Research on charge-transport properties of TTF-TTP derivatives and organic interfaces

Table S1. Measured geometric parameters (in Å) and the maximum values of calculated intermolecular transfer integral (in meV) for compound 1-6

Compound	d(C=C)	d(S-S)	d(min)	d(cen)	d(S^1-S)	V_{hole}(max)	V_{ele}(max)
1	1.35	3.24	4.15	7.41	5.03	107.64	11.19
2	1.34	3.22	3.77	4.11	4.11	64.46	24.81
3	1.31	3.17	3.76	4.63	5.99	80.46	26.69
4	1.35	3.23	3.76	6.11	4.00	75.52	92.99
5	1.33	3.23	3.82	6.14	4.04	75.36	33.25
6	1.35	3.23	3.72	6.32	4.09	49.99	33.25

Table S2 Measured geometric parameters (in Å) and the maximum values of calculated intermolecular transfer integral (in meV) for compound 7-12

Compound	d(C=C)	d(S-S)	d(min)	θ	d(cen)	d(S_1-S)	V_{hole}(max)	V_{ele}(max)
7	1.348	3.21	3.497	68.687	3.854	4.728	61.697	57.30035
8	1.348	3.189	3.742	79.244	3.855	3.855	29.737	99.4274
9	1.334	3.187	3.452		10.87	7.412	40.691	12.37225
10	1.443		3.818	65.128	4.732	3.746	16.221	36.70412
11	1.335	3.216	3.578		4.624	4.624	69.064	18.93624
12	1.339	3.21	3.351	77.425	6.093	3.758	16.666	14.96019

Table S3 Measured geometric parameters (in Å) and the maximum values of calculated intermolecular transfer integral (in meV) for compound 13-17

Compound	d(C=C)	d(S-S)	d(min)	d(cen)	d(S^1-S)	V_{hole}(max)	V_{ele}(max)
13	1.34	3.252	3.78	6	4.972	22.	0.67
14	1.345	3.171	3.763	6.166	4.541	69.58	25.69
15	1.327	3.338	3.672	9.916	5.358	5.70	17.72
16	1.344	3.215	6.355	8.443	7.934	17.21	3.18
17	1.343	3.313	3.609	5.422	3.784	30.41	23.91

Table S4 Measured geometric parameters (in Å) and the maximum values of calculated intermolecular transfer integral (in meV) for compound 18 and 19

Compound	d(C=C)	d(S-S)	d(min)	d(cen)	d(S^1-S)	V_{hole}(max)	V_{ele}(max)
18	1.341	3.071	4.52	5.216	5.216	43.40	37.40
19	1.343	3.066	3.628	6.116	4.037	99.22	37.40

Table S5. Calculated HOMOs, LUMOs, HOMO-LUMO gaps, reorganization energies (λ_{hole} and λ_{ele}), IPs and EAs for TTF derivatives using B3LYP/6-31 G(d) (in eV)

Compound	HOMO	LUMO	H-L gap	λ_{hole}	λ_{ele}	EA	IP
1	-4.32	-0.72	3.60	0.28	0.45	0.59	5.76
2	-4.81	-1.24	3.57	0.23	0.14	-0.23	6.03
3	-4.68	-1.13	3.54	0.25	0.23	-1.42	6.74
4	-4.26	-0.69	3.57	0.24	0.20	-1.69	6.84
5	-4.27	-0.68	3.59	0.27	0.44	0.57	5.65
6	-4.25	-0.68	3.57	0.16	0.47	-3.19	6.54
7	-4.83	-1.32	3.51	0.30	0.48	0.04	6.22
8	-5.58	-2.52	3.06	0.32	0.69	-0.29	6.03
9	-5.73	-2.74	2.99	0.42	0.27	-1.43	6.57
10	-5.35	-2.83	2.47	0.18	0.63	0.69	6.03
11	-5.49	-2.46	3.04	0.31	0.71	0.77	6.14
12	-4.32	-0.96	3.36	0.28	0.45	0.58	5.66
13	-5.01	-1.93	3.08	0.27	0.44	0.58	5.63
14	-5.44	-2.60	2.84	0.29	0.47	0.18	5.53
15	-5.29	-2.35	2.94	0.52	0.54	-1.52	6.56
16	-5.47	-2.65	2.82	0.52	0.90	-1.08	6.20
17	-5.42	-2.57	2.85	0.31	0.79	-2.52	4.57
18	-4.62	-0.50	4.12	0.51	0.53	-1.61	6.56
19	-4.74	-0.45	4.29	0.54	0.55	-1.55	6.53

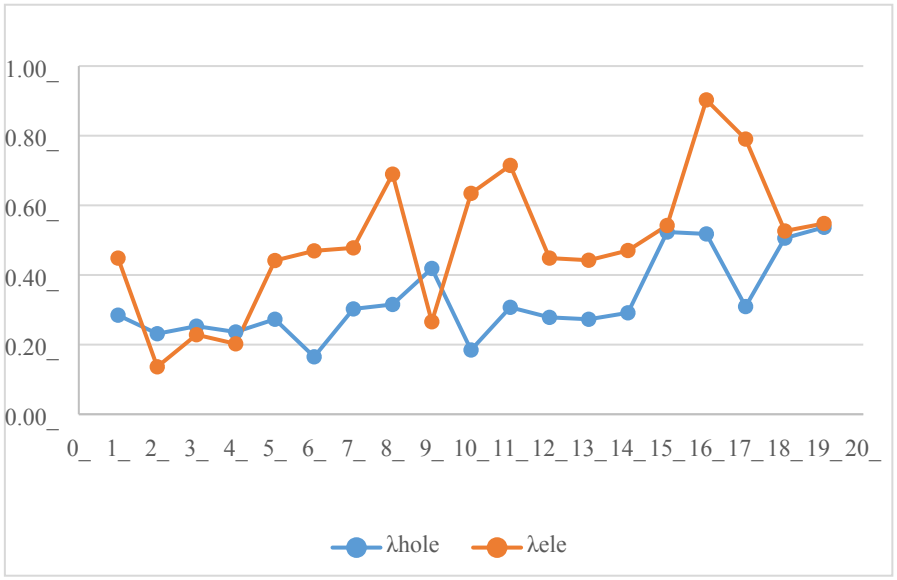

Figure S1. Reorganization energies for all compounds

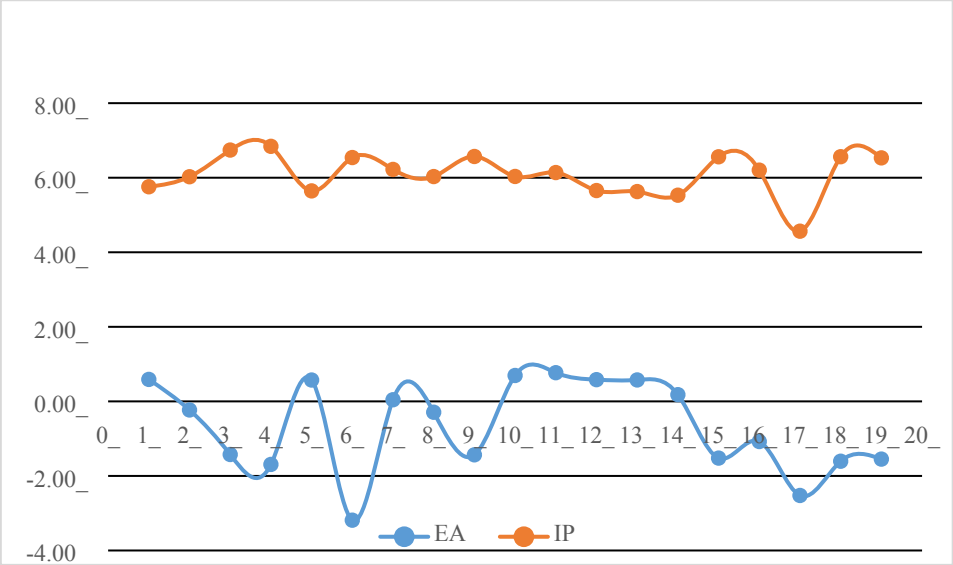

Figure S2. Calaulated energies of EA and IP for all compunds

Table S6. Simulated maximum charge transfer mobilities for all compounds 1-19

	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**
E	0.002	0.004	6.92×10^{-12}	0.190	0.846	0.020	1.709	1.090	0.058	4.03×10^{-5}
H	1.821	0.338	0.370	0.606	0.024	0.451	0.658	0.168	0.414	0.096
	11	**12**	**13**	**14**	**15**	**16**	**17**	**18**	**19**	
E	0.046	0.004	0.000	0.024	4.73×10^{-4}	0.148	0.003	0.003	1.03×10^{-4}	
H	0.094	0.035	0.006	0.902	0.008	0.006	0.005	0.670	0.950	