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

Supporting Information for:

Super-exchange-Induced High Performance Charge Transport in Donor-Acceptor Copolymers

Changli Cheng[a], Hua Geng*[b], Yuanping Yi[b], Zhigang Shuai*[a, b]

(a) MOE Key Laboratory of Organic OptoElectronics and Molecular Engineering, Department of Chemistry, Tsinghua University, Beijing 100084, China

(b) Beijing National Laboratory for Molecular Sciences, CAS Key Laboratory of Organic Solids, Institute of Chemistry, Chinese Academy of Sciences, Beijing 100190, China

*Email - hgeng@iccas.ac.cn , zgshuai@tsinghua.edu.cn

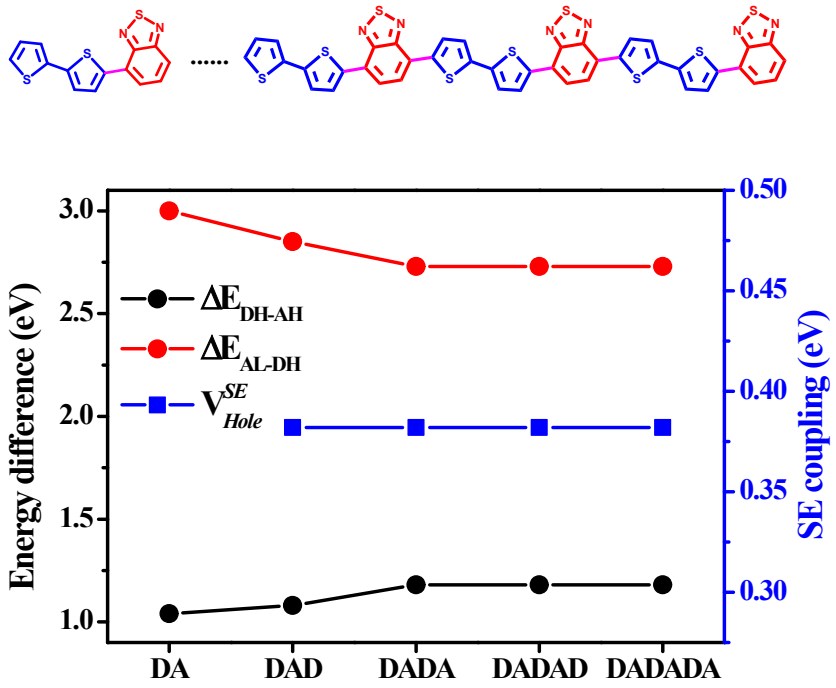

Figure S1. The site energy difference and SE coupling dependence on the length of oligomer chain.

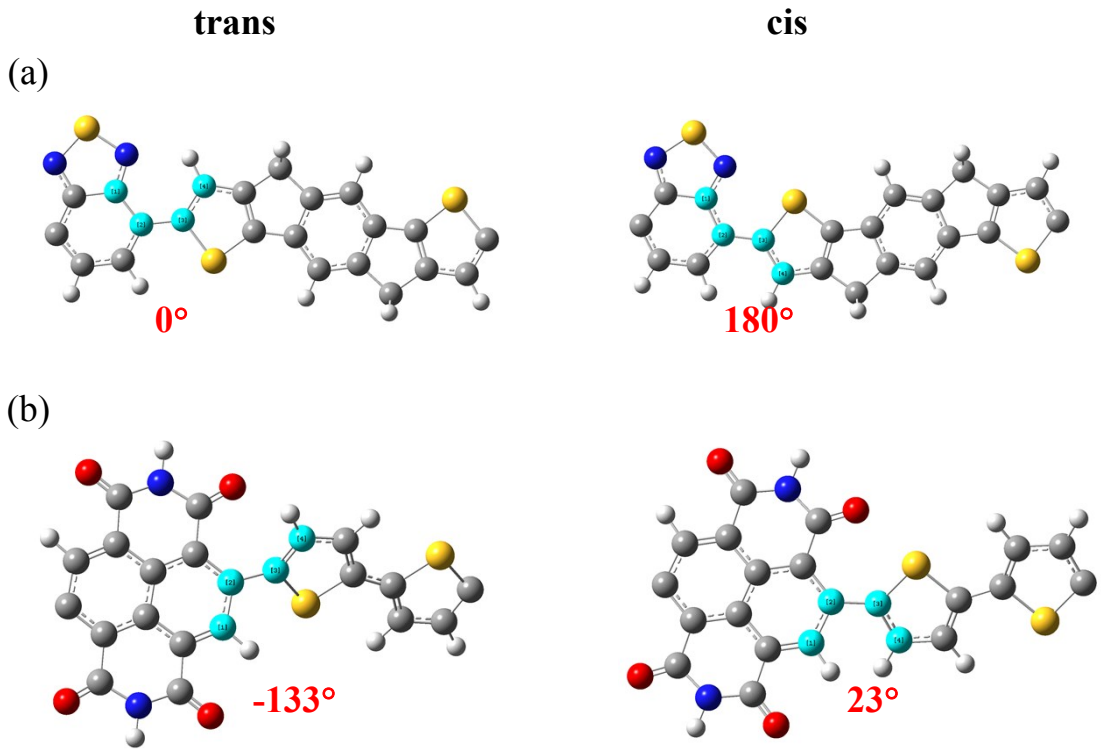

Figure S2. Unit cell of IDT-BT (a) and 2T-NDT (b). Trans/Cis conformations and corresponding dihedrals between donor and acceptor unit are shown.

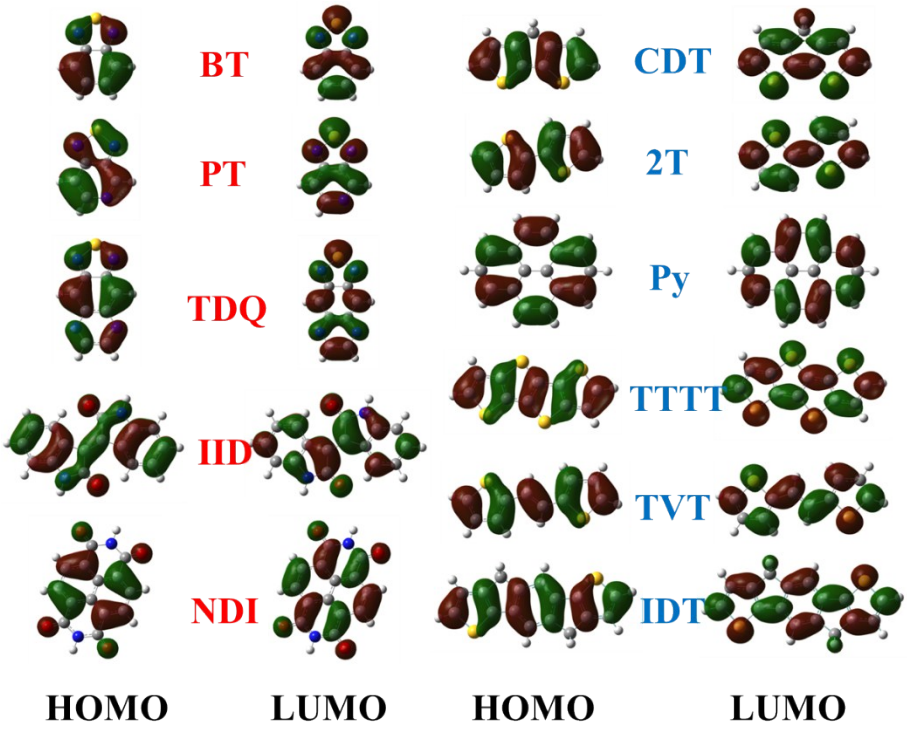

Figure S3. HOMO and LUMO of isolated Donors and Acceptors moieties.

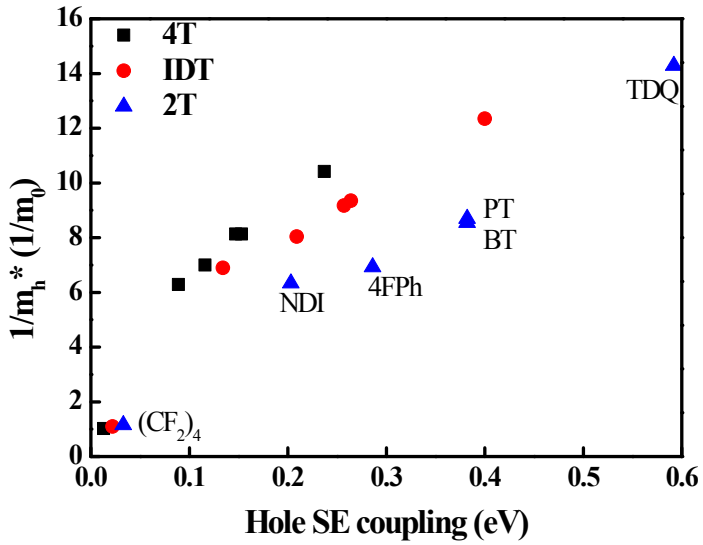

Figure S4. The inverse of hole effective mass as a function of super-exchange coupling for hole.

Table S1. Unit cell energy and hole effective mass for each conformation.

Conformation	Energy (hartree/cell)	Hole effective mass (m_0)
IDT-BT trans	-2147.0071	0.109
IDT-BT cis	-2147.0068	0.109
2T-NDI trans	-2048.2214	0.193
2T-NDI cis	-2048.2219	0.158

Table S2. The optimized bond length (dihedral angle) connecting donor and acceptor. Units in Å (degree).

	BT	**PT**	**TDQ**	**NDI**	**IID**	**$(CF_2)_4$**	**4FPh**
CDT	1.451(0°)	1.445(0°)	1.448(0°)	1.473(28°)	1.461(24°)	1.491	1.457(0°)
2T	1.455(0°)	1.452(0)	1.444(0°)	1.476(23°)	1.463(6°)	1.493	1.458(0°)
Flu	1.483(36°)	1.481(31°)	1.482(41°)	1.495(59°)	1.484(36°)	1.504	1.487(28°)
Py	1.485(38°)	1.484(34°)	1.484(29°)	1.497(54°)	1.487(41°)	1.504	1.489(28°)
TTTT	1.454(0°)	1.451(0°)	1.446(0°)	1.474(36°)	1.463(18°)	1.494	1.459(0°)
TVT	1.454(0°)	1.449(0°)	1.444(0°)	1.475(26°)	1.462(13°)	1.494	1.458(0°)
IDT	1.456(0°)	1.451(0°)	1.448(0°)	1.475(29°)	1.462(11°)	1.492	1.459(0°)
4T	1.455(0°)	1.451(0°)	1.449(0°)	1.475(26°)	1.463(23°)	1.492	1.458(0°)

Table S3. List of $1/m^*$ in Figure 2(a) of main manuscript.

A / D	TDQ	PT	BT	4FPh	IID	NDI	$(CF_2)_4$
Py	0.100	0.100	0.078	0.100	0.100	0.068	0.010
Flu	5.291	5.780	5.128	5.460	4.808	2.519	1.200
4T	10.417	8.130	8.130	7.000	6.250	6.289	1.020
IDT	12.346	9.346	9.174	8.040	8.197	6.897	1.100
TVT	14.286	9.709	9.346	7.900	7.813	6.944	1.100
TTTT	14.286	10.204	9.524	8.420	7.752	6.211	1.200
2T	14.286	8.696	8.547	6.920	7.463	6.329	1.150
CDT	12.658	10.989	10.526	8.440	7.407	7.407	1.320

Table S4. Frontier orbital energies, HOMO and LUMO charge density at linkage atom ($\rho_{HOMO/LUMO}$) and the length of isolated donor or acceptor, all calculated at B3LYP/6-31G* level.

Acceptors	ρ_{HOMO}	ρ_{LUMO}	*a* (Å)	LUMO (eV)	HOMO (eV)
BT	0.250	0.103	2.9	-2.346	-6.610
PT	0.239	0.109	2.8	-2.821	-7.090
TDQ	0.244	0.122	2.9	-3.197	-6.402
NDI	0.054	0.068	5.1	-3.555	-7.196
IID	0.072	0.062	9.6	-2.712	-5.698
4FPh	0.334(H-1)	0.310	2.8	-0.823	-6.783
$(CF_2)_4$	0.077	0.138	4.0	1.006	-8.967
Donors	ρ_{HOMO}	ρ_{LUMO}	*a* (Å)	LUMO (eV)	HOMO (eV)
CDT	0.196	0.161	6.4	-0.985	-5.220
2T	0.183	0.150	6.4	-1.247	-5.475
Flu	0.165	0.160	6.9	-0.713	-5.756
Py	0.002	0.003	7.0	-1.480	-5.326
TTTT	0.149	0.139	8.4	-1.337	-5.419
TVT	0.140	0.104	8.9	-1.593	-5.202
IDT	0.121	0.111	10.6	-1.180	-5.028
4T	0.068	0.055	14.3	-1.930	-4.963