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

Supporting Information

On the Impact of Isomer Structure and Packing Disorder in Thienoacene Organic Semiconductors

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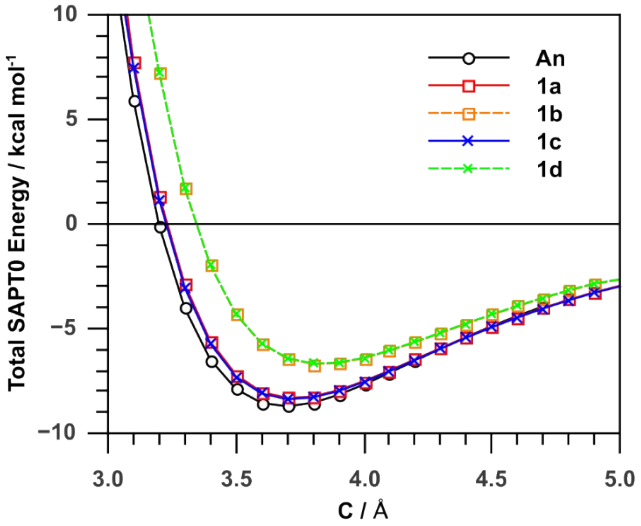


Figure S1. Total SAPT0/jun-cc-pVDZ interaction energies for anthracene as a function of the plane-to-plane *C*-distance. Data for ordered and disordered *anti*- and *syn*-BDT is repeated from the main manuscript for comparison.

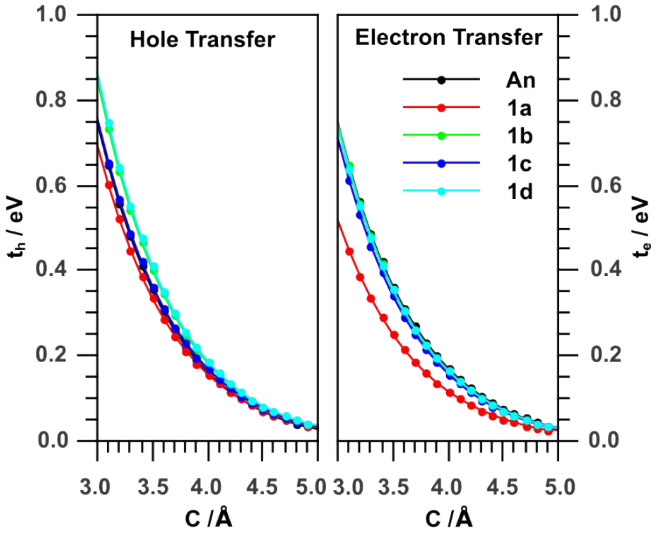


Figure S2. Transfer integrals for holes (t_h, left) and electrons (t_e, right) for anthracene as a function of intermolecular separation as determined at the B3LYP/6-31G(d) level of theory. Data for ordered and disordered *anti*- and *syn*-BDT is repeated from the main manuscript for comparison.

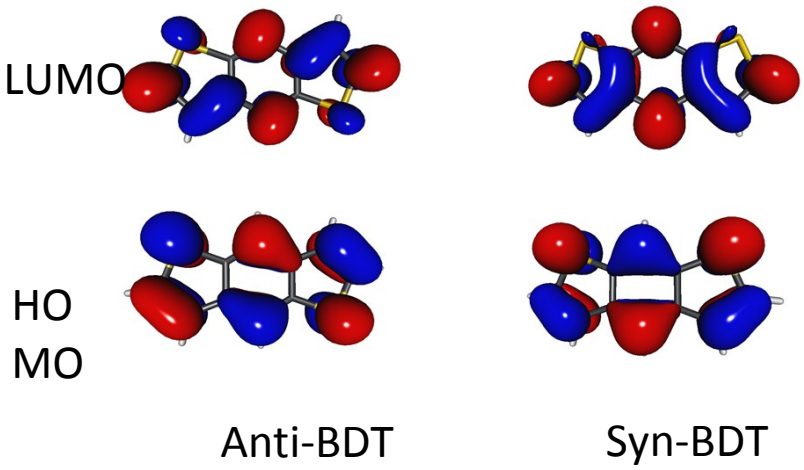


Figure S3. Pictorial representation of the HOMO and LUMO for (left) *anti*- and (right) *syn*-BDT as determined at the B3LYP/6-31G(d) level of theory.

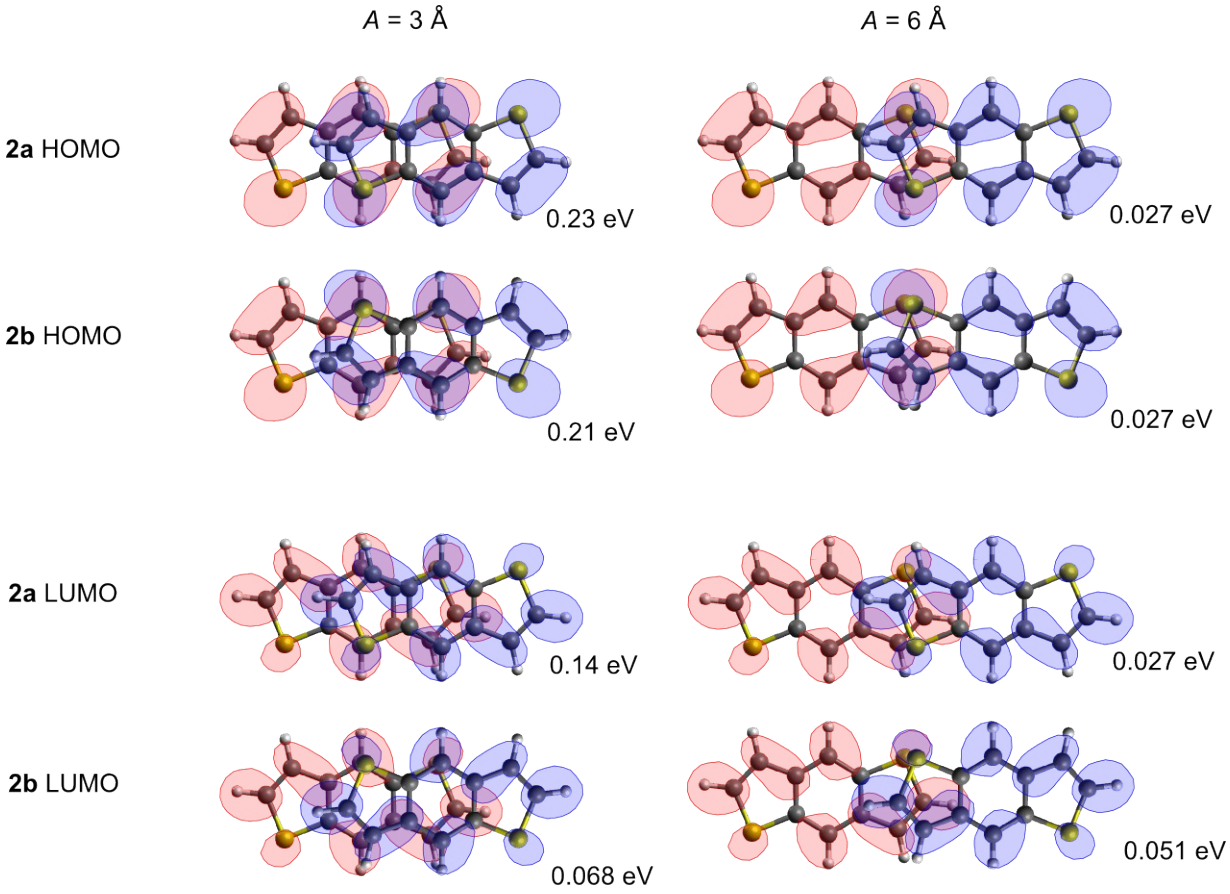


Figure S4. Selected *A* displacements of the *anti*-BDT disordermer pairs 2a and 2b showing the orbital overlap and calculated intermolecular electronic couplings as determined at the B3LYP/6-31G(d) level of theory. The (dimer) molecular orbitals are displayed such that the blue orbitals belong to the top molecule and the red orbitals to the bottom molecule in the stack.

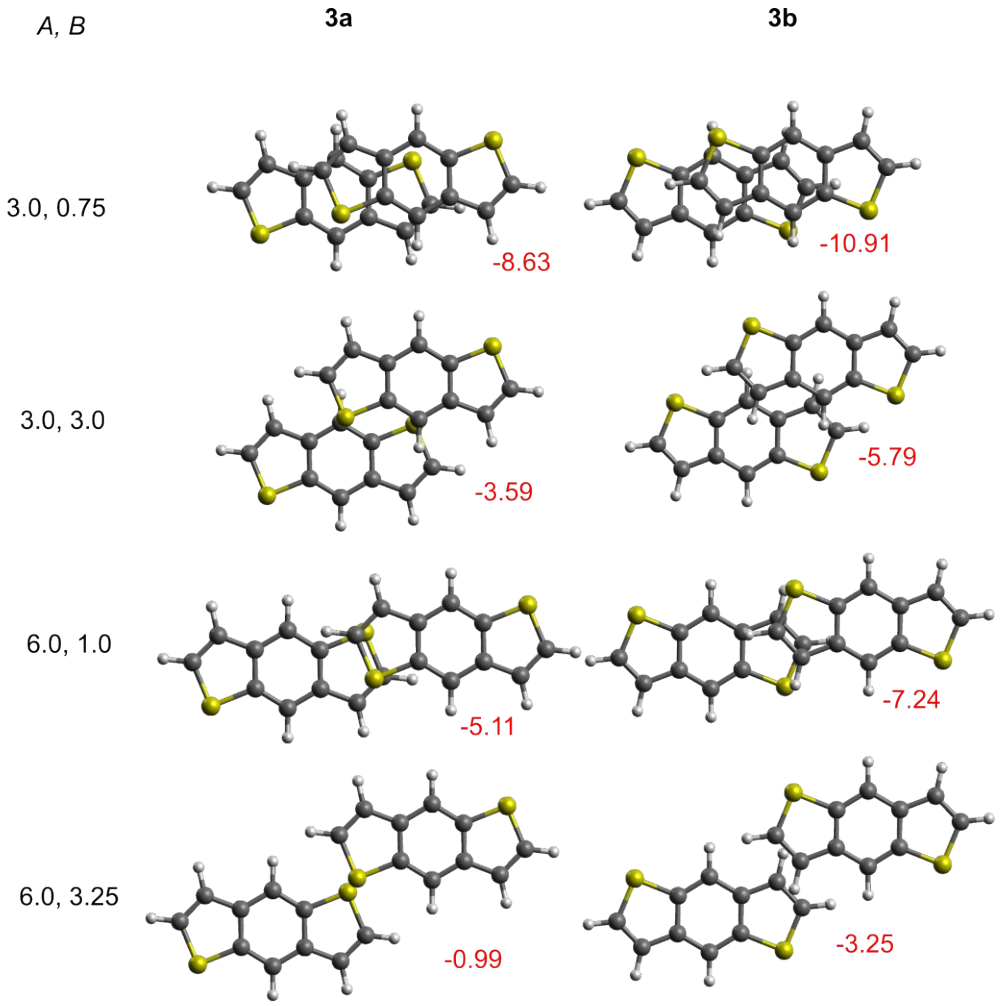


Figure S5. Molecular alignments from *A,B* displacements in Table 1 of the main manuscript for disordermer pairs 3a and 3b, highlighting the contacts involving sulfur. SAPT0/ jun-cc-pVDZ interaction energies are given in red in kcal mol^{-1}.

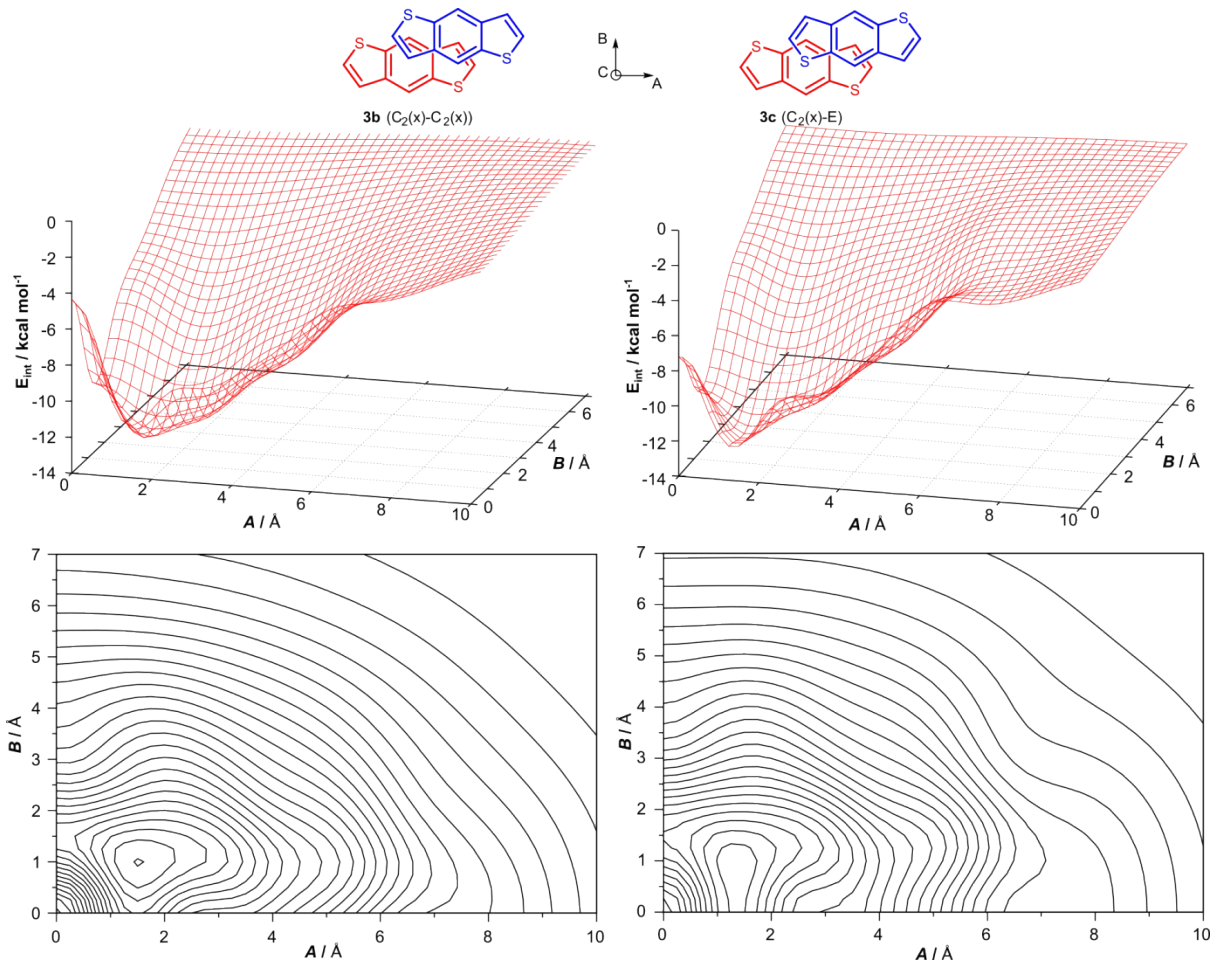


Figure S6. 3D surface (top) and contour (bottom) plots of the SAPT0/ jun-cc-pVDZ interaction energy as a function of *A* and *B* displacement for *anti*-BDT disordermer pairs 3b (left) and 3c (right). Contour lines represent changes in energy of 0.5 kcal mol^{-1}.

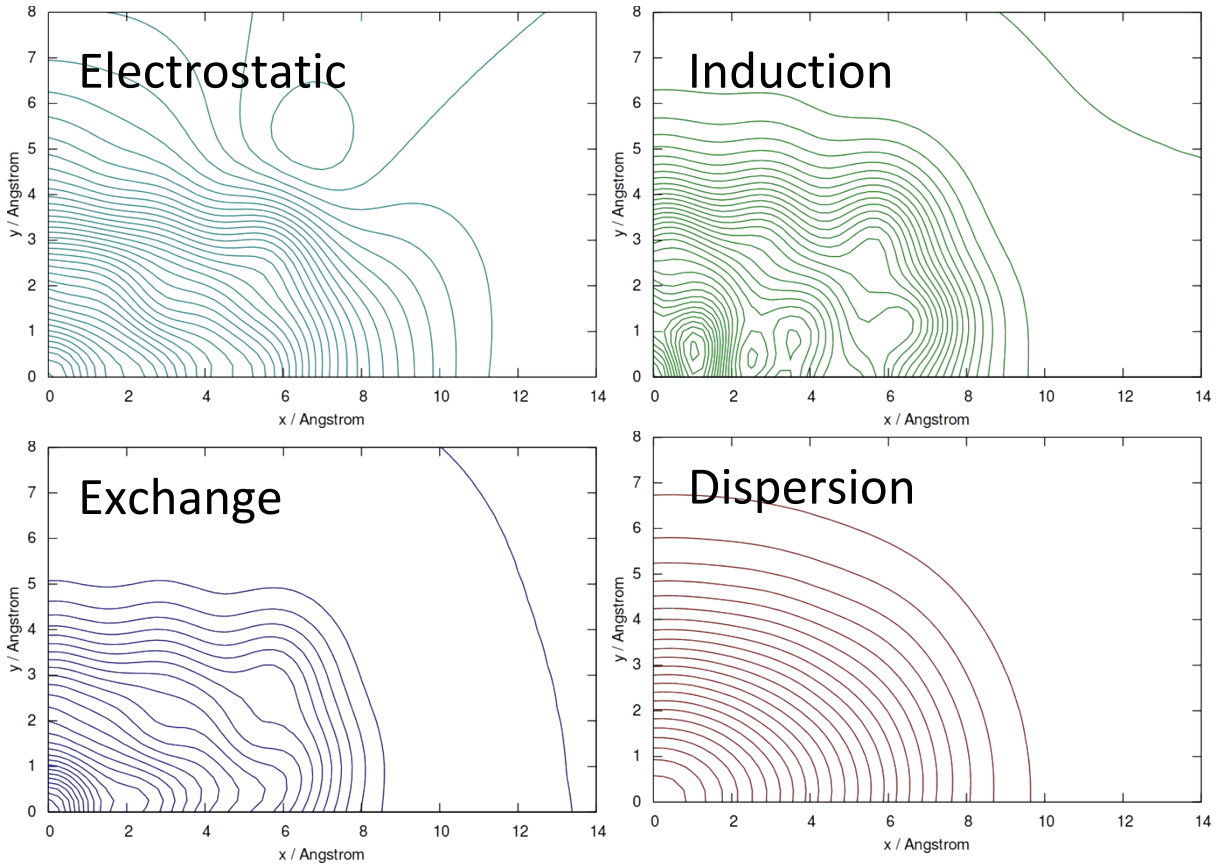
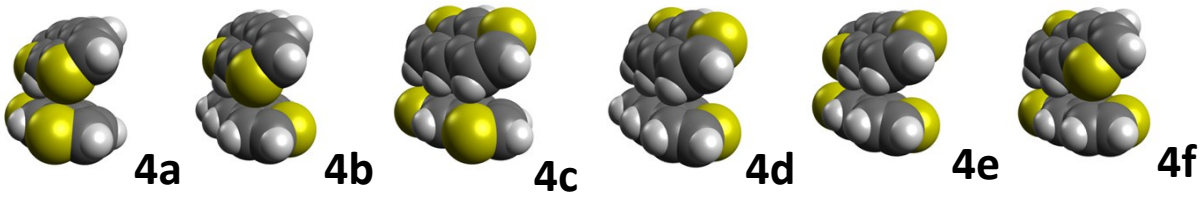


Figure S7. SAPT0/ jun-cc-pVDZ component energies E_{elec} (contour = 0.2 kcal mol^{-1}), E_{ind} (contour = 0.05 kcal mol^{-1}), E_{exch} (contour = 1 kcal mol^{-1}), and E_{disp} (contour = 1 kcal mol^{-1}) for disordermer pair 3a as a function of *A* and *B* displacement. *C* displacement is constant at 3.5 Å.

Table S1. SAPT0/ jun-cc-pVDZ energies for disordermer pairs of *syn* and *anti*-BDT with one molecule rotated by the angle θ. These are equivalent to one molecule rotated by 45°, and then applying a disorder transformation as described in the table. All energies are in kcal mol^{-1} and angles in degrees.



	***Syn*-BDT**				***Anti*-BDT**	
	4a	**4b**	**4c**	**4d**	**4e**	**4f**
θ	45	135	225	315	45/315	135/225
Disordermers	E-E	E-C_2	C_2-E	C_2-C_2	E-E	C_2-E
E_{elec}	-3.39	-2.45	-3.38	-1.56	-2.48	-2.91
E_{exch}	11.17	9.32	8.15	6.44	8.78	8.73
E_{ind}	-1.19	-0.92	-1.16	-0.83	-1.01	-1.06
E_{disp}	-11.77	-11.35	-10.49	-10.10	-10.94	-10.94
E_{int}	**-5.18**	**-5.41**	**-6.88**	**-6.05**	**-5.65**	**-6.18**