Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information:

From Y6 to BTPT-4F: a theoretical insight into the influence of the individual change of fused-ring skeleton length or side alkyl chains on molecular arrangements and electron mobility

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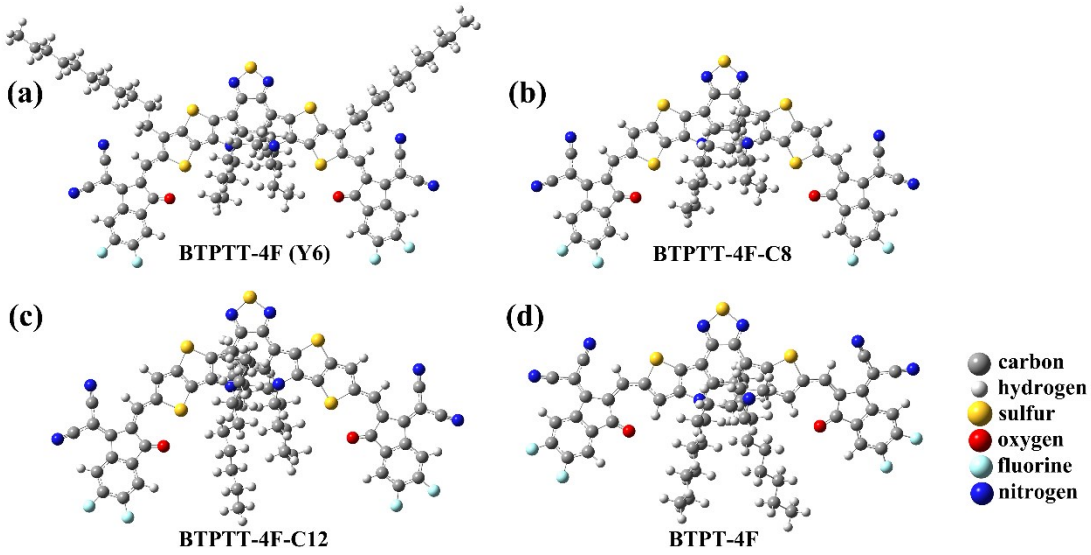

Figure S1. Optimized structures of (a) BTPTT-4F (Y6), (b) BTPTT-4F-C8, (c) BTPTT-4F-C12, and (d) BTPT-4F. Color of codes: grey-carbon, white-hydrogen, yellow-sulfur, red-oxygen, light blue-fluorine and blue-nitrogen.

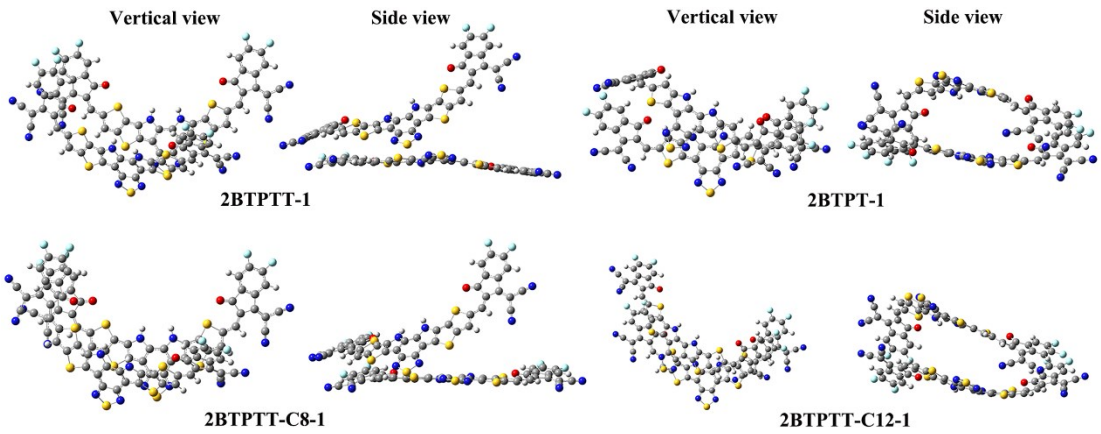

Figure S2. Optimized dimer configurations with bimolecular parallel. The alkyl side chains are omitted for clarity.

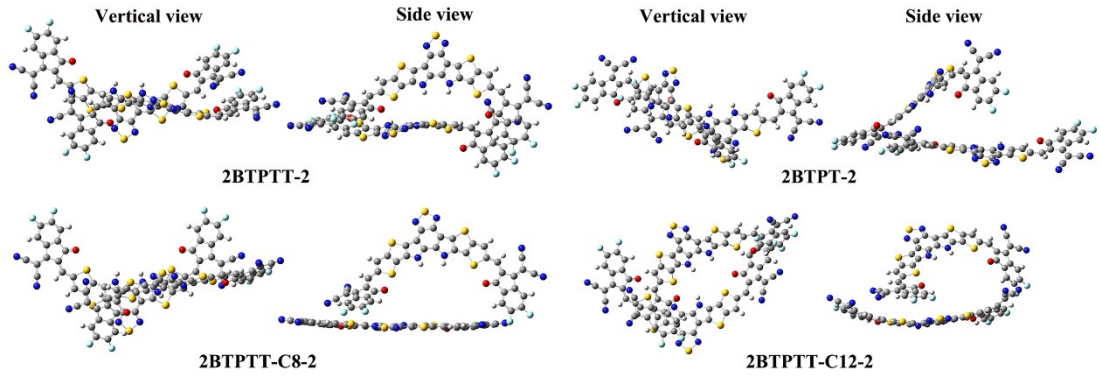

Figure S3. Optimized dimer configurations with bimolecular anti-parallel. The alkyl side chains are omitted for clarity.

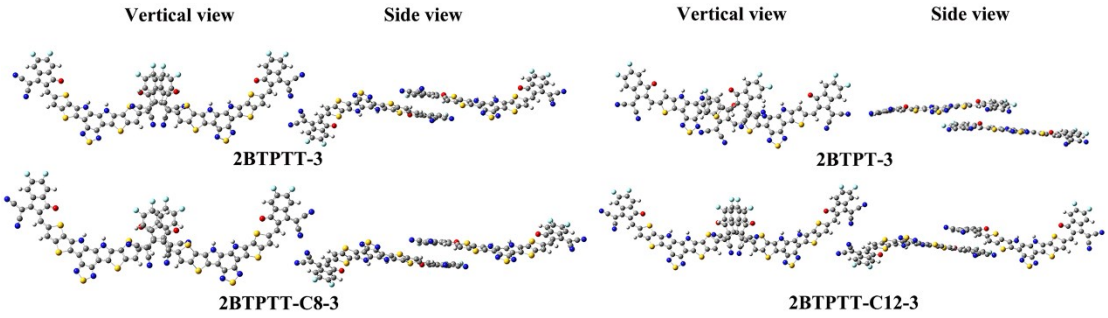

Figure S4. Optimized dimer configurations with end-group overlap. The alkyl side chains are omitted for clarity.

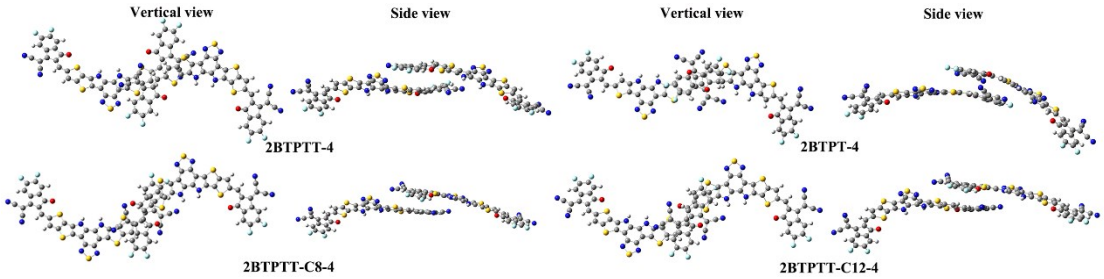

Figure S5. Optimized dimer configurations with end-group anti-overlap. The alkyl side chains are omitted for clarity.

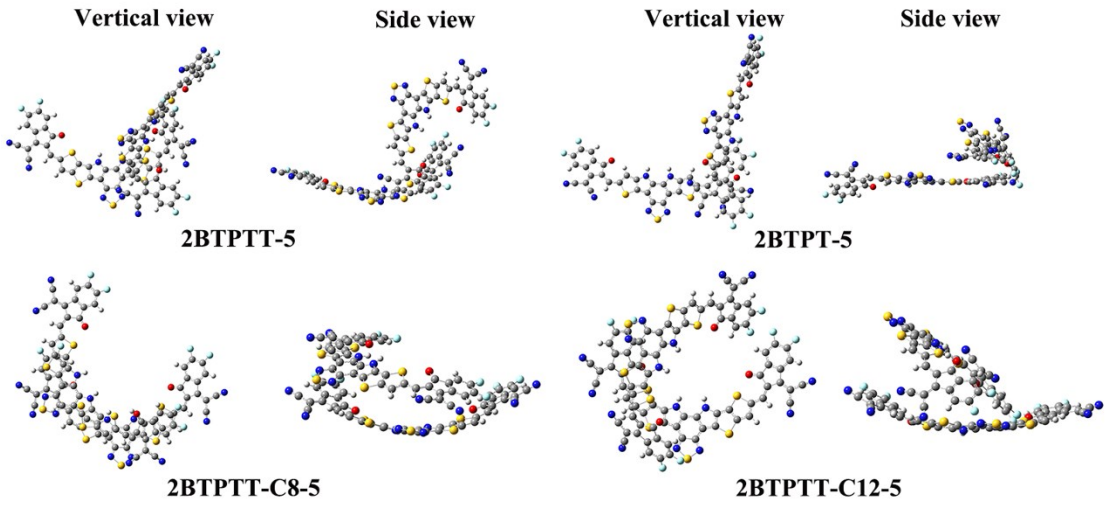

Figure S6. Optimized dimer configurations with bimolecular vertical and central sulfur atom pointing left. The alkyl side chains are omitted for clarity.

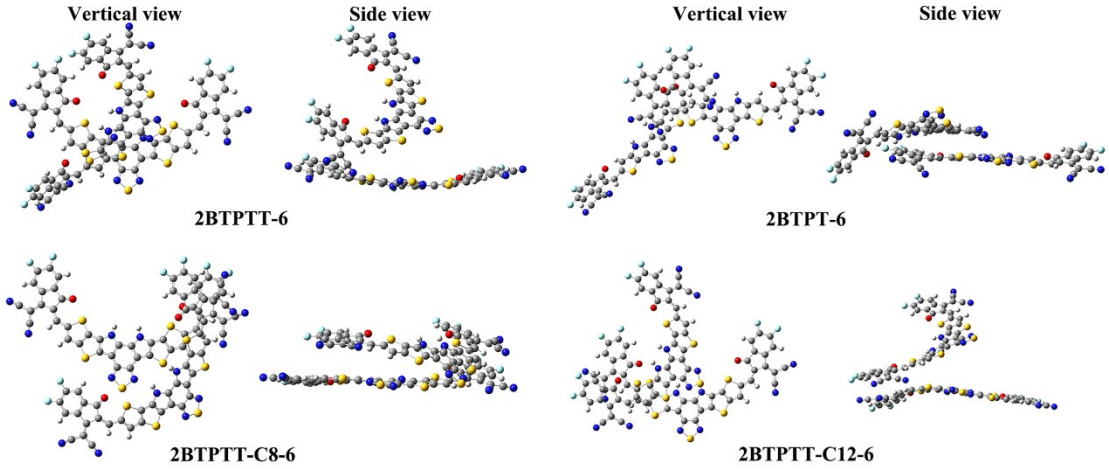

Figure S7. Optimized dimer configurations with bimolecular vertical and central sulfur atom pointing right. The alkyl side chains are omitted for clarity.

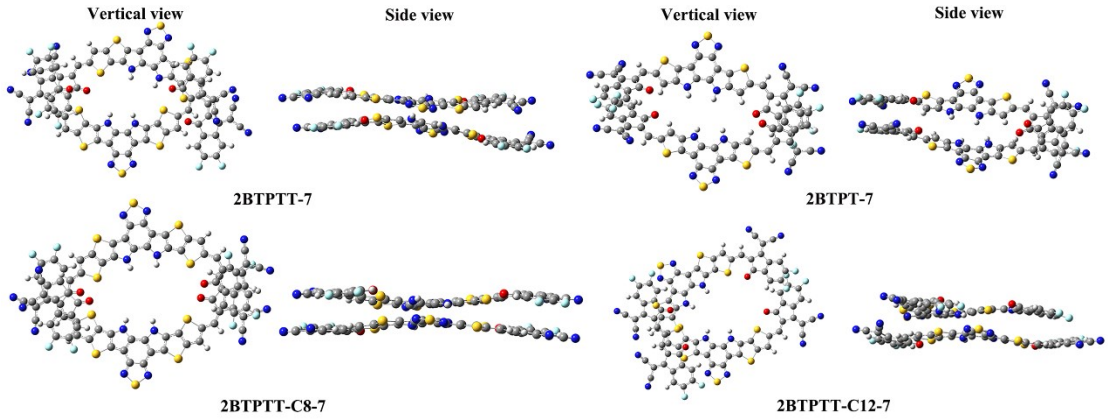

Figure S8. Optimized dimer configurations with tail to tail overlap. The alkyl side chains are omitted for clarity.

Table S1. Dihedral angles of BTPTT-4F (α_1, β_1 and γ_1), BTPTT-4F-C8 (α_2, β_2 and γ_2), BTPTT-4F-

C12 (α_3, β_3 and γ_3), and BTPT-4F (α_4, β_4 and γ_4). Unit: degree.

System	α_1	β_1	Average(α_1, β_1)	γ_1
BTPTT-4F(Y6)	1.27	0.22	0.75	11.15
2BTPTT-1	1.07	6.36	3.72	7.63
	1.81	11.28	6.55	16.29
2BTPTT-2	19.87	8.24	14.06	21.41
	6.55	23.96	15.26	23.87
2BTPTT-3	8.14	0.88	4.51	11.67
	8.95	1.04	5.00	12.09
2BTPTT-4	4.64	0.69	2.67	15.01
	0.42	5.78	3.10	8.45
2BTPTT-5	16.33	1.33	8.83	15.86
	0.45	10.81	5.63	13.40
2BTPTT-6	11.64	2.01	6.83	10.16
	18.03	0.69	9.36	8.54
2BTPTT-7	3.73	5.83	4.78	10.50
	1.01	12.13	6.57	8.08

System	α_2	β_2	Average(α_2, β_2)	γ_2
BTPTT-4F-C8	0.27	0.05	0.16	11.43
2BTPTT-C8-1	3.15	2.17	2.66	7.84
	4.31	8.13	6.22	16.72
2BTPTT-C8-2	13.73	1.39	7.56	12.65
	0.18	2.25	1.22	6.33
2BTPTT-C8-3	9.88	1.22	5.55	11.19
	8.49	0.81	4.65	10.87
2BTPTT-C8-4	6.50	0.27	3.39	13.26
	3.78	0.56	2.17	10.16
2BTPTT-C8-5	9.97	2.36	6.17	14.46
	8.78	5.42	7.10	10.69
2BTPTT-C8-6	10.03	10.94	10.49	10.10
	0.79	0.29	0.54	12.19
2BTPTT-C8-7	1.16	3.09	2.13	9.35
	7.08	1.31	4.20	8.69

System	α_3	β_3	Average(α_3, β_3)	γ_3
BTPTT-4F-C12	0.03	0.47	0.25	11.66
2BTPTT-C12-1	10.26	5.11	7.69	15.63
	6.26	10.54	8.40	13.54
2BTPTT-C12-2	5.48	12.19	8.84	11.85
	4.72	1.29	3.01	0.18
2BTPTT-C12-3	15.55	0.53	8.04	12.12
	4.63	1.44	3.04	11.59

2BTPTT-C12-4	8.09	1.86	4.98	12.82
	0.05	0.23	0.14	12.76
2BTPTT-C12-5	13.44	2.46	7.95	9.27
	5.85	1.74	3.80	12.80
2BTPTT-C12-6	5.88	0.17	3.03	12.17
	0.79	1.20	1.00	9.66
2BTPTT-C12-7	7.19	5.22	6.21	7.57
	3.68	2.93	3.31	5.91

System	α_4	β_4	Average(α_4, β_4)	γ_4
BTPT-4F	5.22	2.63	3.93	11.38
2BTPT-1	33.69	0.92	17.31	11.90
	5.79	10.44	8.12	12.14
2BTPT-2	4.32	4.50	4.41	9.60
	22.00	13.06	17.53	12.82
2BTPT-3	3.85	2.20	3.03	5.85
	0.63	4.99	2.81	4.51
2BTPT-4	4.47	10.56	7.52	9.61
	4.76	6.11	5.44	10.87
2BTPT-5	5.05	2.79	3.92	11.35
	11.31	8.30	9.81	14.04
2BTPT-6	7.40	6.35	6.88	12.27
	4.68	3.03	3.86	10.54
2BTPT-7	9.21	18.03	13.62	10.25
	9.29	18.61	13.95	12.32

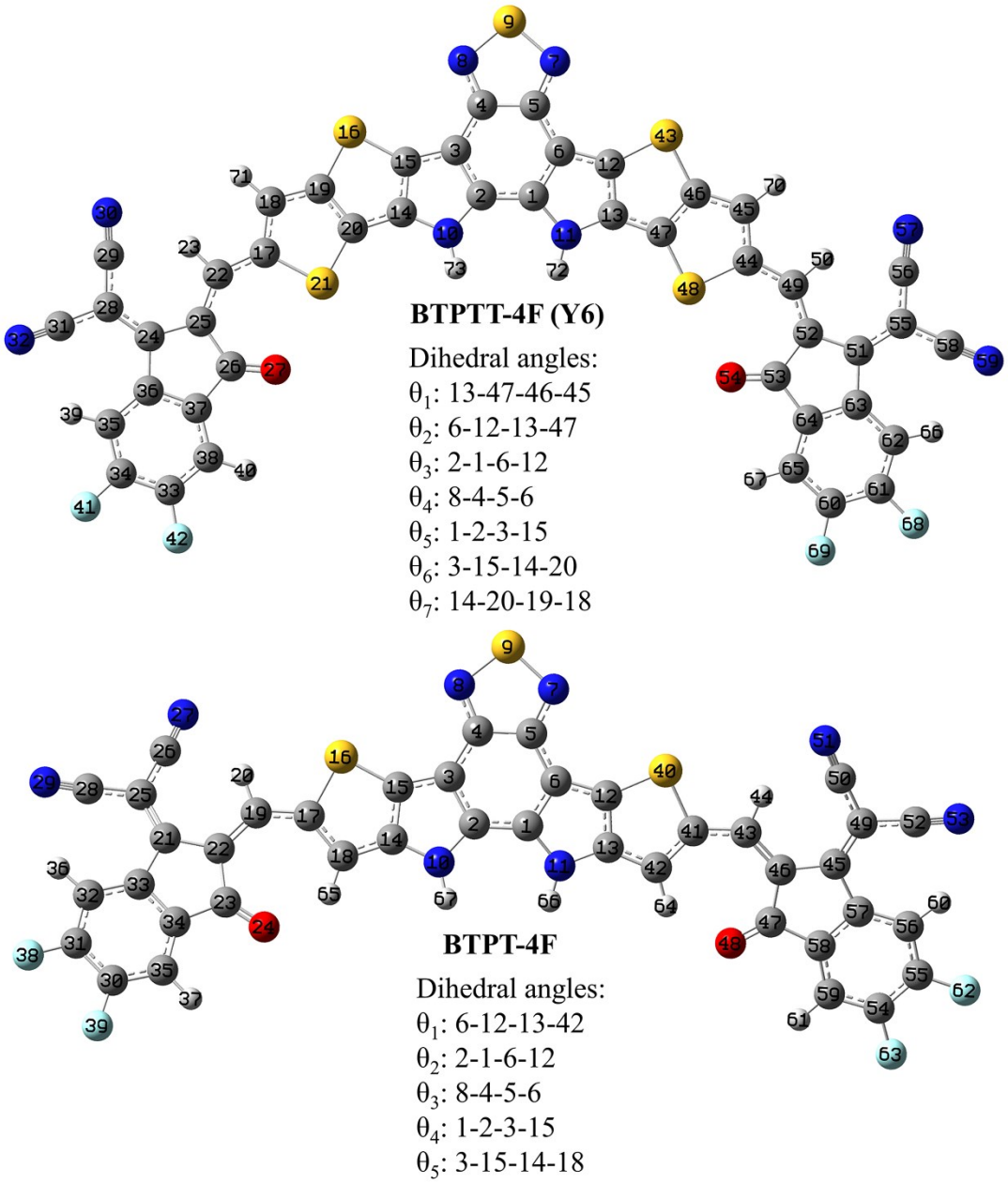

Figure S9. Illustration of selected dihedral angles of central fused-ring skeleton of BTPTT-4F (θ_1-θ_7) and BTPT-4F (θ_1-θ_5). Color of codes: grey-carbon, white-hydrogen, yellow-sulfur, red-oxygen, light blue-fluorine and blue-nitrogen. The side alkyl side chains are omitted for clarity.

Table S2. Dihedral angles of central fused-ring skeleton of BTPTT-4F (θ_1-θ_7) and BTPT-4F (θ_1-θ_5). Unit: degree.

System	θ_1	θ_2	θ_3	θ_4	θ_5	θ_6	θ_7
BTPTT-4F	0.66	0.58	5.31	3.41	4.30	0.16	0.11
2BTPTT-1	0.36	2.45	0.11	3.06	8.67	1.55	2.57
	1.06	1.53	5.08	2.97	6.90	3.14	4.94
2BTPTT-2	3.79	4.81	3.22	5.07	3.95	8.50	2.41
	1.30	9.75	1.86	5.01	2.77	7.79	3.93
2BTPTT-3	0.16	2.31	3.31	3.92	4.29	1.63	0.20

	0.08	2.06	3.43	3.58	3.73	2.54	1.16
2BTPTT-4	0.36	2.11	5.28	2.47	1.10	7.45	4.84
	0.56	0.30	7.64	2.18	0.24	2.00	1.17
2BTPTT-5	0.16	2.68	5.61	3.48	1.23	4.83	4.43
	9.13	8.75	0.64	5.76	3.75	0.88	1.48
2BTPTT-6	1.23	4.89	2.64	4.58	9.26	3.05	1.34
	0.89	1.05	4.06	3.93	4.71	1.03	2.42
2BTPTT-7	2.52	1.33	6.15	2.51	1.32	1.09	0.46
	4.73	3.75	9.01	1.52	3.25	4.14	0.19

System	θ_1	θ_2	θ_3	θ_4	θ_5
BTPT-4F	0.76	5.64	3.46	4.69	1.63
2BTPT-1	3.91	9.75	1.19	0.60	7.76
	8.17	0.05	4.93	7.35	1.84
2BTPT-2	1.78	4.62	4.12	4.21	2.24
	5.73	3.56	3.39	1.86	9.31
2BTPT-3	2.17	1.24	0.10	2.98	0.68
	2.21	1.91	1.93	2.60	3.44
2BTPT-4	3.59	6.41	3.45	4.24	3.06
	1.27	4.73	3.85	5.46	2.65
2BTPT-5	3.55	2.23	4.16	6.02	2.61
	4.63	1.77	4.63	6.63	2.74
2BTPT-6	3.99	3.74	4.26	5.29	3.69
	3.24	0.32	4.55	8.28	1.70
2BTPT-7	7.71	0.36	5.06	9.68	0.61
	8.22	0.82	4.96	8.38	1.33

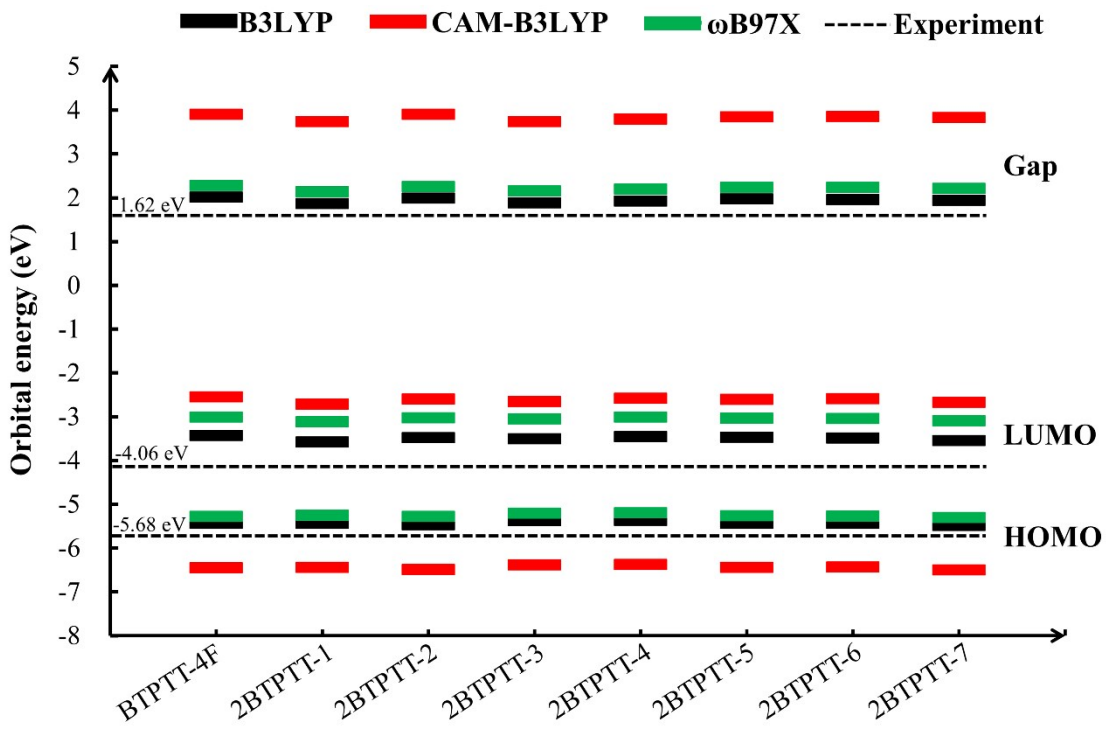

Figure S10. Calculated HOMO, LUMO and corresponding gap energy of BTPTT-4F monomer and dimers obtained with functionals B3LYP, CAM-B3LYP, and tuned ωB97X and basis set 6-31G(d) via PCM (ε=3.0). The experimental data are from reference 1.[1]

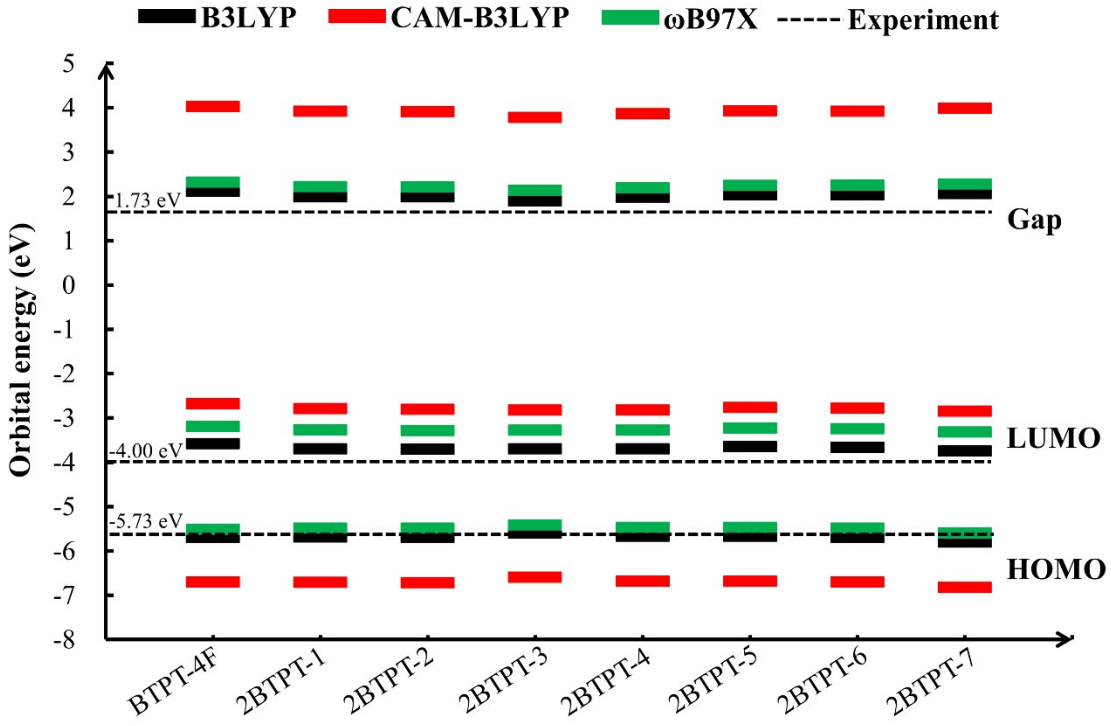

Figure S11. Calculated HOMO, LUMO and corresponding gap energy of BTPT-4F monomer and dimers obtained with functionals B3LYP, CAM-B3LYP, and tuned ωB97X and basis set 6-31G(d) via PCM (ε=3.0). The experimental data are from reference 1.[1]

Table S3. Calculated HOMO, LUMO and corresponding gap energy of BTPTT-4F and BTPT-4F

monomers and dimers obtained with functionals B3LYP, CAM-B3LYP, and tuned ωB97X and basis set 6-31G(d) via PCM (ε=3.0).

Functional	System	HOMO	LUMO	Gap	System	HOMO	LUMO	Gap
B3LYP	BTPTT-4F	-5.44	-3.44	2.01	BTPT-4F	-5.70	-3.59	2.11
	2BTPTT-1	-5.44	-3.58	1.86	2BTPT-1	-5.69	-3.70	1.99
	2BTPTT-2	-5.48	-3.49	1.99	2BTPT-2	-5.69	-3.71	1.98
	2BTPTT-3	-5.38	-3.51	1.88	2BTPT-3	-5.60	-3.71	1.90
	2BTPTT-4	-5.38	-3.46	1.92	2BTPT-4	-5.67	-3.70	1.97
	2BTPTT-5	-5.44	-3.48	1.96	2BTPT-5	-5.68	-3.65	2.03
	2BTPTT-6	-5.44	-3.49	1.95	2BTPT-6	-5.70	-3.67	2.03
	2BTPTT-7	-5.49	-3.55	1.94	2BTPT-7	-5.80	-3.75	2.06
CAM-B3LYP	BTPTT-4F	-6.45	-2.56	3.90	BTPT-4F	-6.71	-2.69	4.02
	2BTPTT-1	-6.45	-2.72	3.73	2BTPT-1	-6.71	-2.80	3.91
	2BTPTT-2	-6.50	-2.60	3.89	2BTPT-2	-6.72	-2.81	3.91
	2BTPTT-3	-6.39	-2.66	3.73	2BTPT-3	-6.60	-2.82	3.78
	2BTPTT-4	-6.38	-2.59	3.79	2BTPT-4	-6.69	-2.82	3.86
	2BTPTT-5	-6.45	-2.61	3.84	2BTPT-5	-6.69	-2.77	3.92
	2BTPTT-6	-6.44	-2.60	3.84	2BTPT-6	-6.70	-2.79	3.91
	2BTPTT-7	-6.50	-2.68	3.82	2BTPT-7	-6.83	-2.85	3.98
ωB97X	BTPTT-4F	-5.28	-3.01	2.27	BTPT-4F	-5.52	-3.20	2.32
	2BTPTT-1	-5.26	-3.13	2.13	2BTPT-1	-5.49	-3.28	2.22
	2BTPTT-2	-5.29	-3.04	2.25	2BTPT-2	-5.50	-3.29	2.21
	2BTPTT-3	-5.21	-3.06	2.15	2BTPT-3	-5.42	-3.28	2.13
	2BTPTT-	-5.20	-3.01	2.19	2BTPT-4	-5.47	-3.28	2.19

	4							
	2BTPTT-5	-5.27	-3.04	2.23	2BTPT-5	-5.48	-3.23	2.24
	2BTPTT-6	-5.28	-3.05	2.23	2BTPT-6	-5.49	-3.24	2.25
	2BTPTT-7	-5.31	-3.10	2.21	2BTPT-7	-5.60	-3.33	2.27

Table S4. Calculated HOMO, LUMO and corresponding gap energy of BTPTT-4F and BTPT-4F monomers and dimers obtained with functional B3LYP and basis sets 6-31G(d), 6-311G(d), and 6-311G(d, p) via PCM (ε=3.0).

Basis set	System	HOMO	LUMO	Gap	System	HOMO	LUMO	Gap
6-31G(d)	BTPTT-4F	-5.44	-3.44	2.01	BTPT-4F	-5.70	-3.59	2.11
	2BTPTT-1	-5.44	-3.58	1.86	2BTPT-1	-5.69	-3.70	1.99
	2BTPTT-2	-5.48	-3.49	1.99	2BTPT-2	-5.69	-3.71	1.98
	2BTPTT-3	-5.38	-3.51	1.88	2BTPT-3	-5.60	-3.71	1.90
	2BTPTT-4	-5.38	-3.46	1.92	2BTPT-4	-5.67	-3.70	1.97
	2BTPTT-5	-5.44	-3.48	1.96	2BTPT-5	-5.68	-3.65	2.03
	2BTPTT-6	-5.44	-3.49	1.95	2BTPT-6	-5.70	-3.67	2.03
	2BTPTT-7	-5.49	-3.55	1.94	2BTPT-7	-5.80	-3.75	2.06
	Average	-5.44	-3.50	1.94	Average	-5.69	-3.68	2.01
6-311G(d)	BTPTT-4F	-5.66	-3.68	1.98	BTPT-4F	-5.93	-3.83	2.09
	2BTPTT-1	-5.66	-3.83	1.84	2BTPT-1	-5.92	-3.96	1.97
	2BTPTT-2	-5.69	-3.73	1.97	2BTPT-2	-5.92	-3.95	1.97
	2BTPTT-3	-5.60	-3.74	1.85	2BTPT-3	-5.83	-3.95	1.88
	2BTPTT-4	-5.59	-3.70	1.89	2BTPT-4	-5.90	-3.95	1.95
	2BTPTT-5	-5.66	-3.72	1.94	2BTPT-5	-5.91	-3.89	2.01
	2BTPTT-6	-5.66	-3.73	1.94	2BTPT-6	-5.92	-3.91	2.01
	2BTPTT-7	-5.70	-3.79	1.92	2BTPT-7	-6.02	-3.99	2.04

	Average	-5.65	-3.74	1.92	Average	-5.92	-3.93	1.99
6-311G(d, p)	BTPTT-4F	-5.66	-3.68	1.98	BTPT-4F	-5.92	-3.84	2.09
	2BTPTT-1	-5.66	-3.83	1.83	2BTPT-1	-5.92	-3.96	1.96
	2BTPTT-2	-5.69	-3.73	1.96	2BTPT-2	-5.92	-3.95	1.97
	2BTPTT-3	-5.60	-3.75	1.85	2BTPT-3	-5.83	-3.95	1.88
	2BTPTT-4	-5.59	-3.70	1.89	2BTPT-4	-5.90	-3.95	1.95
	2BTPTT-5	-5.66	-3.72	1.94	2BTPT-5	-5.90	-3.90	2.01
	2BTPTT-6	-5.66	-3.73	1.93	2BTPT-6	-5.92	-3.91	2.01
	2BTPTT-7	-5.70	-3.79	1.91	2BTPT-7	-6.02	-3.99	2.03
	Average	-5.65	-3.74	1.91	Average	-5.92	-3.93	1.99

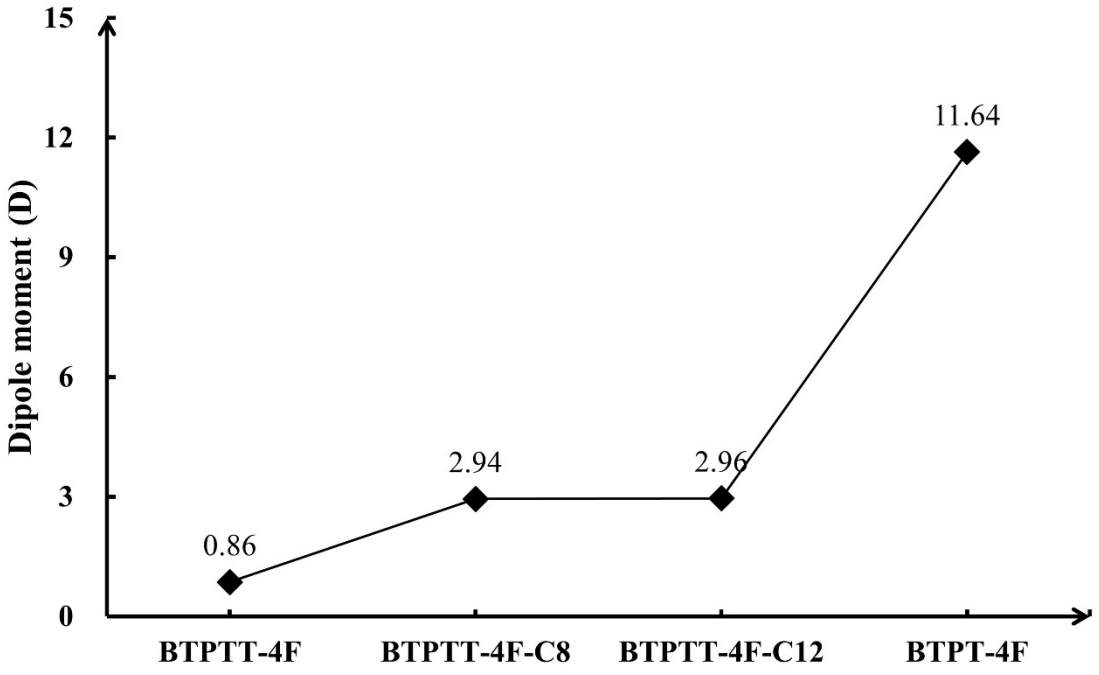

Figure S12. Dipole moments of BTPTT-4F, BTPTT-4F-C8, BTPTT-4F-C12, and BTPT-4F monomers.

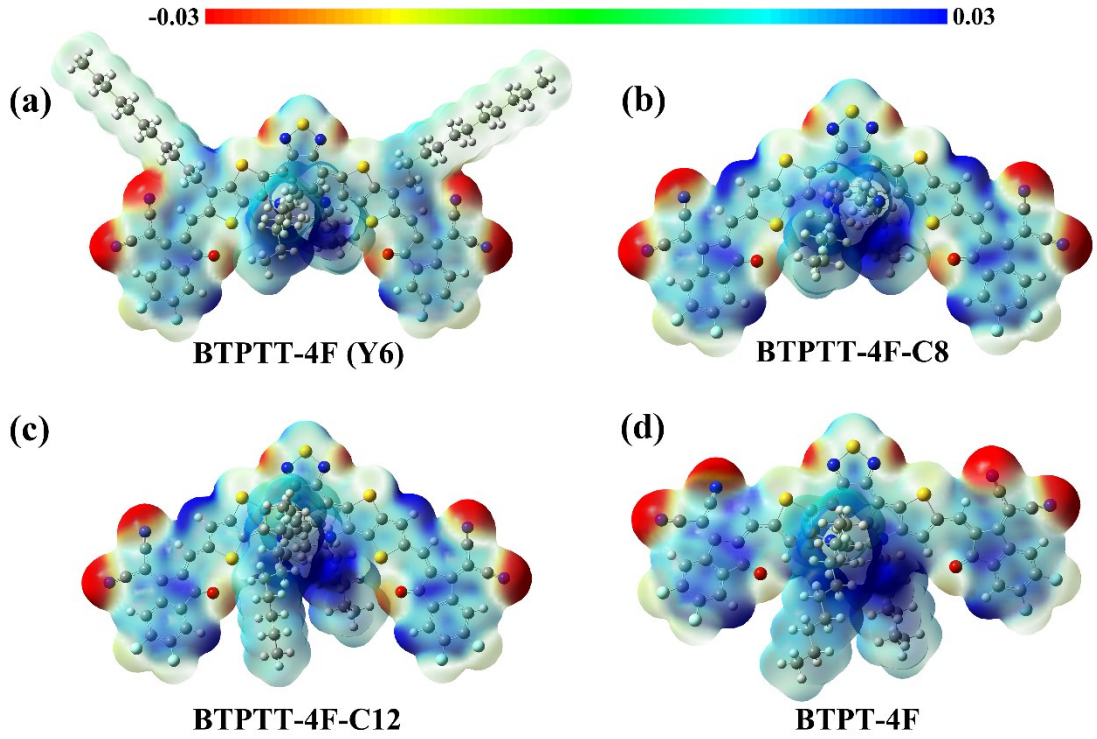

Figure S13. Molecular electrostatic potential of (a) BTPTT-4F (Y6); (b) BTPTT-4F-C8; (c) BTPTT-4F-C12; (d) BTPT-4F based on B3LYP/6-31G(d)/PCM (ε=3.0) theory level. Density=0.001 a.u. The color of code: red-negative; blue-positive; green-neutral.

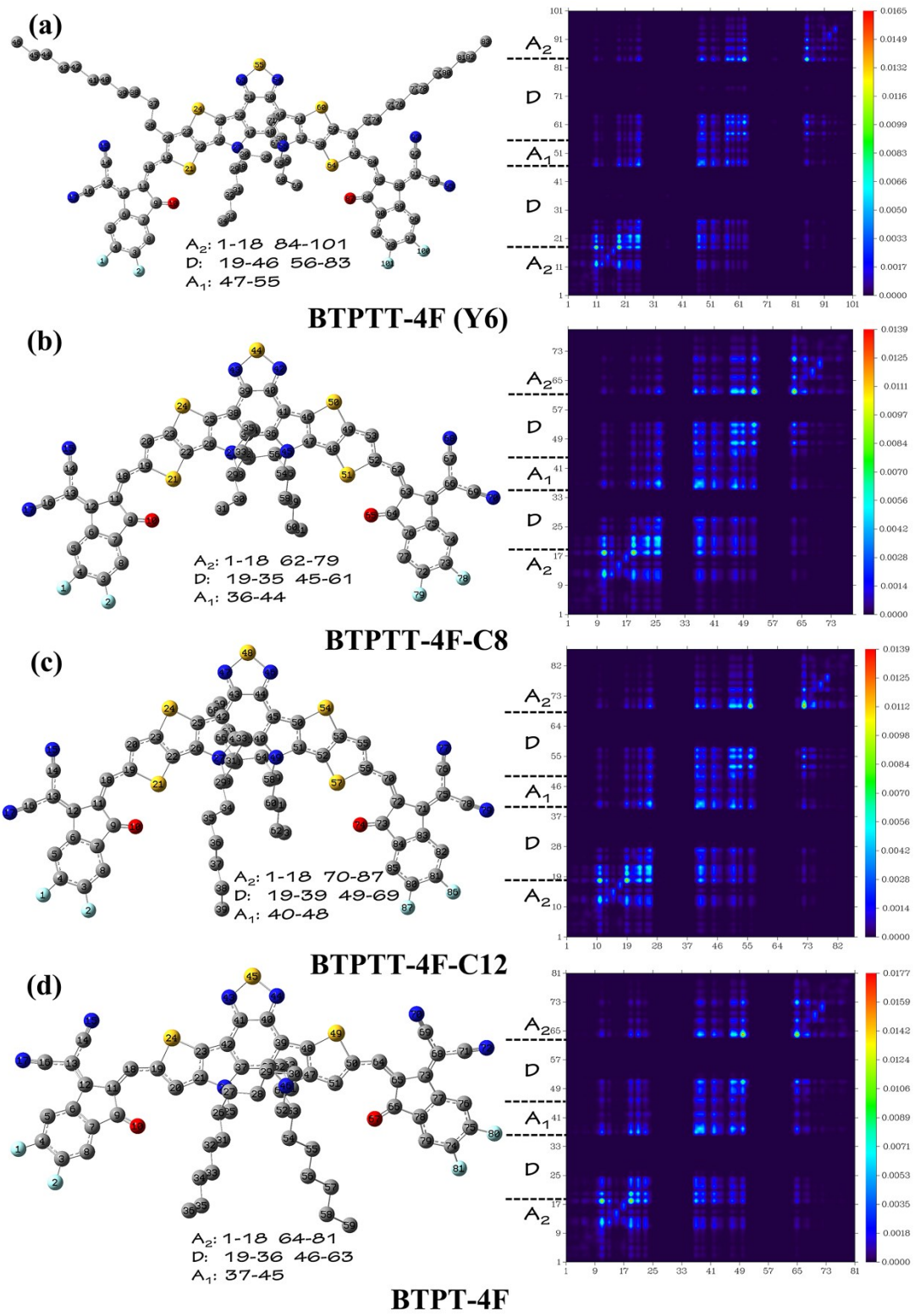

Figure S14. Excitation density matrix and the corresponding atom labels of (a) BTPTT-4F (Y6); (b) BTPTT-4F-C8; (c) BTPTT-4F-C12; (d) BTPT-4F obtained with CAM-B3LYP/6-31G(d)/PCM (ε=3.0) theory level. The abscissa and ordinate correspond to the hole and electron positions, respectively.

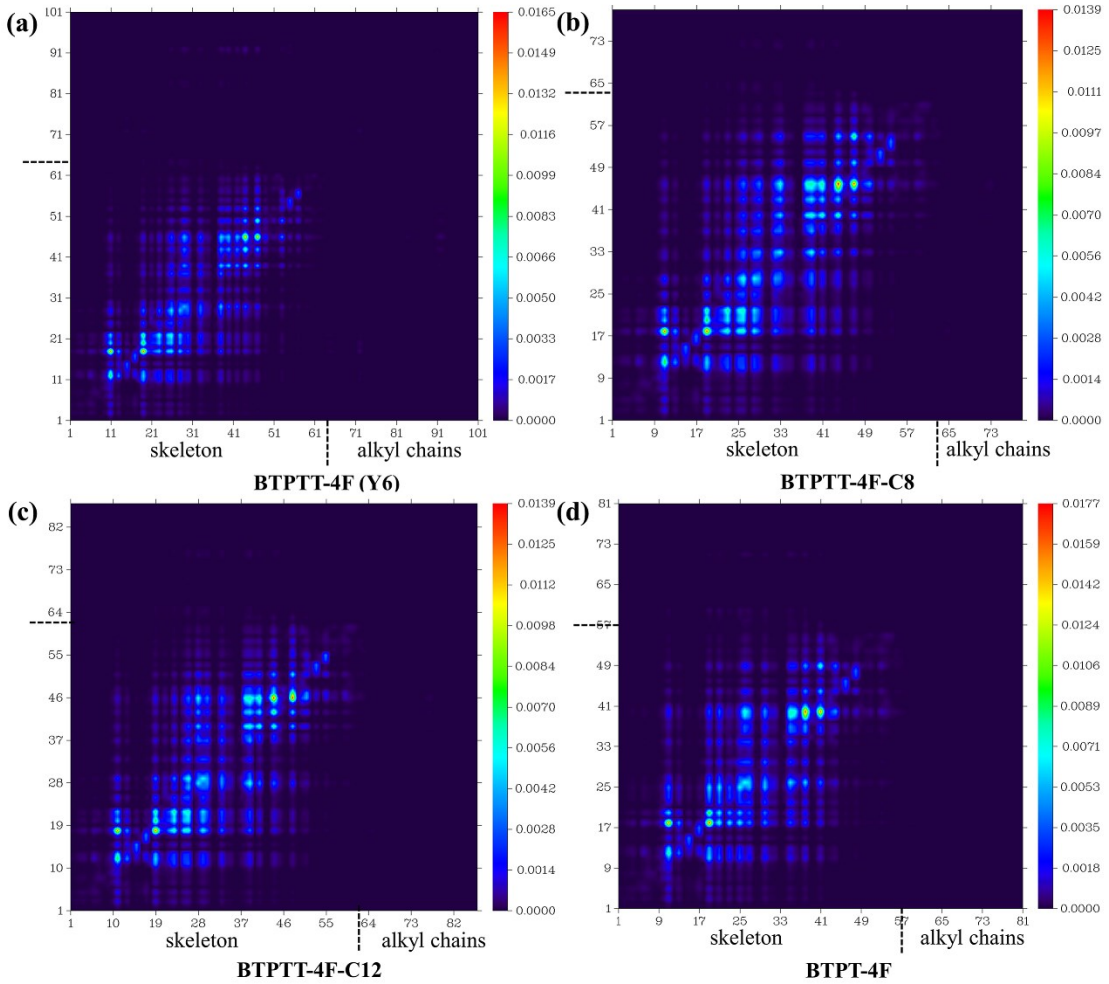

Figure S15. Excitation density matrix of (a) BTPTT-4F (Y6); (b) BTPTT-4F-C8; (c) BTPTT-4F-C12; (d) BTPT-4F obtained with CAM-B3LYP/6-31G(d)/PCM (ε=3.0) theory level. The abscissa and ordinate correspond to the hole and electron positions, respectively.

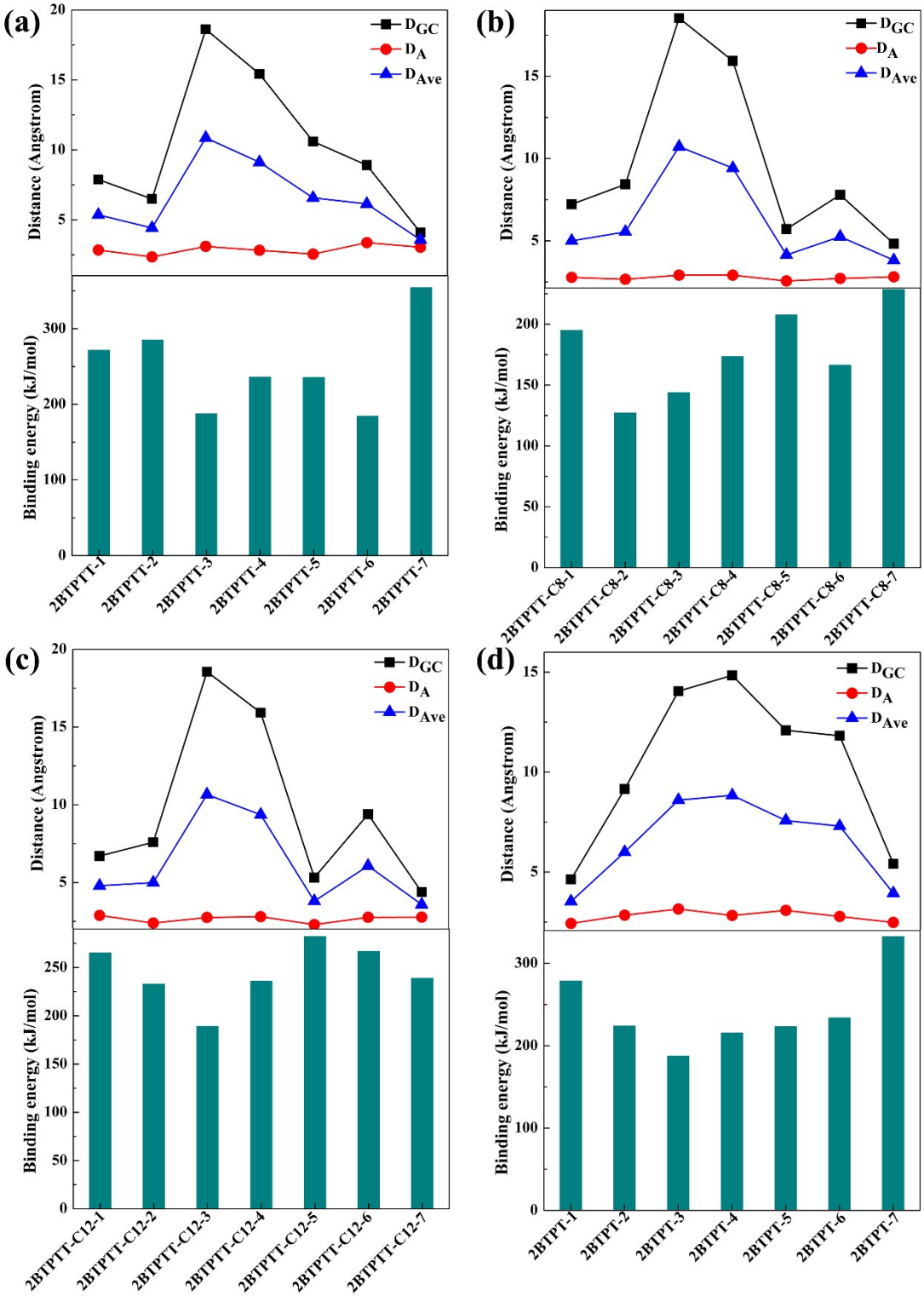

Figure S16. Binding energy and intermolecular distances $^{D_{GC}}$, ^{D_A}, and $^{D_{Ave}}$ of (a) BTPTT-4F; (b) BTPTT-4F-C8; (c) BTPTT-4F-C12; (d) BTPT-4F. $^{D_{GC}}$: the geometry center distance of dimers; ^{D_A}: the shortest atom distance of dimers; $^{D_{Ave}}$: the average distance of ^{D_A} and $^{D_{GC}}$. The side alkyl side chains are omitted when measuring these distances.

Table S5. Binding energies ($^{E_{binding}}$) of BTPTT-4F, BTPTT-4F-C8, BTPTT-4F-C12, and BTPT-4F dimers obtained by B3LYP+GD3 with 6-31G (d) basis set in di-butyl ether (Ɛ=3.0). Unit: kJ/mol

System	$E_{binding}$	System	$E_{binding}$
2BTPTT-1	271.76	2BTPTT-C8-1	194.93
2BTPTT-2	285.36	2BTPTT-C8-2	127.11
2BTPTT-3	187.60	2BTPTT-C8-3	143.84
2BTPTT-4	236.33	2BTPTT-C8-4	173.47
2BTPTT-5	235.52	2BTPTT-C8-5	207.65
2BTPTT-6	184.46	2BTPTT-C8-6	166.51
2BTPTT-7	354.38	2BTPTT-C8-7	228.57
2BTPTT-C12-1	265.14	2BTPT-1	278.60
2BTPTT-C12-2	232.98	2BTPT-2	223.84
2BTPTT-C12-3	189.13	2BTPT-3	187.48
2BTPTT-C12-4	235.60	2BTPT-4	215.57
2BTPTT-C12-5	282.24	2BTPT-5	223.10
2BTPTT-C12-6	266.55	2BTPT-6	233.80
2BTPTT-C12-7	238.64	2BTPT-7	332.32

Table S6. Distances (D_{GC}, D_A and D_{Ave}) of BTPTT-4F, BTPTT-4F-C8, BTPTT-4F-C12, and BTPT-4F dimers. D_{GC}: the geometry center distance of dimers; D_A: the shortest atom distance of dimers; D_{Ave}: the average distance of D_A and D_{GC}. The alkyl side chains were removed when calculating the distances. Unit: Å

System	D_{GC}	D_A	D_{Ave}	System	D_{GC}	D_A	D_{Ave}
2BTPTT-1	7.88	2.84	5.36	2BTPTT-C8-1	7.22	2.78	5.00
2BTPTT-2	6.49	2.35	4.42	2BTPTT-C8-2	8.43	2.66	5.54
2BTPTT-3	18.62	3.10	10.86	2BTPTT-C8-3	18.53	2.91	10.72
2BTPTT-4	15.43	2.82	9.12	2BTPTT-C8-4	15.93	2.91	9.42
2BTPTT-5	10.60	2.55	6.57	2BTPTT-C8-5	5.71	2.56	4.14
2BTPTT-6	8.91	3.37	6.14	2BTPTT-C8-6	7.79	2.71	5.25
2BTPTT-7	4.09	3.04	3.57	2BTPTT-C8-7	4.82	2.81	3.82
2BTPTT-C12-1	6.70	2.88	4.79	2BTPT-1	4.63	2.43	3.53
2BTPTT-C12-2	7.59	2.39	4.99	2BTPT-2	9.15	2.84	6.00
2BTPTT-C12-3	18.56	2.75	10.66	2BTPT-3	14.05	3.15	8.60
2BTPTT-C12-4	15.92	2.80	9.36	2BTPT-4	14.84	2.83	8.84
2BTPTT-C12-5	5.31	2.29	3.80	2BTPT-5	12.09	3.08	7.58
2BTPTT-C12-6	9.39	2.76	6.07	2BTPT-6	11.82	2.78	7.30
2BTPTT-C12-7	4.38	2.77	3.58	2BTPT-7	5.41	2.48	3.94

Table S7. Internal reorganization energy (λ_i) of BTPTT-4F, BTPTT-4F-C8, BTPTT-4F-C12, and BTPT-4F obtained with B3LYP functional and 6-31G(d) and 6-311G(d, p) basis sets via PCM (ε=3.0). Unit: eV.

System	Basis set	
	6-31G(d)	6-311G(d, p)
BTPTT-4F	0.134	0.131
BTPTT-4F-C8	0.132	0.130
BTPTT-4F-C12	0.132	0.130
BTPT-4F	0.189	0.186

Table S8. External reorganization energy of BTPTT-4F, BTPTT-4F-C8, BTPTT-4F-C12, and BTPT-4F dimers obtained with B3LYP/6-31G(d)/PCM (ε=3.0) theory level.

System	$R_{A/}$Å	$r_{DA/}$Å	$\lambda_{o/}$eV	System	$R_{A/}$Å	$r_{DA/}$Å	$\lambda_{o/}$eV
2BTPTT-1	7.47	9.380	0.0652	2BTPTT-C8-1	6.67	8.372	0.0731
2BTPTT-2	7.47	9.363	0.0648	2BTPTT-C8-2	6.67	8.380	0.0734
2BTPTT-3	7.47	9.388	0.0654	2BTPTT-C8-3	6.67	8.376	0.0732
2BTPTT-4	7.47	9.384	0.0653	2BTPTT-C8-4	6.67	8.368	0.0729
2BTPTT-5	7.47	9.385	0.0654	2BTPTT-C8-5	6.67	8.377	0.0732
2BTPTT-6	7.47	9.385	0.0654	2BTPTT-C8-6	6.67	8.370	0.0730
2BTPTT-7	7.47	9.370	0.0650	2BTPTT-C8-7	6.67	8.366	0.0729
2BTPTT-C12-1	6.98	8.754	0.0693	2BTPT-1	6.82	8.553	0.0709
2BTPTT-C12-2	6.98	8.770	0.0698	2BTPT-2	6.82	8.570	0.0715
2BTPTT-C12-3	6.98	8.767	0.0697	2BTPT-3	6.82	8.555	0.0710
2BTPTT-C12-4	6.98	8.762	0.0696	2BTPT-4	6.82	8.561	0.0712
2BTPTT-C12-5	6.98	8.763	0.0696	2BTPT-5	6.82	8.565	0.0713
2BTPTT-C12-6	6.98	8.762	0.0695	2BTPT-6	6.82	8.561	0.0712
2BTPTT-C12-7	6.98	8.762	0.0696	2BTPT-7	6.82	8.541	0.0705

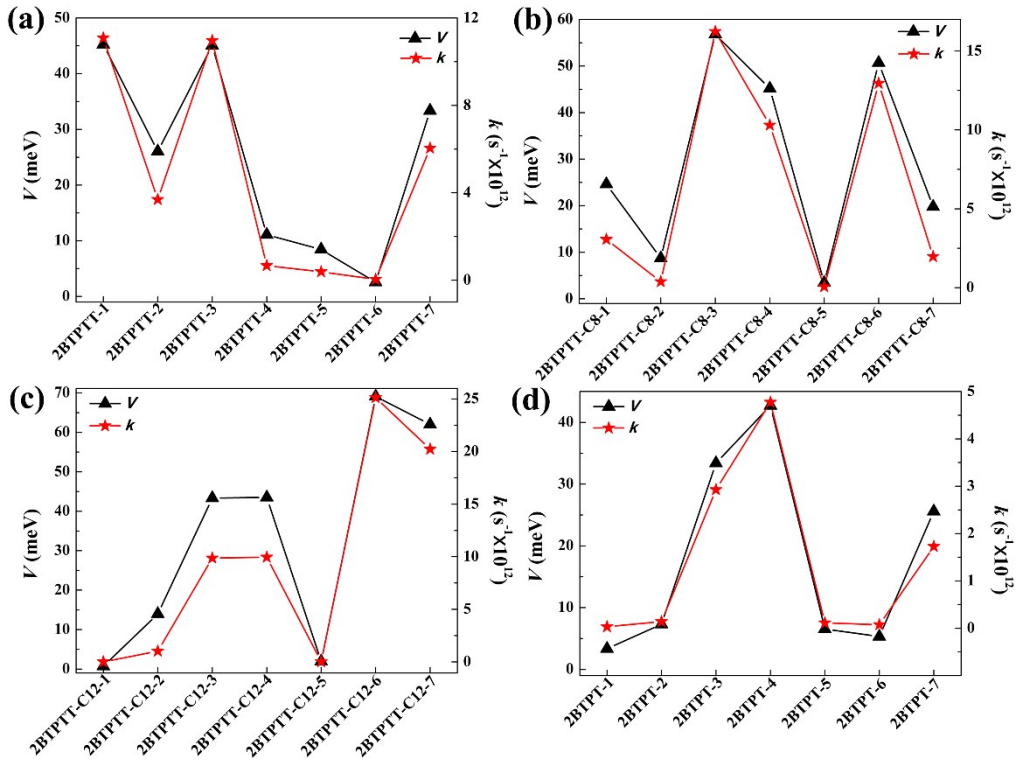

Figure S17. Absolute values of electronic coupling ($|V|$, in meV) and charge transfer rate constants (k, in $s^{-1}\times10^{12}$) of (a) BTPTT-4F; (b) BTPTT-4F-C8; (c) BTPTT-4F-C12; (d) BTPT-4F dimer configurations. 1-bimolecular parallel; 2-anti-parallel; 3-end-group overlap; 4-end-group anti-overlap;5-vertical-left; 6-vertical-right; 7-tail to tail overlap.

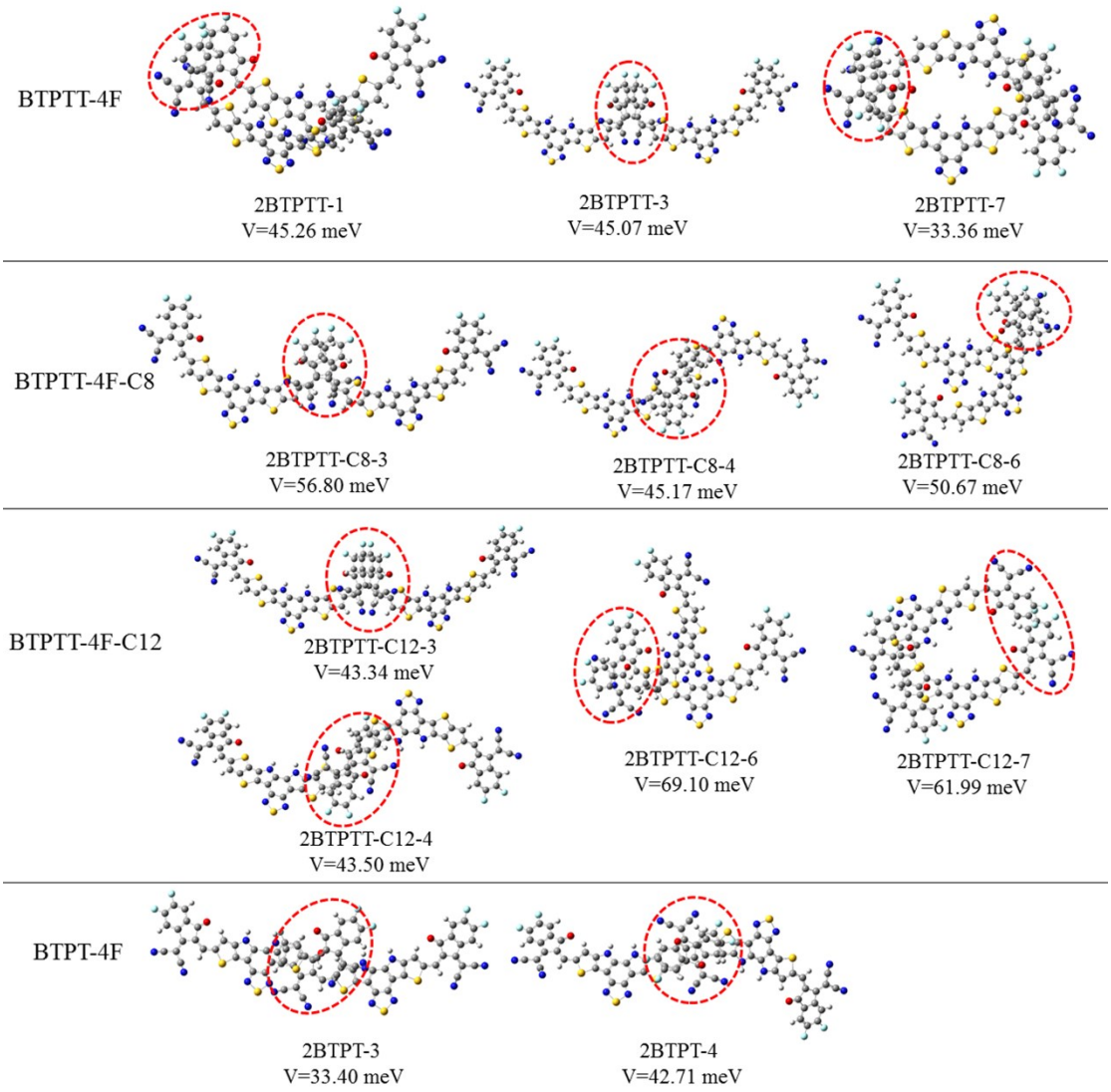

Figure S18. Dimers with high electron coupling. The end groups with face-on orientation and good stacking are circled in red. The side alkyl chains are omitted for clarity.

Table S9. Calculated geometric center distances between the end groups ($D_{end-group}$, in Å) and absolute values of electronic coupling ($|V|$, in meV) of all dimer configurations with high electron coupling.

System	$D_{end-group}$	$\|V\|$	System	$D_{end-group}$	$\|V\|$
2BTPTT-1	4.25	45.26	2BTPTT-C8-3	3.54	56.80
2BTPTT-3	3.61	45.07	2BTPTT-C8-4	5.80	45.17
2BTPTT-7	3.53	33.36	2BTPTT-C8-6	4.31	50.67
2BTPTT-C12-3	3.75	43.34	2BTPT-3	6.80	33.40
2BTPTT-C12-4	5.74	43.50	2BTPT-4	4.32	42.71
2BTPTT-C12-6	5.68	69.10			

2BTPTT-C12-7	7.69	61.99

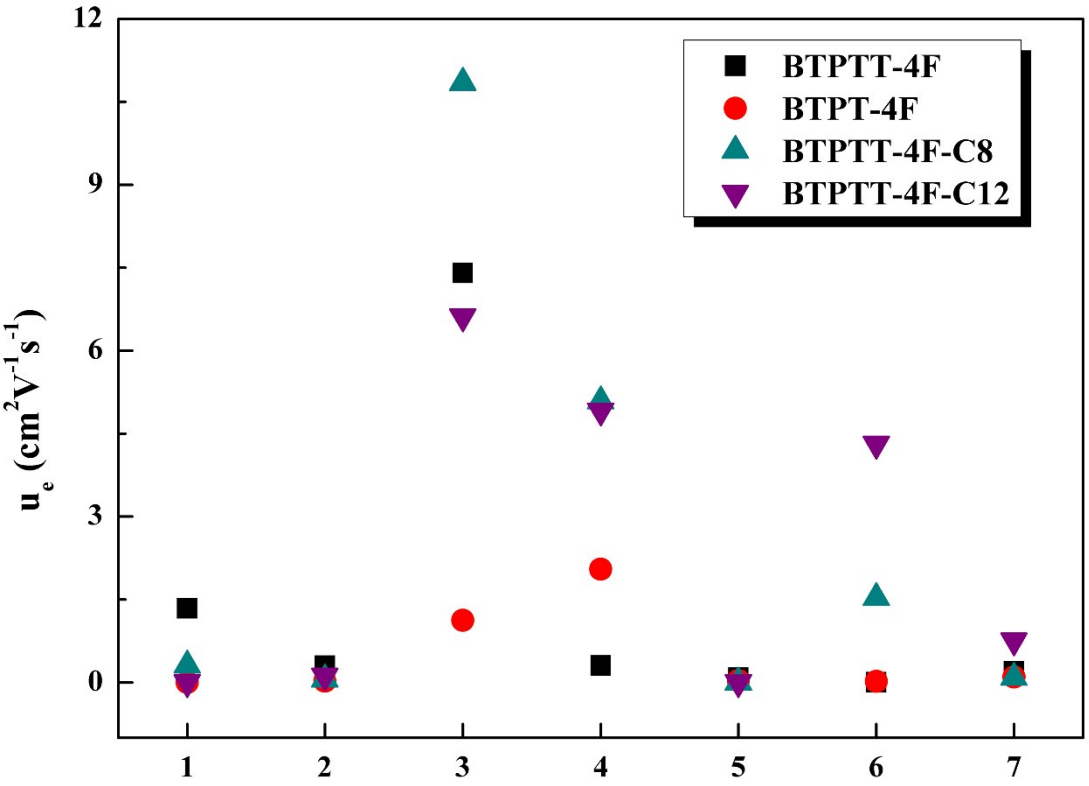

Figure S19. Charge carrier mobility (μ_e, in $cm^2V^{-1}s^{-1}$) of BTPTT-4F, BTPTT-4F-C8, BTPTT-4F-C12, and BTPT-4F dimer configurations. 1-bimolecular parallel; 2-anti-parallel; 3-end-group overlap; 4-end-group anti-overlap;5-vertical-left; 6-vertical-right; 7-tail to tail overlap.

Table S10. Charge transfer distances (r, in Å), absolute values of electronic coupling ($|V|$, in meV), reorganization energy (λ, in eV), charge transfer rate constants (k, in s^{-1}), and charge carrier mobility (μ_e, in $cm^2V^{-1}s^{-1}$) of BTPTT-4F, BTPTT-4F-C8, BTPTT-4F-C12, and BTPT-4F dimers.

System	r	$\|V\|$	λ	k	μ_e
2BTPTT-1	7.88	45.26	0.199	1.11×10^{13}	1.34
2BTPTT-2	6.49	26.05	0.199	3.69×10^{12}	3.03×10^{-1}
2BTPTT-3	18.62	45.07	0.199	1.10×10^{13}	7.40
2BTPTT-4	15.43	11.09	0.199	6.64×10^{11}	3.08×10^{-1}
2BTPTT-5	10.60	8.43	0.199	3.84×10^{11}	8.40×10^{-2}
2BTPTT-6	8.91	2.55	0.199	3.52×10^{10}	5.43×10^{-3}
2BTPTT-7	4.09	33.36	0.199	6.04×10^{12}	1.97×10^{-1}
2BTPTT-C8-1	7.22	24.63	0.205	3.06×10^{12}	3.10×10^{-1}
2BTPTT-C8-2	8.43	8.72	0.205	3.81×10^{11}	5.27×10^{-2}

2BTPTT-C8-3	18.53	56.80	0.205	1.62×10^{13}	10.84
2BTPTT-C8-4	15.93	45.17	0.205	1.03×10^{13}	5.09
2BTPTT-C8-5	5.71	3.45	0.205	6.00×10^{10}	3.81×10^{-3}
2BTPTT-C8-6	7.79	50.67	0.205	1.30×10^{13}	1.53
2BTPTT-C8-7	4.82	19.77	0.205	1.97×10^{12}	8.93×10^{-2}
2BTPTT-C12-1	6.70	0.72	0.202	2.71×10^{9}	2.37×10^{-4}
2BTPTT-C12-2	7.59	13.96	0.202	1.02×10^{12}	1.15×10^{-1}
2BTPTT-C12-3	18.56	43.34	0.202	9.86×10^{12}	6.61
2BTPTT-C12-4	15.92	43.50	0.202	9.96×10^{12}	4.91
2BTPTT-C12-5	5.31	1.93	0.202	1.95×10^{10}	1.07×10^{-3}
2BTPTT-C12-6	9.39	69.10	0.202	2.51×10^{13}	4.31
2BTPTT-C12-7	4.38	61.99	0.202	2.02×10^{13}	7.55×10^{-1}
2BTPT-1	4.63	3.34	0.260	2.93×10^{10}	1.22×10^{-3}
2BTPT-2	9.15	7.30	0.260	1.39×10^{11}	2.27×10^{-2}
2BTPT-3	14.05	33.40	0.260	2.93×10^{12}	1.12
2BTPT-4	14.84	42.71	0.260	4.77×10^{12}	2.05
2BTPT-5	12.09	6.53	0.260	1.11×10^{11}	3.17×10^{-2}
2BTPT-6	11.82	5.31	0.260	7.38×10^{10}	2.01×10^{-2}
2BTPT-7	5.41	25.59	0.260	1.73×10^{12}	9.82×10^{-2}

Table S11. Charge transfer rate constants (k_{M-L-J}, in s^{-1}) and charge carrier mobility ($\mu_{e,M-L-J}$, in $cm^2V^{-1}s^{-1}$) of BTPTT-4F, BTPTT-4F-C8, BTPTT-4F-C12, and BTPT-4F dimers obtained with M-L-J formula.

System	k_{M-L-J}	$\mu_{e,M-L-J}$	System	k_{M-L-J}	$\mu_{e,M-L-J}$
2BTPTT-1	3.53×10^{13}	4.26	2BTPTT-C8-1	9.24×10^{12}	9.38×10^{-1}
2BTPTT-2	1.18×10^{13}	9.67×10^{-1}	2BTPTT-C8-2	1.15×10^{12}	1.59×10^{-1}
2BTPTT-3	3.49×10^{13}	23.54	2BTPTT-C8-3	4.90×10^{13}	32.77
2BTPTT-4	2.11×10^{12}	9.79×10^{-1}	2BTPTT-C8-4	3.12×10^{13}	15.39
2BTPTT-5	1.22×10^{12}	2.67×10^{-1}	2BTPTT-C8-5	1.81×10^{11}	1.15×10^{-2}
2BTPTT-6	1.12×10^{11}	1.73×10^{-2}	2BTPTT-C8-6	3.92×10^{13}	4.62
2BTPTT-7	1.93×10^{13}	6.28×10^{-1}	2BTPTT-C8-7	5.98×10^{12}	2.70×10^{-1}
2BTPTT-C12-1	8.35×10^{9}	7.17×10^{-4}	2BTPT-1	1.31×10^{11}	5.45×10^{-3}
2BTPTT-C12-2	3.14×10^{12}	3.52×10^{-1}	2BTPT-2	6.18×10^{11}	1.01×10^{-1}
2BTPTT-C12-3	3.03×10^{13}	20.30	2BTPT-3	1.30×10^{13}	5.01
2BTPTT-C12-4	3.06×10^{13}	15.09	2BTPT-4	2.13×10^{13}	9.11

2BTPTT-C12-5	6.00×10^{10}	3.30×10^{-3}	2BTPT-5	4.95×10^{11}	1.41×10^{-1}
2BTPTT-C12-6	7.72×10^{13}	13.24	2BTPT-6	3.29×10^{11}	8.94×10^{-2}
2BTPTT-C12-7	6.21×10^{13}	2.32	2BTPT-7	7.71×10^{12}	4.38×10^{-1}

References

1. B. Fan, D. Zhang, M. Li, W. Zhong, Z. Zeng, L. Ying, F. Huang and Y. Cao, *Sci. China Chem.*, 2019, **62**, 746-752.