Supporting Information

Impact of Solvent-Processing for PM6/Y6 Morphology and Charge transfer in Organic Solar Cells

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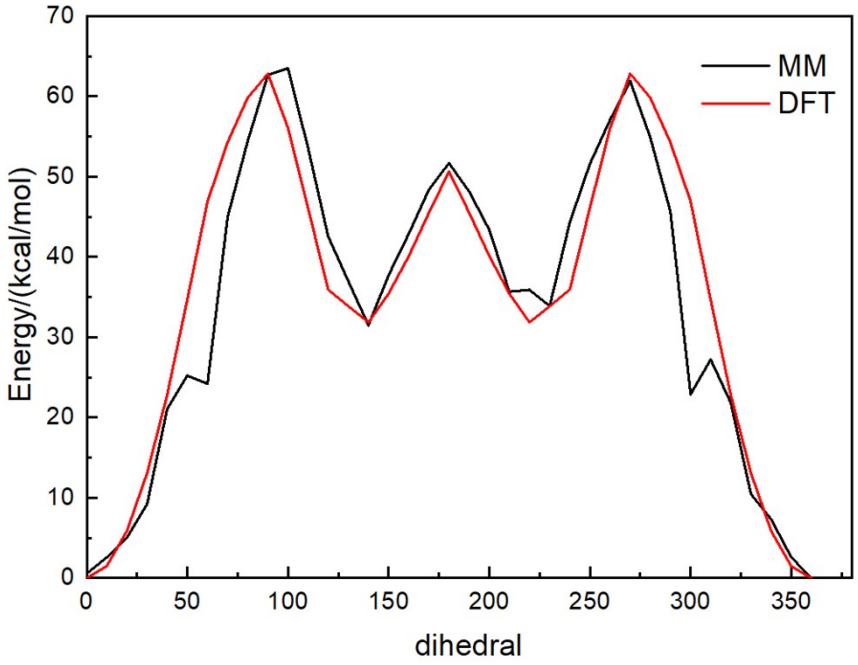

Figure S1. Potential energy cures for the dihedral angle S-C-C-C calculated by DFT and OPLS-AA along with the fitted intrinsic torsion potential

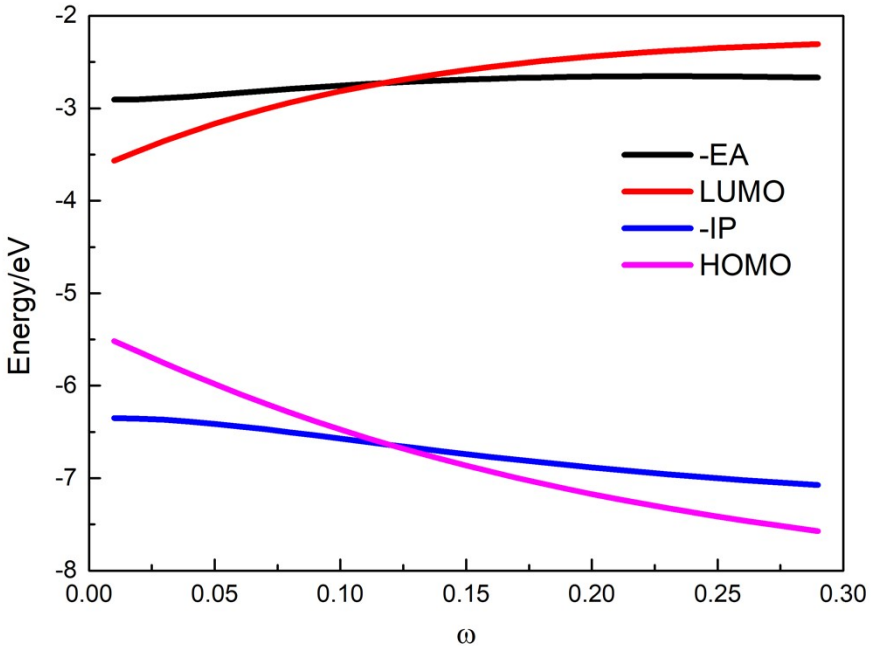

Figure S2. Dependence of -IP, -EA, HOMO, and LUMO energies for the PM6:Y6 complex as a function of the RS parameter, ω. The calculations were performed at the ωB97XD/def2-SVP level.

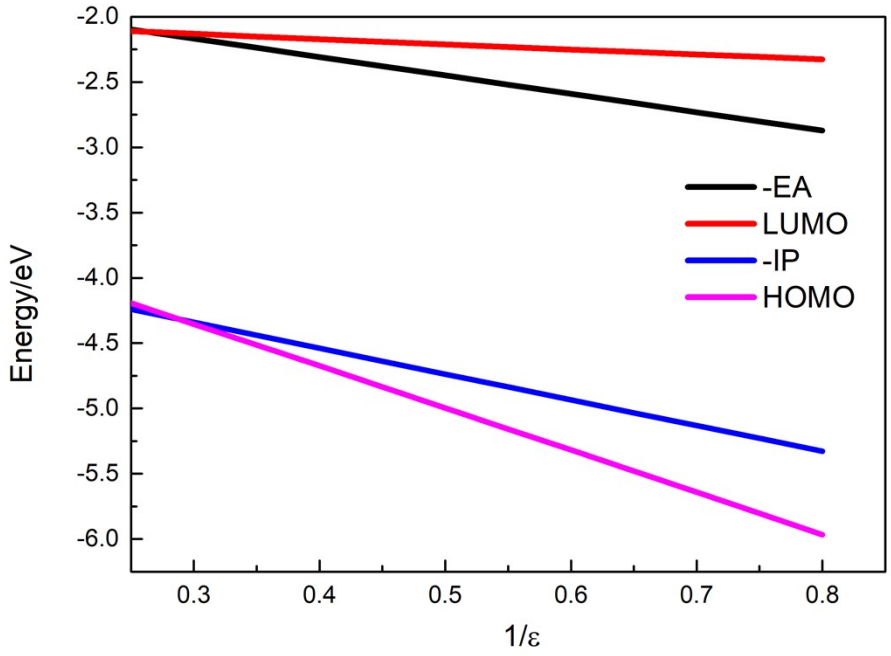

Figure S3. Dependence of -IP, -EA, HOMO, and LUMO energies for the PM6:Y6 complex as a function of 1/ε (1/ε = 0.2222 + β) in a dielectric medium with ε= 4. The calculations were performed at the ωB97XD/def2-SVP level with ω = ω_{vac}.

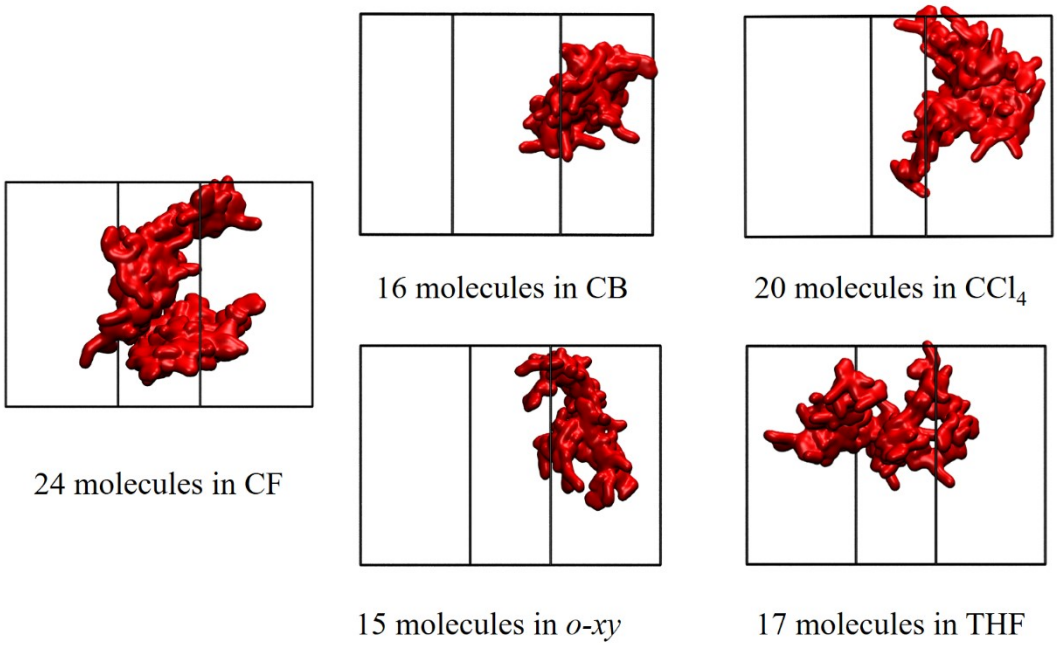

Figure S4: The largest clusters of electron transport network of Y6 acceptors in films treated with different solvents.

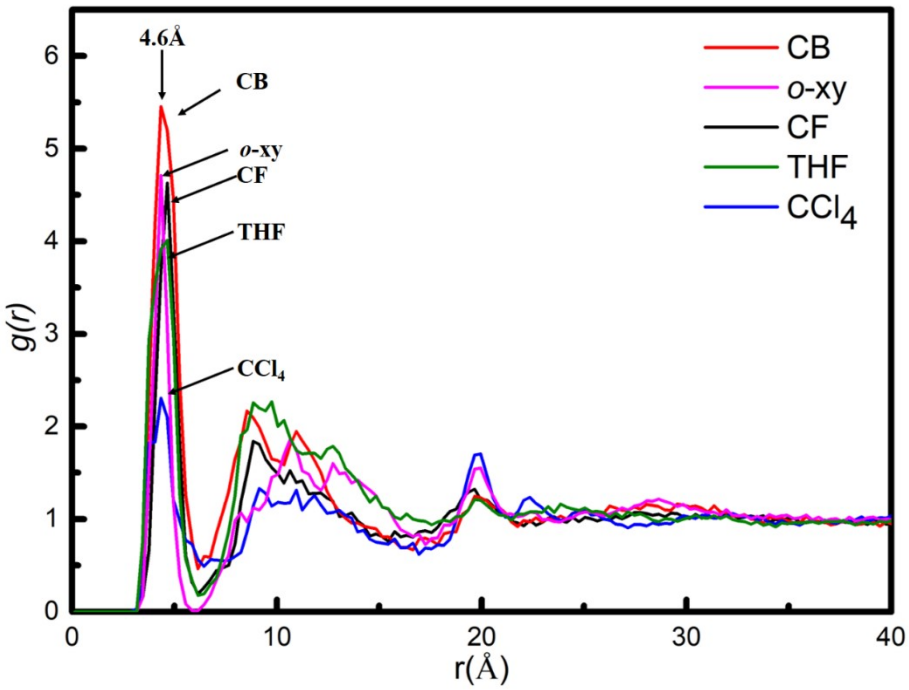

Figure S5. center-of-mass radial distribution functions of the Y6 dimer.

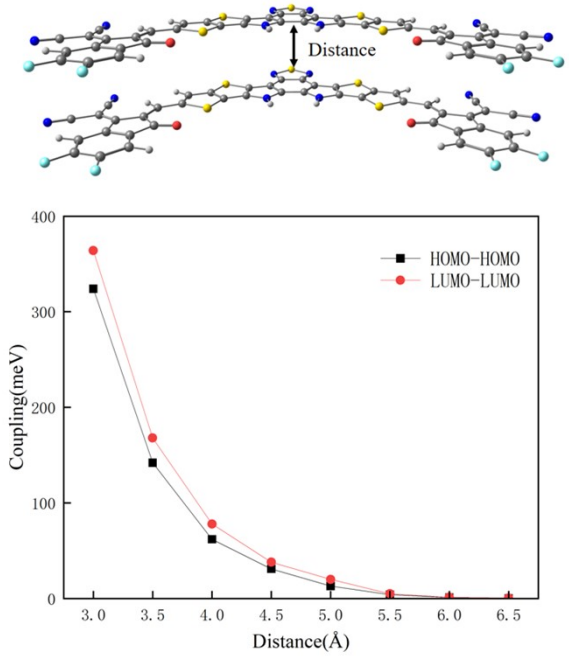

Figure S6. Relationships between distances and coupling of completely face-on Y6 dimers. In general, only some fragments of Y6 will overlap. Thus, we chose 5Å as the dividing line, below which part of the dimer is still coupled as having a strong coupling.

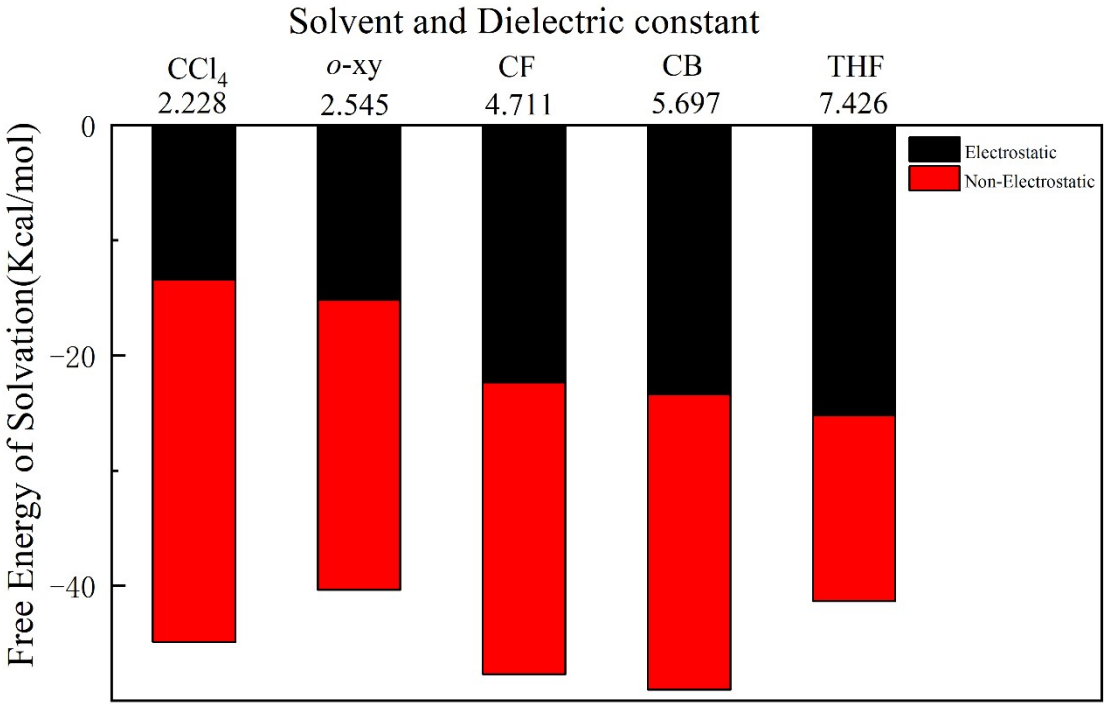

Figure S7. Free energy of solvation for Y6 in different solvents.

Table S1. The solubility limit of Y6 in different solvents.[1]

Solvents	Solubility (mg/mL)
CF	20
THF	12
CB	26

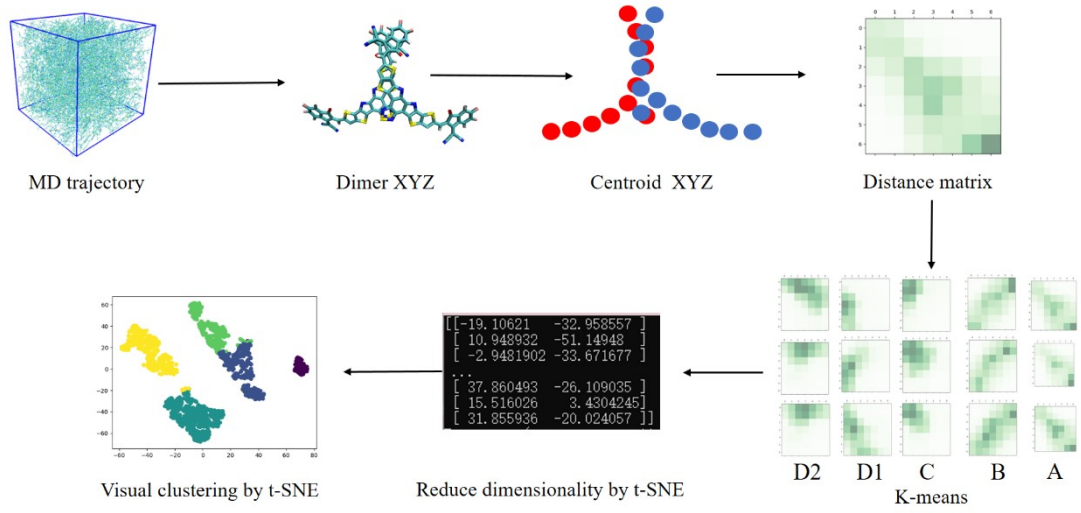

Figure S8. Classification of Y6 dimers or PM6/Y6 complexes by K-means method.[2]

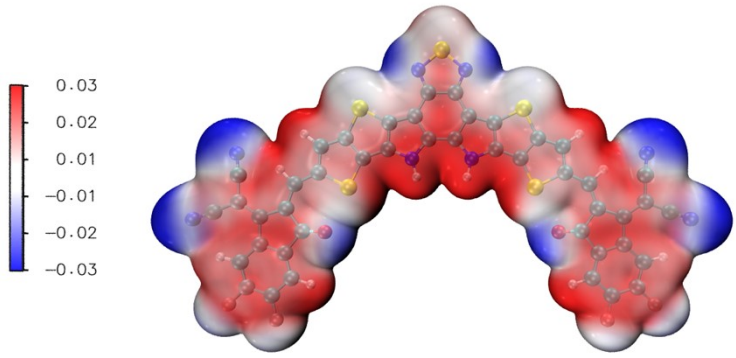

Figure S9. Electrostatic potential graphs of the Y6.

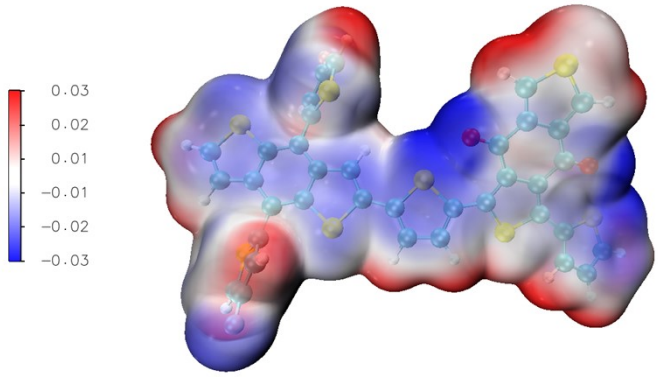

Figure S10. Electrostatic potential graphs of the PM6.

HOMO LUMO

Figure S11. The HOMO and LUMO orbital for the PM6.

HOMO LUMO

Figure S12. The HOMO and LUMO orbital for the Y6.

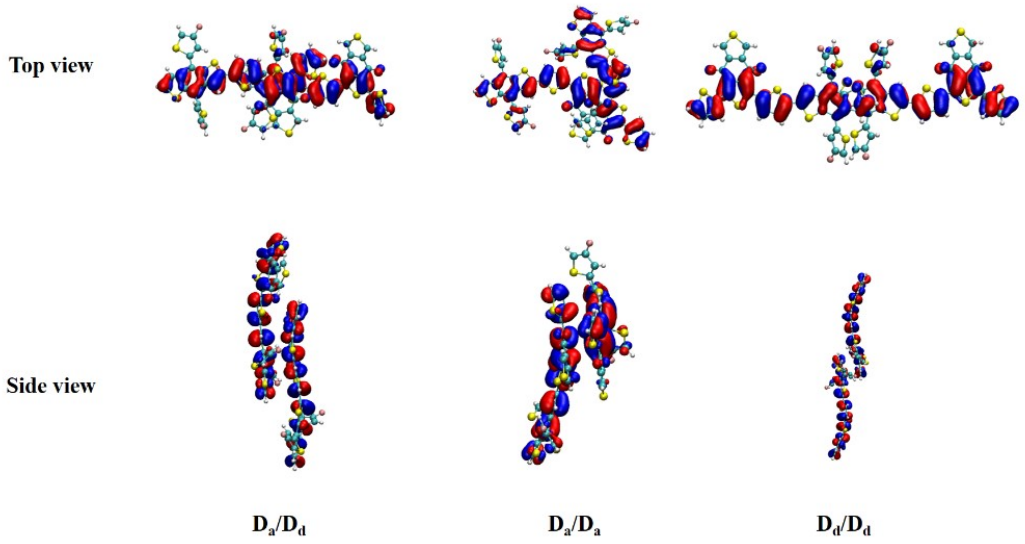

Figure S13. HOMO orbitals in PM6 dimer.

Table S2: Reorganization energies (in meV) for electron transport in A/A domain, hole transport in D/D domain, as well as, charge transfer at D/A interface.

	λ(meV)
$DD^+ \rightarrow D^+D$	246.5
$AA^- \rightarrow A^-A$	147.1
$D^*A \rightarrow D^+A^-$	122.6
$DA^* \rightarrow D^+A^-$	197.8

Tab. S3. Electronic coupling and rate of A_{ad}-A_{ad} type Y6 dimer

pairN	V	Ecombin	rate
pair0	94.88307	-28.1855	3.57E+13
pair1	0.782344	-18.6207	2.42E+09
pair2	3.308569	-22.7677	4.34E+10
pair3	44.9698	-21.8743	8.01E+12
pair4	8.766366	-19.4716	3.04E+11
pair5	67.19391	-26.2283	1.79E+13
pair6	54.35013	-27.2048	1.17E+13
pair7	22.26485	-24.6617	1.96E+12
pair8	81.89039	-22.6742	2.66E+13
pair9	61.52578	-23.0122	1.5E+13
pair10	46.84845	-23.7888	8.69E+12
pair11	60.43332	-21.862	1.45E+13
pair12	16.22132	-25.8217	1.04E+12
pair13	68.17207	-23.8419	1.84E+13
pair14	47.42475	-23.4317	8.91E+12
pair15	31.28633	-22.7568	3.88E+12
pair16	28.48218	-17.1802	3.21E+12
pair17	48.18482	-27.054	9.2E+12
pair18	74.03536	-25.5268	2.17E+13
pair19	73.89593	-26.8296	2.16E+13
pair20	81.52713	-24.0476	2.63E+13
pair21	29.98096	-18.2045	3.56E+12
pair22	88.43267	-25.3292	3.1E+13
pair23	55.96389	-23.3325	1.24E+13
pair24	62.69095	-21.5255	1.56E+13
pair25	50.03325	-26.3667	9.91E+12
pair26	31.60108	-24.7636	3.96E+12
pair27	36.80788	-24.7898	5.37E+12
pair28	18.77247	-20.9705	1.4E+12
pair29	72.99502	-25.3625	2.11E+13
pair30	2.174919	-21.7693	1.87E+10
pair31	53.92431	-24.0898	1.15E+13
pair32	17.86129	-22.7135	1.26E+12
pair33	33.94886	-20.2692	4.56E+12
pair34	35.72006	-23.649	5.05E+12
pair35	31.18817	-24.6966	3.85E+12
pair36	65.11426	-27.0824	1.68E+13
pair37	36.57966	-18.331	5.3E+12
pair38	67.11196	-25.1986	1.78E+13
pair39	90.65593	-26.6024	3.25E+13
pair40	57.28805	-25.4856	1.3E+13

pair41	76.42453	-27.9132	2.31E+13
pair42	10.84502	-18.7454	4.66E+11
pair43	51.31838	-24.0067	1.04E+13
pair44	53.34649	-25.8904	1.13E+13
pair45	22.63134	-21.0553	2.03E+12
pair46	19.15313	-23.4386	1.45E+12
pair47	21.44348	-15.0085	1.82E+12
pair48	31.11048	-18.0755	3.83E+12
pair49	34.97047	-20.315	4.84E+12
Average	45.53072	-23.2365	8.21E+12

Tab. S4. Electronic coupling and rate of A_{ad}-A_{da} type Y6 dimer

pairN	V	Ecombin	rate
pair0	47.55564	-30.0007	8.96E+12
pair1	12.60184	-17.6689	6.29E+11
pair2	2.461198	-29.1976	2.4E+10
pair3	28.11581	-28.132	3.13E+12
pair4	7.817681	-21.6862	2.42E+11
pair5	27.86537	-28.2644	3.08E+12
pair6	10.38353	-20.3831	4.27E+11
pair7	1.914442	-23.3884	1.45E+10
pair8	14.09456	-27.7278	7.87E+11
pair9	28.95152	-29.7347	3.32E+12
pair10	1.897673	-22.4853	1.43E+10
pair11	56.9093	-30.3929	1.28E+13
pair12	10.74778	-23.8126	4.57E+11
pair13	26.27409	-19.2267	2.73E+12
pair14	11.18128	-25.7401	4.95E+11
pair15	1.589608	-26.3259	1E+10
pair16	11.3227	-24.5697	5.08E+11
pair17	26.7853	-28.1856	2.84E+12
pair18	4.974719	-13.1306	9.8E+10
pair19	18.63467	-30.4564	1.38E+12
pair20	7.015593	-21.3555	1.95E+11
pair21	3.647131	-23.1586	5.27E+10
pair22	11.77549	-24.7781	5.49E+11
pair23	42.32999	-29.2549	7.1E+12
pair24	21.13558	-21.5872	1.77E+12
pair25	3.647496	-21.2293	5.27E+10
pair26	16.33348	-26.9361	1.06E+12
pair27	13.72005	-19.3254	7.46E+11
pair28	14.06871	-24.1734	7.84E+11
pair29	45.38532	-28.0352	8.16E+12

pair30	26.39946	-26.6555	2.76E+12
pair31	33.64436	-29.0234	4.48E+12
pair32	35.17767	-24.7944	4.9E+12
pair33	3.629686	-18.1874	5.22E+10
pair34	10.93702	-21.6298	4.74E+11
pair35	22.72602	-26.8254	2.05E+12
pair36	54.88849	-23.3193	1.19E+13
pair37	8.50104	-23.326	2.86E+11
pair38	0.42409	-28.9016	7.12E+08
pair39	22.71675	-23.9701	2.04E+12
pair40	26.69592	-25.9972	2.82E+12
pair41	39.7601	-26.8324	6.26E+12
pair42	43.45401	-31.7007	7.48E+12
pair43	5.725936	-16.5158	1.3E+11
pair44	8.523273	-16.2341	2.88E+11
pair45	42.94084	-25.6963	7.3E+12
pair46	14.09611	-19.6353	7.87E+11
pair47	6.347657	-13.0271	1.6E+11
pair48	2.593955	-20.9912	2.66E+10
pair49	42.21205	-15.5058	7.06E+12
Average	19.65064	-23.9822	1.53E+12

Tab. S5. Electronic coupling and rate of A_a-A_a type Y6 dimer

pairN	V	Ecombin	rate
pair0	11.46974	-12.0921	5.21E+11
pair1	27.14757	-14.8758	2.92E+12
pair2	5.94844	-13.6322	1.4E+11
pair3	30.55777	-14.7542	3.7E+12
pair4	13.69279	-13.8998	7.43E+11
pair5	5.513226	-16.335	1.2E+11
pair6	12.34747	-13.579	6.04E+11
pair7	43.68645	-14.0292	7.56E+12
pair8	25.01195	-15.9203	2.48E+12
pair9	5.782777	-13.2137	1.32E+11
pair10	10.11304	-13.9327	4.05E+11
pair11	0.261754	-8.77592	2.71E+08
pair12	27.93816	-12.5126	3.09E+12
pair13	2.929248	-14.4212	3.4E+10
pair14	5.468518	-12.6091	1.18E+11
pair15	19.00423	-14.4597	1.43E+12
pair16	34.91926	-16.1144	4.83E+12
pair17	11.64038	-11.9305	5.37E+11
pair18	43.99712	-14.7781	7.67E+12
pair19	36.28401	-14.5513	5.21E+12

pair20	21.10077	-15.7932	1.76E+12
pair21	31.26154	-11.0593	3.87E+12
pair22	12.70566	-19.8243	6.39E+11
pair23	53.67129	-14.8213	1.14E+13
pair24	2.986808	-12.2014	3.53E+10
pair25	18.86896	-10.5472	1.41E+12
pair26	16.55239	-11.9704	1.09E+12
pair27	51.34737	-15.7599	1.04E+13
pair28	42.31346	-12.9409	7.09E+12
pair29	10.39335	-15.7981	4.28E+11
pair30	12.36625	-14.1526	6.06E+11
pair31	54.79315	-15.1229	1.19E+13
pair32	13.83767	-13.5097	7.58E+11
pair33	0.644623	-13.3685	1.65E+09
pair34	9.762175	-13.6402	3.77E+11
pair35	2.581558	-14.8452	2.64E+10
pair36	12.30772	-8.41238	6E+11
pair37	4.749698	-9.2309	8.93E+10
pair38	5.1434	-12.2484	1.05E+11
pair39	14.7566	-14.9119	8.62E+11
pair40	19.37558	-14.8946	1.49E+12
pair41	0.22726	-12.7293	2.05E+08
pair42	3.35533	-11.994	4.46E+10
pair43	2.599421	-15.5428	2.68E+10
pair44	13.04851	-13.4842	6.74E+11
pair45	10.94682	-14.9559	4.75E+11
pair46	2.001959	-9.41835	1.59E+10
pair47	25.90745	-14.3418	2.66E+12
pair48	43.01963	-14.3202	7.33E+12
pair49	15.13225	-13.5903	9.07E+11
Average	18.02945	-13.6369	1.29E+12

Tab. S6. Electronic coupling and rate of A_a-A_d type Y6 dimer

pairN	V	Ecombin	rate
pair0	13.55671	-13.8463	7.28E+11
pair1	32.51245	-18.5564	4.19E+12
pair2	4.818774	-13.5977	9.2E+10
pair3	26.28229	-11.4992	2.74E+12
pair4	2.105516	-12.0063	1.76E+10
pair5	53.02524	-16.8446	1.11E+13
pair6	8.482583	-16.9415	2.85E+11
pair7	6.606184	-14.3284	1.73E+11
pair8	1.060411	-14.5502	4.45E+09

pair9	18.51473	-12.8845	1.36E+12
pair10	11.6832	-10.8618	5.41E+11
pair11	1.679035	-18.7476	1.12E+10
pair12	15.04642	-14.4428	8.97E+11
pair13	1.937146	-9.99812	1.49E+10
pair14	34.33691	-12.6262	4.67E+12
pair15	12.64309	-13.95	6.33E+11
pair16	21.26763	-11.8743	1.79E+12
pair17	9.840019	-15.3269	3.83E+11
pair18	19.37589	-16.4501	1.49E+12
pair19	33.45533	-18.3655	4.43E+12
pair20	22.70181	-17.9937	2.04E+12
pair21	2.058907	-15.0846	1.68E+10
pair22	13.99826	-12.3026	7.76E+11
pair23	1.909559	-14.7179	1.44E+10
pair24	7.321059	-12.6938	2.12E+11
pair25	24.95029	-16.637	2.47E+12
pair26	32.74203	-18.3598	4.25E+12
pair27	3.989205	-12.759	6.3E+10
pair28	17.99647	-14.6182	1.28E+12
pair29	9.636609	-12.7514	3.68E+11
pair30	36.41597	-19.2397	5.25E+12
pair31	3.358607	-14.3059	4.47E+10
pair32	19.69425	-13.2991	1.54E+12
pair33	6.216829	-12.0727	1.53E+11
pair34	7.447183	-15.5399	2.2E+11
pair35	1.146748	-10.6582	5.21E+09
pair36	13.83432	-14.7442	7.58E+11
pair37	1.279979	-16.3785	6.49E+09
pair38	26.36809	-8.44396	2.75E+12
pair39	24.08351	-12.9466	2.3E+12
pair40	24.83266	-15.621	2.44E+12
pair41	30.92771	-16.4951	3.79E+12
pair42	6.847868	-17.1784	1.86E+11
pair43	26.89696	-10.4024	2.87E+12
pair44	26.39736	-18.5187	2.76E+12
pair45	28.44072	-15.3148	3.2E+12
pair46	9.734804	-15.2271	3.75E+11
pair47	35.76587	-11.9731	5.07E+12
pair48	12.61675	-16.8713	6.3E+11
pair49	29.90331	-20.7067	3.54E+12
Average	16.75486	-14.6311	1.11E+12

Table. S7. Hole coupling and hole-transform rate of D_a-D_d type PM6 dimer

DDN	V	Ecombin	rate
DD0	34.60851	-11.9056	1.2E+12
DD1	15.32442	-14.1573	2.36E+11
DD2	22.44266	-12.0571	5.05E+11
DD3	17.61577	-11.7652	3.11E+11
DD4	30.41234	-12.3379	9.28E+11
DD5	23.23323	-12.1404	5.41E+11
DD6	1.291811	-11.4436	1.67E+09
DD7	22.81889	-12.1166	5.22E+11
DD8	38.42225	-13.308	1.48E+12
DD9	26.43751	-11.0429	7.01E+11
DD10	35.16674	-12.3344	1.24E+12
DD11	12.60955	-11.1555	1.59E+11
DD12	17.89472	-14.2069	3.21E+11
DD13	31.53266	-17.6241	9.97E+11
DD14	33.89273	-17.8708	1.15E+12
DD15	54.18921	-17.7035	2.95E+12
DD16	76.23091	-16.0953	5.83E+12
DD17	47.9932	-19.0585	2.31E+12
DD18	66.48768	-19.4351	4.43E+12
DD19	44.42823	-17.0975	1.98E+12
DD20	63.36648	-16.6384	4.03E+12
DD21	38.17766	-18.8274	1.46E+12
DD22	59.70493	-18.3636	3.58E+12
DD23	70.98859	-13.4253	5.05E+12
DD24	5.165785	-12.7376	2.68E+10
DD25	26.96312	-16.1284	7.29E+11
DD26	24.07251	-13.8903	5.81E+11
DD27	34.84144	-13.2455	1.22E+12
DD28	27.3102	-10.909	7.48E+11
DD29	11.55613	-12.869	1.34E+11
DD30	20.60165	-12.7983	4.26E+11
DD31	1.239107	-13.223	1.54E+09
DD32	6.917662	-13.2567	4.8E+10
DD33	5.18174	-14.0072	2.69E+10
DD34	38.01983	-14.6674	1.45E+12
DD35	2.537771	-16.2043	6.46E+09
DD36	17.45027	-18.8189	3.05E+11
DD37	19.41391	-26.6014	3.78E+11
DD38	20.93175	-11.7957	4.39E+11
DD39	60.51373	-15.3523	3.67E+12
DD40	64.29762	-13.6912	4.15E+12
DD41	16.3323	-13.923	2.68E+11
DD42	7.197228	-8.5001	5.2E+10

DD43	19.92836	-14.6973	3.98E+11
DD44	62.39584	-23.8962	3.9E+12
DD45	16.94183	-11.9475	2.88E+11
DD46	10.82727	-13.3821	1.18E+11
DD47	5.081872	-13.1067	2.59E+10
DD48	1.753917	-12.9326	3.09E+09
DD49	28.46165	-15.0068	8.12E+11
Average	28.8241	-14.594	8.33E+11

Table S8. Hole coupling and hole-transform rate of D_d-D_d type PM6 dimer

DDN	V	Ecombin	rate
DD0	3.229337	6142523	1.05E+10
DD1	1.125507	6142521	1.27E+09
DD2	0.189667	6142483	36080425
DD3	12.06103	6142497	1.46E+11
DD4	19.84233	6142501	3.95E+11
DD5	4.316867	6142503	1.87E+10
DD6	11.88422	6142504	1.42E+11
DD7	2.037642	6142533	4.16E+09
DD8	0.415564	6142561	1.73E+08
DD9	2.940152	6142530	8.67E+09
DD10	7.065553	6142499	5.01E+10
DD11	3.0423	6142508	9.28E+09
DD12	3.873404	6142515	1.5E+10
DD13	7.476416	6142525	5.61E+10
DD14	22.85717	6142507	5.24E+11
DD15	7.958293	6142524	6.35E+10
DD16	7.295163	6142523	5.34E+10
DD17	1.975372	6142557	3.91E+09
DD18	12.40452	6142553	1.54E+11
DD19	13.88806	6142489	1.93E+11
DD20	4.316284	6142517	1.87E+10
DD21	19.53043	6142561	3.83E+11
DD22	54.23889	6142542	2.95E+12
DD23	18.6726	6142570	3.5E+11
DD24	41.60882	6142507	1.74E+12
DD25	1.674778	6142555	2.81E+09
DD26	25.77844	6142540	6.67E+11
DD27	25.00218	6142546	6.27E+11
DD28	6.466278	6142532	4.19E+10
DD29	1.975372	6142557	3.91E+09
DD30	13.25205	6142508	1.76E+11
DD31	2.17263	6142543	4.73E+09
DD32	0.470611	6142522	2.22E+08

DD33	3.77264	6142532	1.43E+10
DD34	1.816722	6142566	3.31E+09
DD35	8.840285	6142580	7.84E+10
DD36	8.219979	6142561	6.78E+10
DD37	2.382556	6142595	5.69E+09
DD38	0.826715	6142490	6.85E+08
DD39	21.53503	6142528	4.65E+11
DD40	2.908676	6142481	8.49E+09
DD41	3.017071	6142482	9.13E+09
DD42	3.96442	6142532	1.58E+10
DD43	2.715342	6142524	7.39E+09
DD44	15.09313	6142559	2.28E+11
DD45	15.09313	6142559	2.28E+11
DD46	59.33879	6142531	3.53E+12
DD47	15.82525	6142542	2.51E+11
DD48	3.124743	6142535	9.79E+09
DD49	12.33067	6142514	1.52E+11
Average	10.83686	6142529	1.18E+11

Table S9. Hole coupling and hole-transform rate of D_a-D_a type PM6 dimer

DDN	V	Ecombin	rate
DD0	0.301672	6142522	91276314
DD1	0.432885	6142491	1.88E+08
DD2	13.34149	6142505	1.79E+11
DD3	2.536635	6142547	6.45E+09
DD4	3.167545	6142547	1.01E+10
DD5	4.89377	6142558	2.4E+10
DD6	16.2489	6142528	2.65E+11
DD7	1.764092	6142567	3.12E+09
DD8	0.427529	6142521	1.83E+08
DD9	2.546768	6142543	6.51E+09
DD10	3.923932	6142524	1.54E+10
DD11	25.61059	6142513	6.58E+11
DD12	18.91301	6142546	3.59E+11
DD13	52.47206	6142514	2.76E+12
DD14	21.93807	6142481	4.83E+11
DD15	21.93807	6142481	4.83E+11
DD16	4.984584	6142566	2.49E+10
DD17	43.43424	6142524	1.89E+12
DD18	25.73851	6142531	6.64E+11
DD19	44.98276	6142574	2.03E+12
DD20	9.583659	6142550	9.21E+10
DD21	55.71208	6142548	3.11E+12
DD22	30.52819	6142554	9.35E+11

DD23	0.400047	6142523	1.61E+08
DD24	23.26554	6142519	5.43E+11
DD25	9.226142	6142527	8.54E+10
DD26	7.016583	6142541	4.94E+10
DD27	35.12697	6142579	1.24E+12
DD28	19.68566	6142526	3.89E+11
DD29	51.48054	6142534	2.66E+12
DD30	5.591926	6142544	3.14E+10
DD31	27.28504	6142554	7.47E+11
DD32	2.590128	6142544	6.73E+09
DD33	0.184788	6142515	34248032
DD34	0.441734	6142474	1.96E+08
DD35	0.829392	6142500	6.9E+08
DD36	1.18669	6142490	1.41E+09
DD37	47.8417	6142548	2.3E+12
DD38	32.0206	6142592	1.03E+12
DD39	0.3989	6142575	1.6E+08
DD40	76.12438	6142503	5.81E+12
DD41	50.09278	6142561	2.52E+12
DD42	68.84911	6142553	4.75E+12
DD43	17.85704	6142527	3.2E+11
DD44	4.27767	6142559	1.84E+10
DD45	61.3335	6142552	3.77E+12
DD46	1.020088	6142517	1.04E+09
DD47	50.77305	6142533	2.59E+12
DD48	89.52005	6142540	8.04E+12
DD49	21.69239	6142517	4.72E+11
Average	22.23067	6142534	4.96E+11

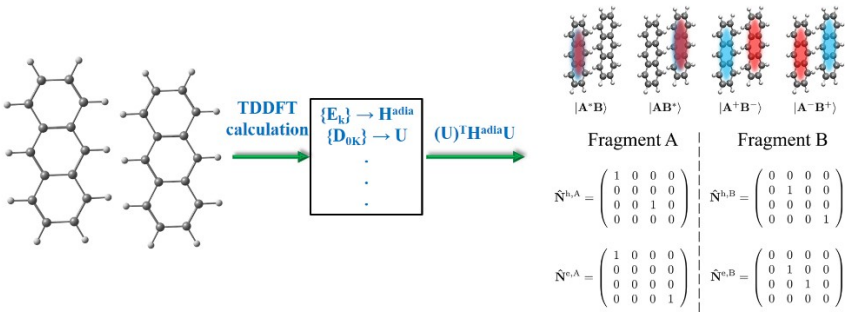

Figure S14. The process of constructing dimeric exciton states and CT states.[3]

Table S10. Coupling (meV) of A_a-D_a type PM6:Y6 complexes.

DAN	Y6_CT1	PM6_CT1	PM6_CT2	PM6_CT3	PM6_CT4	PM6_CT5
DA0	41.25	39.03	34.92	0.9	22.13	1.93
DA1	22.53	40.83	23.78	0.91	9.48	9.45

DA2	3.47	5.63	2.52	13.01	22.09	7.54
DA3	11.87	16.41	34.45	8.59	29.31	18.49
DA4	10.13	12.36	0.54	0.91	3.9	3.6
DA5	24.91	28.41	19.8	4	19.88	0.25
DA6	11.87	4.19	7.87	7.28	9.39	0.71
DA7	10.17	8.8	9.03	2.29	0.49	17.9
DA8	16.45	7.1	3.24	3.25	12.38	16.17
DA9	41.83	104.35	50.95	48.61	29.89	7.72
DA10	17.51	16.91	12.4	0.12	2.15	4.82
DA11	17.77	10.09	9.34	1.06	18.76	18.86
DA12	27.79	50.26	30.84	14.49	3.87	6.62
DA13	50.45	84.55	82.12	6.05	101.55	40.2
DA14	54.59	26.01	26.72	5.49	27.96	26.15
DA15	6.63	11.09	6.38	3.17	37.25	7.15
DA16	10.02	19.26	28.64	7.05	36.8	30.75
DA17	24.15	16.34	0.09	13.43	22.35	3.55
DA18	12.12	72.2	45.86	3.93	18.16	4.42
DA19	34.93	27.42	18.27	10.66	23.88	7.87
DA20	24.89	27.2	1.75	10.32	84.08	23.21
DA21	49.31	16.94	1.69	0.66	9.79	8
DA22	23.97	20.23	10.65	6.25	7.83	1.51
DA23	14.9	53.51	60.28	25.43	70.02	14.01
DA24	36.04	47.91	43.47	9.22	19.69	5.51
DA25	20.5	2.47	19.89	10.87	47.35	22.45
DA26	25.94	0.62	54.54	6.17	94.54	21.52
DA27	72.14	74.51	62.11	1.26	45.77	3.76
DA28	54.09	45.65	11.51	17.52	25.15	20.09
DA29	49.35	12.87	8	3.57	3.03	12.61
DA30	38.5	130.82	54.65	4.34	43.08	26.87
DA31	4.4	4.53	2.26	0.33	14.35	32.28
DA32	27.42	1	30.67	54.24	81.67	40.19
DA33	5.99	2.71	0.25	2.96	28.18	34.2
DA34	10.58	16.33	15.86	5.38	35.13	5.15
DA35	34.05	73.49	46.89	14.27	34.88	6.18
DA36	21.87	14.07	29.31	12.49	60.53	22.9
DA37	10.22	82.17	92.71	34.72	91.66	24.15
DA38	9.39	22.89	11.47	14.97	14.47	87.47
DA39	10.16	5.05	10.92	2.66	31.52	18.32
DA40	39.18	25.65	3.6	9.6	8.91	5.13
DA41	5.18	43.65	40.76	11.43	55.9	27.56
DA42	97.11	6.93	34.11	14.72	99.83	47.56
DA43	60.98	14.27	2	3.75	12.66	3.01
DA44	62.36	46.47	24.21	9.69	28.29	2.21
DA45	21.41	44.9	27.16	6.53	9.71	12.17

DA46	50.76	31.4	26.2	6.29	29.8	3.91
DA47	15.86	33.64	26.92	0.13	8.84	8.75
DA48	2.03	3.04	28.4	23.21	55.58	42.63
DA49	36.89	34.21	26.16	0.35	36.1	32.54
Average	27.71	30.80	25.12	9.57	32.80	17.00

Table S11. Coupling (meV) of A_a-D_d type PM6:Y6 complexes.

DAN	Y6_CT1	PM6_CT1	PM6_CT2	PM6_CT3	PM6_CT4	PM6_CT5
DA0	0.08	0.63	10.52	5.44	39.82	1.84
DA1	22.17	21.08	3.84	7.73	7.2	7.61
DA2	20.2	0.34	11.19	7.98	19.41	24.83
DA3	19.59	2.96	2.46	1.47	5.51	0.27
DA4	4.64	2.16	5.88	2.69	9.19	1.38
DA5	16.67	15.75	11.17	13.49	19.8	10.11
DA6	41.95	8.76	3.44	13.68	3.63	11.81
DA7	10.15	15.92	11.64	4.36	5.64	0.74
DA8	2.23	1.59	2.19	2.46	9.09	0.16
DA9	14.95	40.8	42.35	0.52	11.43	2.58
DA10	35.2	34.27	21.89	5.51	23.94	0.29
DA11	17.67	11.2	6.75	1.22	1.7	5.27
DA12	20.36	29.67	0.23	27.74	30.14	2.94
DA13	13.42	9.96	0.99	10.97	10.61	8.34
DA14	31.74	20.95	10.43	13.99	0.78	6.37
DA15	7.02	20.59	9.7	24.41	17.64	2.1
DA16	8.27	31.03	12.16	19.38	14.05	16.11
DA17	12.26	25.78	18.64	9.98	18.12	4.16
DA18	53.46	31.55	0.35	24.28	7.41	1.12
DA19	23.35	6.44	12.06	1.75	1.27	27.25
DA20	29.69	19.97	9.74	3.32	1.24	3.71
DA21	27.08	16.72	7.35	5.22	8.11	1.6
DA22	7.94	43.69	7.46	12.66	63.78	0.09
DA23	0.23	1.59	4.32	0.15	8.53	14.56
DA24	22	62.02	42.43	49.31	1.69	5.31
DA25	22.28	14.78	13.04	4.97	0.38	4.48
DA26	37.04	37.97	27.89	0.01	15.29	2.91
DA27	4.86	8.52	5.9	9.82	17.4	4.72
DA28	0.8	3.08	2.57	7.69	7.83	9.22
DA29	21.24	1.2	1.85	2.97	1.8	0.17
DA30	40.54	30.76	1.91	3.83	5.35	1.02
DA31	5.73	26.04	9.09	7.21	21.84	5.24
DA32	16.51	41.27	1.84	7.22	3.94	33.22
DA33	15.03	43.36	15.38	0.36	1.91	1.11
DA34	10.07	14.48	0.73	9.62	1.63	6.86
DA35	40.91	18.66	9.18	9.07	23.33	5.25

DA36	1.49	9.56	0.08	10.51	5	3.77
DA37	7.5	18.77	6.01	18.83	27.84	16.07
DA38	17.3	10.26	2.09	16.23	57.56	27.37
DA39	2.55	1.94	0.66	5.1	1.16	0.12
DA40	1.41	0.15	1.38	1.64	15.03	15.86
DA41	18.24	19.02	11.43	15.34	23.11	11.97
DA42	1.31	4.25	4.22	11.28	23.23	8.52
DA43	20.65	17.19	5.41	13.44	26.91	1.8
DA44	18.82	44.03	31.87	15.44	53.88	3.98
DA45	38.17	69.08	52.96	28.72	27.3	6.22
DA46	76.08	69.78	22.13	18.53	17.48	3.66
DA47	43.22	30.15	27.83	8.91	4.27	0.45
DA48	21.98	38.51	29.65	10.29	21.51	4.3
DA49	31.83	34.1	5.22	19.62	6.83	1.09
Average	19.55	21.64	11.19	10.52	15.03	6.79

Table S12. Coupling (meV) of A_d-D_a type PM6:Y6 complexes.

DAN	Y6_CT1	PM6_CT1	PM6_CT2	PM6_CT3	PM6_CT4	PM6_CT5
DA0	24.95	2.01	2.51	1.7	8.87	4.82
DA1	8.4	23.08	6.02	17.48	38.29	1.13
DA2	49.37	7.33	2.5	5.05	13.79	4.16
DA3	58.8	71.31	27.5	8.34	10.65	11.29
DA4	20.27	18.35	10.17	2.05	33.77	12.06
DA5	43.72	28.82	33.6	6.11	11.97	4.29
DA6	27.04	0.31	18.86	3.6	17.56	3.29
DA7	41.27	16.43	11.69	0.73	2.94	3.01
DA8	27.7	12.84	4.51	2.5	8.55	0.67
DA9	35.82	35.5	10.27	0.04	1.05	0.2
DA10	6.24	14.19	4.87	0.8	7.52	1.97
DA11	26.3	58.33	16.22	2.54	7.92	16.01
DA12	32.45	49.24	24.89	9.01	22.93	24.21
DA13	42.54	27.31	21.1	5.89	8.66	13.53
DA14	63.05	31.57	10.34	0.69	0.79	2.97
DA15	5.49	3.07	4.89	0.53	2.76	2.56
DA16	24.61	16.25	5.97	5.65	51.4	5.56
DA17	15.86	33.64	26.92	0.13	8.84	8.75
DA18	12.58	28.89	2.93	31.58	7.29	46.65
DA19	15.84	2.75	35.88	7.41	48.62	10.79
DA20	25.08	16.33	7.86	3.68	13.54	6.31
DA21	4.02	32.6	12.4	2.99	0.05	5.44
DA22	22.84	28.56	10.99	5.48	0.27	2.15
DA23	6.54	35.4	0.91	2.7	0.22	8.45
DA24	41.08	4.08	6.02	0.73	18.23	0.49
DA25	50.02	6.62	16.57	9.2	15.33	12.27

DA26	24.58	4.39	22.77	0.02	11.87	0.48
DA27	8.4	23.08	6.02	17.48	38.29	1.13
DA28	35.95	0.86	3.83	3.39	13.68	10.95
DA29	4.67	54.31	19.43	16.91	72.16	9.26
DA30	47.74	61.74	43.38	7.76	0.01	37.77
DA31	26.63	41.34	10.12	1.5	6.15	11.63
DA32	58.3	46.63	21.35	3.03	15.31	30.77
DA33	17.63	73.21	32.36	6.95	3.54	7.89
DA34	45.96	26.07	24.11	0.63	26.94	12
DA35	11.82	5.69	2.73	2.05	3.18	7.31
DA36	2.3	40.25	23.42	1.01	0.39	17.56
DA37	48.22	32.82	0.57	4.79	13.2	8.67
DA38	11.06	2.61	18.31	12.35	25.6	39.1
DA39	41.34	18.06	16.8	57.31	65.63	11.4
DA40	27.91	18.71	0.42	1.8	16.46	15.6
DA41	21.28	9.42	3.08	16.87	5.55	1.84
DA42	10.11	32.52	10.48	8.91	4.82	3.65
DA43	15.01	5.3	12.85	4.79	6.22	1.99
DA44	26.28	18.06	15.62	0.25	1.47	0.92
DA45	40.26	66.92	44.55	10.68	4.88	0.47
DA46	11.13	21.08	0.87	11.21	2.31	2.16
DA47	106.03	50.1	32.91	3.84	54.53	49.8
DA48	32.38	43.57	4.12	3.03	50.76	13.34
DA49	18.81	10.14	14.56	8.61	36.99	4.34
Average	28.51	26.23	14.42	6.83	16.83	10.26

Table S13. Coupling (meV) of A_d-D_d type PM6:Y6 complexes.

DAN	Y6_CT1	PM6_CT1	PM6_CT2	PM6_CT3	PM6_CT4	PM6_CT5
DA0	23.78	16.78	6.56	10.55	11.15	4.05
DA1	46.54	20.7	9.69	11.58	7.33	1.8
DA2	51.72	28.73	18.73	13.72	27.11	3.07
DA3	23.22	54.62	59.83	16.13	55.21	5.92
DA4	43.42	21.39	4.29	15.35	17.16	7.51
DA5	47.51	20.76	8.19	3.81	15.27	17.98
DA6	16.58	19.89	40.75	26.35	44.24	8.42
DA7	66.92	32.62	4.32	4.72	24.48	17.78
DA8	33.34	26.71	40.43	33.68	35.07	12.7
DA9	41.7	11.64	22.31	32.39	3.51	4.14
DA10	16.81	22.88	10.18	9.65	1.41	5.57
DA11	31.83	29.4	1.1	16.13	4.78	6.34
DA12	23.15	14.49	38.85	26.19	46.04	20.35
DA13	13.17	43.51	33.31	37.89	46.65	19.14
DA14	7.26	2.44	0.19	0.73	31.48	0.06
DA15	48.21	4.9	0.55	8.05	5.18	3.79

DA16	45.72	29.46	10.63	19.08	28.01	1.75
DA17	16.78	5.7	29.3	16.54	26.01	7.2
DA18	40.54	30.76	1.91	3.83	5.35	1.02
DA19	28.63	0.14	5.34	4.7	26.13	5.97
DA20	8.16	24.28	15	9.2	32.95	16.84
DA21	43.06	32.89	16.13	11.81	20.86	3.59
DA22	69.81	74.4	58.6	31.35	25.92	3.84
DA23	58.29	8.71	11.76	19.05	14.93	0.91
DA24	18.41	10.13	20.99	15.06	10.98	2.14
DA25	11.53	21.71	42.11	11.83	24.91	8.14
DA26	38.83	26.61	24.85	13.61	35.52	12.03
DA27	75.5	46.95	5.74	12.12	12.16	9.42
DA28	29.19	22.29	20.64	15.75	56.2	11.47
DA29	85.47	41.64	2.77	1.5	39.79	11.83
DA30	64.24	29.67	2.26	7.86	34.81	7.66
DA31	13.72	35.27	31.93	40.86	57.26	47.01
DA32	25.31	11.52	13.44	6.09	25.02	4.19
DA33	1.98	32.35	26.58	4.11	55.09	8.95
DA34	9.59	9.92	30.87	26.54	34.06	0.92
DA35	40.24	28.15	7.72	23.06	21.97	0.13
DA36	46.71	47.09	60.23	30	1.24	6.49
DA37	77.77	9.32	4.42	36.53	48.13	25.51
DA38	16.73	35.38	11.29	52.85	1.13	21.47
DA39	43.08	17.96	21.73	15.12	47.33	17.15
DA40	24.5	23.34	28.02	6	34.21	20.12
DA41	37.33	4.28	10.34	16.28	7.66	1.91
DA42	54.48	21.93	8.08	34.86	52.45	38.66
DA43	12.58	20.72	48.8	40.45	33.4	11.64
DA44	20.48	35.38	19.3	20.88	13.25	7.85
DA45	31.95	38.57	1.77	3.21	13.09	16.46
DA46	36.72	11.46	31.18	24.02	43.75	11.38
DA47	50.98	32.59	14.1	3.24	31.27	23.42
DA48	29.28	41.18	8.11	4.78	41.11	12.25
DA49	27.45	17.44	0.6	0.78	14.93	2.03
Average	35.404	25.013	18.9164	16.9974	26.939	10.3994

Table S14. Coupling (meV) of A_{da}-D_{da} type PM6:Y6 complexes.

DAN	Y6_CT1	PM6_CT1	PM6_CT2	PM6_CT3	PM6_CT4	PM6_CT5
DA0	45.36	23.2	35.99	16.39	13.75	4.42
DA1	24.56	2.1	7.4	4.63	2.67	18.57
DA2	51.89	24.87	1.44	6.83	0.54	4.93
DA3	32.64	70.38	23.35	42.11	7.5	43.24
DA4	34.75	26.01	4.94	21.55	33.71	65.36
DA5	52.46	22.97	9.64	5.53	31.15	3.01

DA6	22.94	18.83	4.28	11.52	39.87	13.54
DA7	60.12	58.14	79.48	29.46	7.92	13.21
DA8	47.88	36.1	1.22	2.38	40.85	36.85
DA9	29.98	12.2	7.43	0.87	16.29	6.83
DA10	65.15	50.8	30	70.54	34.08	4.67
DA11	0.29	9.2	1.17	2.2	4.31	19.1
DA12	65.75	46.98	75.94	11.53	3.8	18.53
DA13	86.28	62.24	41.91	20.18	37.85	51.65
DA14	14.66	4.04	9.77	9.14	3.72	0.49
DA15	32.8	34.23	31.77	10.54	11.81	5.33
DA16	37.36	43.8	25.53	10.09	50.08	82.61
DA17	39.11	23.42	18.35	14.99	53.57	41.89
DA18	50.56	2.63	18.6	3.34	2.4	1.29
DA19	30.07	14.52	1.35	15.3	33.42	9.89
DA20	51.71	11.11	29.19	22.45	29.96	12.54
DA21	22.2	1.79	6.34	3.4	13.31	1.02
DA22	13.74	26.96	19.58	12.08	11	121.33
DA23	41.56	23.03	30.21	7.36	4.37	22.24
DA24	16.56	58.78	24.04	27.84	7.23	12.23
DA25	48.62	26.78	41.44	28.33	5.65	21.96
DA26	41.08	73.5	69.02	34.84	4.67	19.53
DA27	86.6	34.79	28.47	33.5	4.12	33.53
DA28	29.98	12.2	7.43	0.87	16.29	6.83
DA29	31.73	56.95	4.51	4.09	3.53	8.63
DA30	74.9	48.97	41.06	11.98	8.15	31.28
DA31	47.98	15	2.75	8.03	15.63	17.65
DA32	25.9	35.18	34.62	25.43	8.68	8.89
DA33	57.64	23.66	39.75	9.24	9.47	0.13
DA34	17.65	8.2	7.44	4.73	12.1	12.45
DA35	37.9	4.51	7.35	5.36	84.66	43.95
DA36	65.75	46.98	75.94	11.53	3.8	18.53
DA37	14.66	4.04	9.77	9.14	3.72	0.49
DA38	19.63	56.24	4.36	6.41	70.66	43.46
DA39	18.93	41.01	8.01	10.88	11.62	24.19
DA40	51.71	11.11	29.19	22.45	29.96	12.54
DA41	66.02	0.84	21.03	24.81	8.74	13.34
DA42	7.31	1.5	2.72	8.85	3.45	6.66
DA43	45.82	25.6	13.73	18.6	53.47	2.85
DA44	43.1	16.06	2.91	1.52	44.34	53.38
DA45	14.4	43.44	22.59	0.29	4.03	72.29
DA46	10.26	3.69	18.54	9.57	21.42	16.73
DA47	10.08	69.47	57.15	27.58	4.51	18.63
DA48	27.95	28.87	25.8	13.05	9.99	15.67
DA49	28.9	11.19	5.68	17.92	18.25	36.69

Average	37.89	28.16	22.40	14.62	19.12	23.10

Table S15. Coupling (meV) of A_{da}-D_{ad} type PM6:Y6 complexes.

DAN	Y6_CT1	PM6_CT1	PM6_CT2	PM6_CT3	PM6_CT4	PM6_CT5
DA0	67.25	19.07	12.35	55.61	33.54	44.75
DA1	0.7	14.4	24.44	0.47	24	9.99
DA2	54.42	21.44	9.56	20.99	9.61	25.41
DA3	10.79	11.87	17.59	14.16	44.49	44.66
DA4	7.22	52.46	52.63	3.68	30.3	12.76
DA5	66.17	74.2	36.28	25.62	19.36	0.5
DA6	23.71	25.86	36.26	17.67	19.21	10.54
DA7	63.86	1.87	31.95	11.93	46.57	19.77
DA8	7.29	12.85	19.89	5.55	34.24	18.78
DA9	59.19	11.85	23.74	11	11.78	26.26
DA10	40.13	31.05	20.39	0.74	21.18	25.25
DA11	44.19	52.81	2.56	42.19	61.08	48.9
DA12	36.01	19.12	55.44	21.32	4.63	20.98
DA13	68.09	48.75	13.55	19.7	9.1	43.88
DA14	54.64	2.84	17.29	1.25	18.21	17.36
DA15	31.74	18.08	0.22	10.97	1.78	6.79
DA16	23.87	36.85	7.07	0.15	32.92	5.25
DA17	54.61	29.74	47.26	47.31	35.23	40.91
DA18	22.09	57.78	56.72	21.87	17.53	13.67
DA19	71.56	78.64	82.15	12.7	9.96	3.66
DA20	49.2	2.94	9.17	0.12	2.37	7.95
DA21	37.2	41.88	11.45	9.16	62.14	47.34
DA22	13.07	27.31	11.76	6.03	16.91	11.74
DA23	73.46	21.76	3.17	0.04	39.73	2.19
DA24	43.96	34.24	57.49	3.79	50.67	32.45
DA25	19.44	10.72	26.05	11.81	14.75	41.77
DA26	41.91	28.92	16.13	10.49	69.71	31.37
DA27	70.73	44.61	17.17	47.01	10.31	14.32
DA28	23.68	59.1	19.91	20.49	31.88	33.66
DA29	21.25	41.93	10.09	3.64	51.98	2.62
DA30	5.87	8.83	1.42	1.86	13.2	7.74
DA31	14.4	34.71	12.76	3.24	48.47	22.02
DA32	60.52	68.42	54.21	1.12	0.29	3.43
DA33	10.56	47.46	3.1	3.61	34	6.98
DA34	29.87	26.72	10.29	20.85	15.91	24.89
DA35	40.64	11.93	24.41	0.1	31.74	5.21
DA36	63.46	69.55	60.24	11.68	21.39	35.15
DA37	14.62	8.63	0.43	1.91	7.74	1.99
DA38	38.6	53.14	68.72	4.73	23.55	12.87

DA39	24.43	32.72	20.34	12.59	25.67	5.75
DA40	42.44	21.88	11.4	18.26	16.29	14.54
DA41	35.01	13.83	43.47	8.94	39.98	14.57
DA42	10.51	3.29	22.85	2.14	61.63	42.46
DA43	64.56	69.08	16.97	10.18	11.44	41.02
DA44	3.17	15.95	4.06	3.76	5.92	5.62
DA45	28.63	39.29	30.56	16.5	10.32	9.5
DA46	77.02	15.61	5.29	35.86	2.34	12.96
DA47	59.09	34.32	14.1	0.03	38.18	56.17
DA48	54.72	21.98	11.57	22.04	6.49	0.94
DA49	33.4	10.07	5.41	17.36	9.97	23.99
Average	38.25	30.84	23.42	13.08	25.19	20.26

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