Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.
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Supporting Information

Theoretical exploration on molecular packing and charge transfer mechanism of organic solar cells based on PM6:Y6

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Table S1 Vertical excitation energy(*E*/eV), excitation wavelength(*λ*/nm) and oscillator intensity(f) of the first twenty excited states of Dimer-1

Dimer-1	*E*/eV	*λ*/nm	f		*E*/eV	λ/nm	f
S_1	1.3362	927.90	0.0017	S_{11}	2.0072	617.69	0.0232
S_2	1.4221	871.82	0.0045	S_{12}	2.0236	612.69	0.0027
S_3	1.5675	790.98	0.0017	S_{13}	2.0264	611.83	0.0197
S_4	1.6369	757.42	0.9465	S_{14}	2.0613	601.50	0.0002
S_5	1.6507	751.08	0.0034	S_{15}	2.0708	598.73	0.0032
S_6	1.8032	687.57	0.0010	S_{16}	2.1096	587.72	0.0266
S_7	1.8252	679.30	0.8509	S_{17}	2.1160	585.95	0.0022
S_8	1.8402	673.74	0.0006	S_{18}	2.1200	584.82	0.0307
S_9	1.8784	660.04	0.5571	S_{19}	2.1644	572.84	0.0891
S_{10}	1.9906	622.84	0.1214	S_{20}	2.1750	570.06	0.0187

Table S2 Vertical excitation energy(*E*/eV), excitation wavelength(*λ*/nm) and oscillator intensity(f) of the first twenty excited states of Dimer-2

Dimer-2	*E*/eV	*λ*/nm	f		*E*/eV	λ/nm	f
S_1	1.4010	884.97	0.0021	S_{11}	2.0030	618.98	0.0014
S_2	1.5347	807.85	0.0187	S_{12}	2.0635	600.86	0.2232
S_3	1.6638	745.20	0.0737	S_{13}	2.0758	597.28	0.0196
S_4	1.7083	725.76	0.0507	S_{14}	2.0946	591.93	0.0047
S_5	1.7491	708.87	0.1443	S_{15}	2.1040	589.27	0.0046
S_6	1.8079	685.81	0.4248	S_{16}	2.1224	584.18	0.0341
S_7	1.8342	675.97	1.3623	S_{17}	2.1281	582.61	0.0183
S_8	1.8735	661.79	0.3332	S_{18}	2.1616	573.58	0.0881
S_9	1.8968	653.64	0.0815	S_{19}	2.1978	564.14	0.0104
S_{10}	1.9295	642.58	0.5797	S_{20}	2.2356	554.58	0.0020

Table S3 Vertical excitation energy(*E*/eV), excitation wavelength(*λ*/nm) and oscillator intensity(f) of the first twenty excited states of Dimer-3

Dimer-3	*E*/eV	*λ*/nm	f		*E*/eV	λ/nm	f
S_1	1.2166	1019.13	0.0061	S_{11}	1.9479	636.50	0.0812
S_2	1.4094	879.68	0.0121	S_{12}	1.9634	631.46	0.1150
S_3	1.5419	804.08	0.0080	S_{13}	1.9991	620.19	0.0305
S_4	1.6273	761.90	0.5684	S_{14}	2.0235	607.51	0.0822
S_5	1.6570	748.23	0.3998	S_{15}	2.0427	606.96	0.2030
S_6	1.7229	719.63	1.6724	S_{16}	2.0427	606.96	0.2030
S_7	1.7326	715.61	0.0715	S_{17}	2.0569	602.78	0.0071
S_8	1.7616	703.81	0.0536	S_{18}	2.0747	597.59	0.1775
S_9	1.8149	683.15	0.0114	S_{19}	2.1646	572.77	0.1369
S_{10}	1.8599	666.61	0.1068	S_{20}	2.1963	564.51	0.0254

Table S4 Vertical excitation energy(*E*/eV), excitation wavelength(*λ*/nm) and oscillator intensity(f) of the first twenty excited states of Dimer-4

Dimer-4	*E*/eV	*λ*/nm	f		*E*/eV	λ/nm	f
S_1	1.3038	950.95	0.0005	S_{11}	2.0217	613.26	0.0002
S_2	1.4561	851.49	0.0006	S_{12}	2.0538	603.67	0.1244
S_3	1.6237	763.58	0.0003	S_{13}	2.0633	600.90	0.2817
S_4	1.7587	704.98	0.0069	S_{14}	2.0714	598.54	0.0105
S_5	1.7747	698.63	0.0294	S_{15}	2.0817	595.58	0.0492
S_6	1.8072	686.06	2.7824	S_{16}	2.1499	576.70	0.0004
S_7	1.8346	675.80	0.4801	S_{17}	2.2195	558.62	0.0009
S_8	1.8635	665.35	0.0002	S_{18}	2.2458	552.08	0.1973
S_9	1.9835	625.07	0.0000	S_{19}	2.2516	550.65	0.0003
S_{10}	1.9911	622.71	0.0001	S_{20}	2.2536	550.15	0.0682

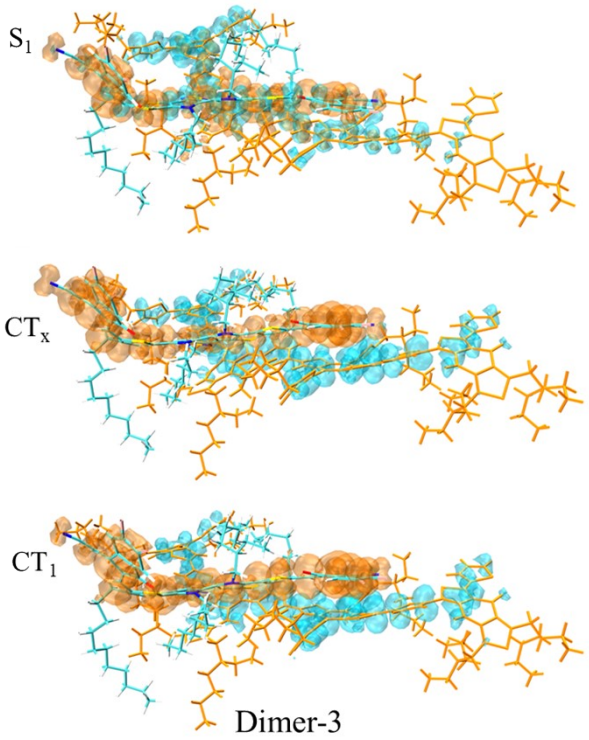

Figure S1. The hole-electron (blue-orange) density distribution of S_1 state, CT_X state, and CT_1 state of Dimer-3.

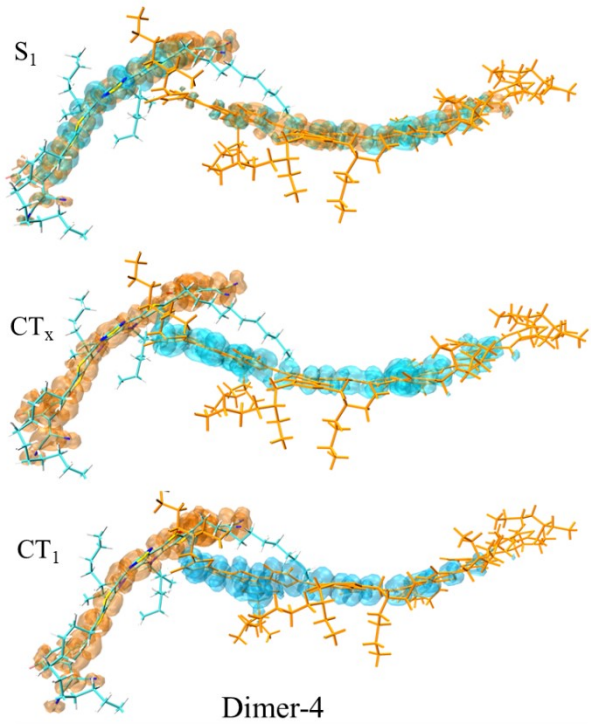

Figure S2. The hole-electron (blue-orange) density distribution of S_1 state, CT_X state, and CT_1 state of Dimer-4.

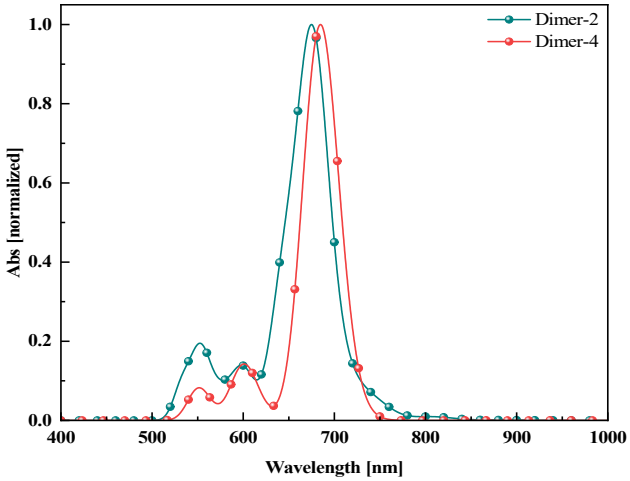

Figure S3. UV-Vis spectroscopy of Dimer-2 and Dimer-4.

Table S5 Electron transfer recombination energy($\lambda_{electron}$/eV), electron transfer Gibbs free energy($\Delta G_{electron}$/eV), electron transfer rates($k_{CT\text{-}electron}$/s^{-1}), hole transfer recombination energy(λ_{hole}/eV), hole transfer Gibbs free energy(ΔG_{hole}/eV), hole transfer rates($k_{CT\text{-}hole}$/s^{-1}) for the first seven excited states of Dimer-1

Dimer-1	$\lambda_{electron}$/eV	$\Delta G_{electron}$/eV	$k_{CT\text{-}electron}$/s^{-1}	λ_{hole}/eV	ΔG_{hole}/eV	$k_{CT\text{-}hole}$/s^{-1}
CT_1	0.9804	-0.5340	2.68×10^{11}	0.8808	-0.2805	3.82×10^{10}
CT_2	0.9804	-0.6539	1.15×10^{12}	0.8808	-0.4636	5.11×10^{11}
CT_3	0.9804	-0.5438	2.67×10^{11}	0.8808	-0.6236	8.98×10^{11}
S_1	0.9804	-0.5706	1.74×10^{15}	0.8808	-0.6393	5.09×10^{15}
CT_4	0.9804	-0.5830	7.63×10^{11}	0.8808	-0.6828	2.50×10^{12}
S_2	0.9804	-0.5528	4.64×10^{10}	0.8808	-0.6399	1.58×10^{11}
S_3	0.9804	-0.5682	1.60×10^{15}	0.8808	-0.6541	5.17×10^{15}

Table S6 Electron transfer recombination energy($\lambda_{electron}$/eV), electron transfer Gibbs free energy($\Delta G_{electron}$/eV), electron transfer rates($k_{CT\text{-}electron}$/s^{-1}), hole transfer recombination energy(λ_{hole}/eV), hole transfer Gibbs free energy(ΔG_{hole}/eV), hole transfer rates($k_{CT\text{-}hole}$/s^{-1}) for the first seven excited states of Dimer-2

Dimer-2	$\lambda_{electron}$/eV	$\Delta G_{electron}$/eV	$k_{CT\text{-}electron}$/s^{-1}	λ_{hole}/eV	ΔG_{hole}/eV	$k_{CT\text{-}hole}$/s^{-1}
CT_1	1.0307	-0.4573	8.46×10^{11}	0.8562	-0.3343	9.36×10^{11}
CT_2	1.0307	-0.6054	7.43×10^{12}	0.8562	-0.4242	5.39×10^{12}
CT_3	1.0307	-0.5390	2.31×10^{13}	0.8562	-0.5207	6.89×10^{13}
CT_4	1.0307	-0.5806	1.71×10^{15}	0.8562	-0.6471	7.73×10^{15}
S_1	1.0307	-0.5802	1.77×10^{15}	0.8562	-0.6415	7.80×10^{15}
S_2	1.0307	-0.5826	2.68×10^{14}	0.8562	-0.6558	1.24×10^{15}
S_3	1.0307	-0.5816	1.17×10^{15}	0.8562	-0.7121	6.78×10^{15}

Table S7 Electron transfer recombination energy($\lambda_{electron}$/eV), electron transfer Gibbs free energy($\Delta G_{electron}$/eV), electron transfer rates($k_{CT\text{-}electron}$/s^{-1}), hole transfer recombination energy(λ_{hole}/eV), hole transfer Gibbs free energy(ΔG_{hole}/eV), hole transfer rates($k_{CT\text{-}hole}$/s^{-1}) for the first seven excited states of Dimer-3

Dimer-3	$\lambda_{electron}$/eV	$\Delta G_{electron}$/eV	$k_{CT\text{-}electron}$/s^{-1}	λ_{hole}/eV	ΔG_{hole}/eV	$k_{CT\text{-}hole}$/s^{-1}
CT_1	1.0121	-0.4537	4.08×10^{11}	0.8036	-0.4558	2.12×10^{12}
CT_2	1.0121	-0.5322	1.04×10^{12}	0.8036	-0.5700	5.53×10^{12}
CT_3	1.0121	-0.4858	5.69×10^{11}	0.8036	-0.6679	7.32×10^{12}
S_1	1.0121	-0.5055	3.07×10^{14}	0.8036	-0.6895	3.47×10^{15}
S_2	1.0121	-0.5770	1.11×10^{14}	0.8036	-0.7518	7.46×10^{14}
S_3	1.0121	-0.5581	1.37×10^{15}	0.8036	-0.7891	1.11×10^{16}
S_4	1.0121	-0.6556	1.17×10^{15}	0.8036	-0.8172	4.45×10^{15}

Table S8 Electron transfer recombination energy($\lambda_{electron}$/eV), electron transfer Gibbs free energy($\Delta G_{electron}$/eV), electron transfer rates($k_{CT\text{-}electron}$/s^{-1}), hole transfer recombination energy(λ_{hole}/eV), hole transfer Gibbs free energy(ΔG_{hole}/eV), hole transfer rates($k_{CT\text{-}hole}$/s^{-1}) for the first seven excited states of Dimer-4

Dimer-4	$\lambda_{electron}$/eV	$\Delta G_{electron}$/eV	$k_{CT\text{-}electron}$/s^{-1}	λ_{hole}/eV	ΔG_{hole}/eV	$k_{CT\text{-}hole}$/s^{-1}
CT_1	1.0641	-0.4712	1.37×10^{10}	0.8496	-0.3998	3.76×10^{10}
CT_2	1.0641	-0.5376	1.20×10^{10}	0.8496	-0.5344	5.44×10^{10}
CT_3	1.0641	-0.4291	1.63×10^{09}	0.8496	-0.5623	2.82×10^{10}
CT_4	1.0641	-0.4312	5.98×10^{10}	0.8496	-0.5690	1.06×10^{12}
CT_5	1.0641	-0.4633	4.00×10^{11}	0.8496	-0.5583	4.59×10^{12}
S_1	1.0641	-0.4619	4.72×10^{14}	0.8496	-0.7096	1.16×10^{16}
S_2	1.0641	-0.5333	2.95×10^{14}	0.8496	-0.7592	3.95×10^{15}