, respectively. Since the integrand in Eq. (3) is an even function, the relationship is only shown here for $t \geq 0$.

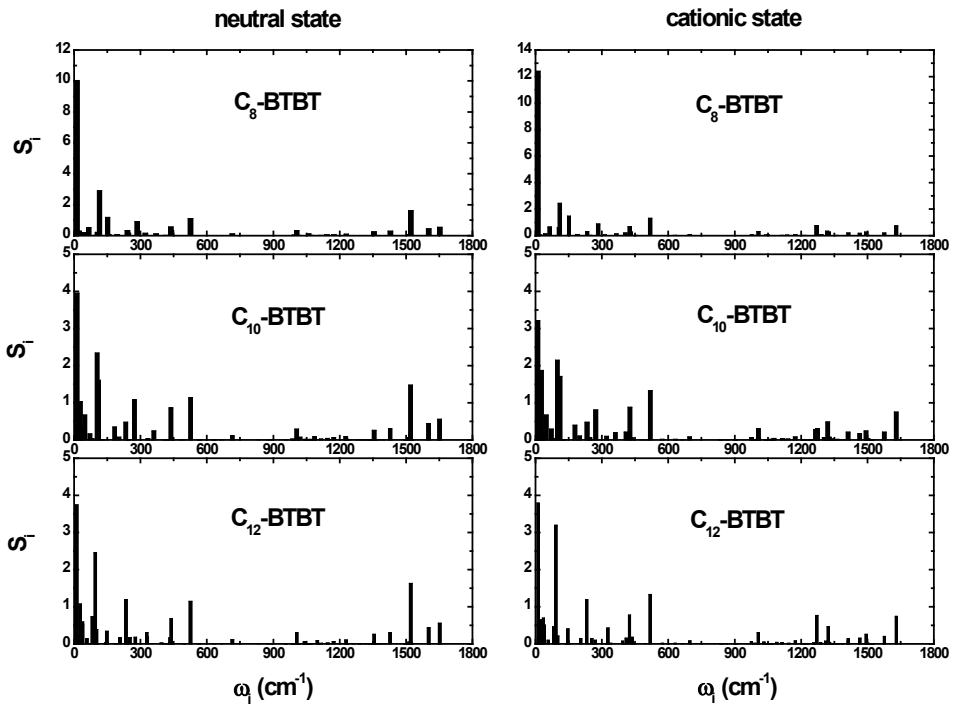

Figure S3. The Huang-Rhys factor $S_i = \lambda_i / \hbar\omega_i$ of each normal mode in C_n-BTBT (n=8, 10, 12) for neutral and cationic states, respectively.