Supporting Information

Effect of Donor Length on the Electronic Structures and Charge Transport Polarity for DTDPP-based D-A Copolymers: a Computational Study Based on Super-Exchange Model

Feifei He[†a], Changli Cheng, [†a] Hua Geng,[*b] Yuanping Yi[c] and Zhigang Shuai[*a]

[a]MOE Key Laboratory of Organic OptoElectronics and Molecular Engineering, Department of Chemistry, Tsinghua University, Beijing 100084, China.

[b]Department of Chemistry, Capital Normal University, Beijing 100048, China.

[c]Beijing National Laboratory for Molecular Sciences, CAS Key Laboratory of Organic Solids, Institute of Chemistry, Chinese Academy of Sciences, Beijing 100190, China.

Figure S1. (a) The molecular orbitals of ADA cluster, DTDPP and 2T; (b) The partial charge density at high symmetry points for DTDPP-2T.

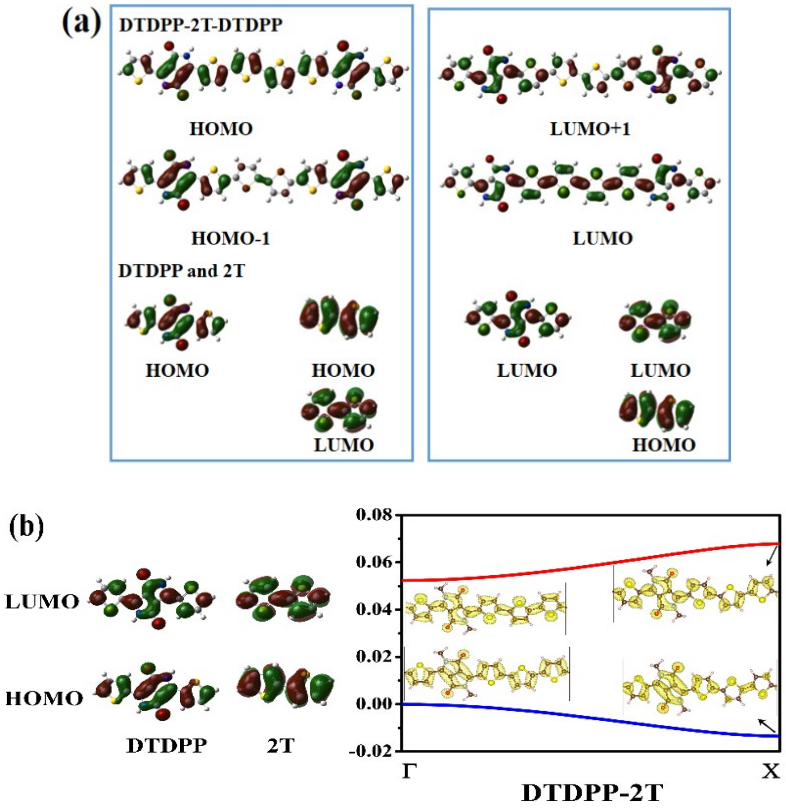

Figure S2. The energy gap of DTDPP-nT (n=1-4) calculated from extrapolation method.

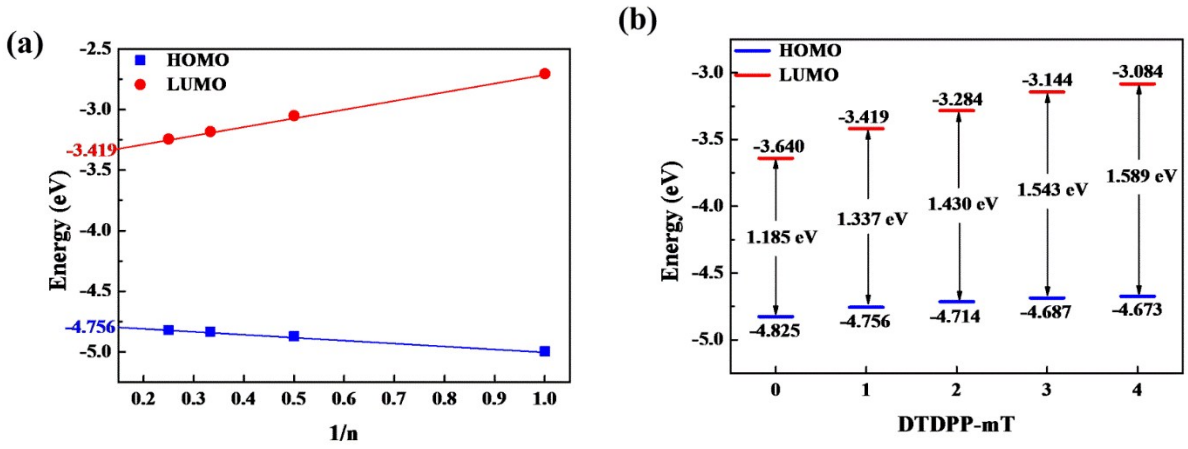

Table S1. The main bridge orbital contribution to the SE coupling at B3LTP/6-31g* level.

Systems	Bridge Orbital	Electron SE coupling (meV)	Hole SE coupling (meV)
DTDPP-T	HOMO-3	-20	-17
	HOMO	83	99
	LUMO	179	61
	LUMO+2	-28	-16
DTDPP-2T	HOMO-3	-52	-40
	HOMO	62	127
	LUMO	167	44
	LUMO+1	-36	-27
DTDPP-3T	HOMO-5	21	20
	HOMO-1	-39	-46
	HOMO	41	108
	LUMO	132	24
	LUMO+1	-55	-22
DTDPP-4T	HOMO-1	-33	-46
	HOMO	29	106
	LUMO	132	21
	LUMO+1	-66	-23
	LUMO+2	32	15
DTDPP-5T	HOMO-2	-24	12
	HOMO-1	30	0.0
	HOMO	-22	-101
	LUMO	-118	-34
	LUMO+1	72	22

Figure S3. The inter-chain binding energy of DTDPP (a), DTDPP-2T (b) and DTDPP-4T (c).

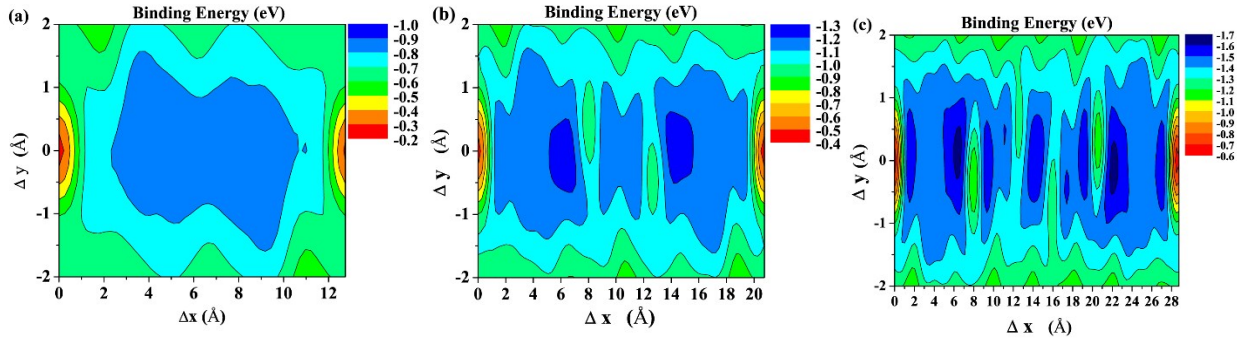

Figure S4.The distribution of electrostatic potential for the most stable structure of DTDPP (a) and DTDPP-2T (b). Red indicates a negative value, and blue indicates a positive value.