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

ESI for Towards Predicting Power Conversion Efficiencies of Organic Solar Cells from Donor and Acceptor Molecule Structures

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Basis benchmark

Table S1: Consumed time and electron-transfer coupling for various basis sets. Each calculation is performed at one node with 12 CPUs. The calculated dimer is molecule 1 ($PC_{71}BM$) and molecule 437 (DERHD7T).

Basis Sets	3-21g*	6-31g	6-31g*	6-31g**	6-311g*	6-311g**
RealTime(HH:MM:SS)	1:06:20	1:09:59	3:03:55	3:51:36	5:50:52	7:02:31
Couplings (meV)	-22.4070	-21.2460	20.9120	21.0390	-21.572	-21.745

DERHD7T thin film

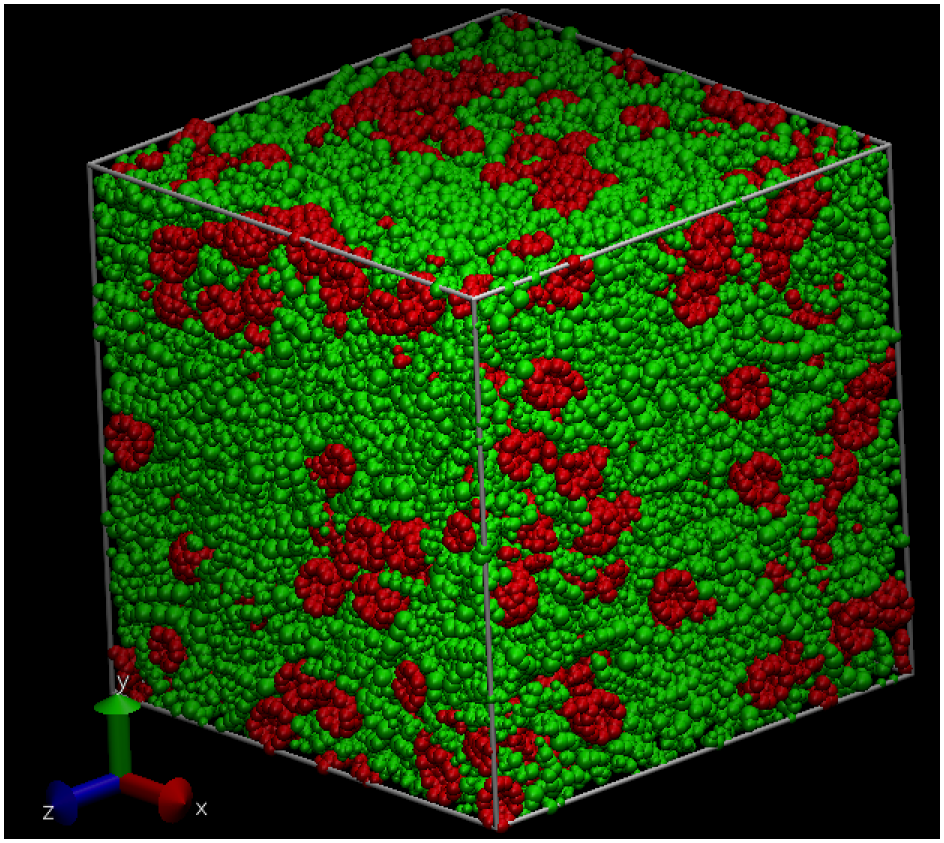

Figure S1: DERHD7T thin film structure. The VDW surfaces of DERHD7T molecules are shown in green and $PC_{71}BM$ VDW surfaces are colored with red.

Site energies

Table S2: The gas phase HOMO and LUMO energy levels of DRCN5T, DRCN7T, DERHD7T, $PC_{71}BM$ molecules at ground states.

Basis	B3LYP/6-311G*		B3LYP/6-31G*	
Molecules	HOMO (eV)	LUMO (eV)	HOMO (eV)	LUMO (eV)
DRCN5T	-5.38	-3.40	-5.21	-3.19
DRCN7T	-5.09	-3.30	-4.93	-3.08
DERHDD7T	-4.93	-3.04	-4.81	-2.87
$PC_{71}BM$	-5.90	-3.40	-5.68	-3.14

Table S3: Distributions of HOMO energy levels of DRCN5T, DRCN7T, DERHD7T molecules in blend and single component thin films. The unit is eV.

Molecules	Blend		Pure	
	Average	σ	Average	σ
DRCN5T	-5.48	0.121	-5.49	0.117
DRCN7T	-5.26	0.138	-5.26	0.135
DERHD7T	-5.18	0.116	-5.15	0.114

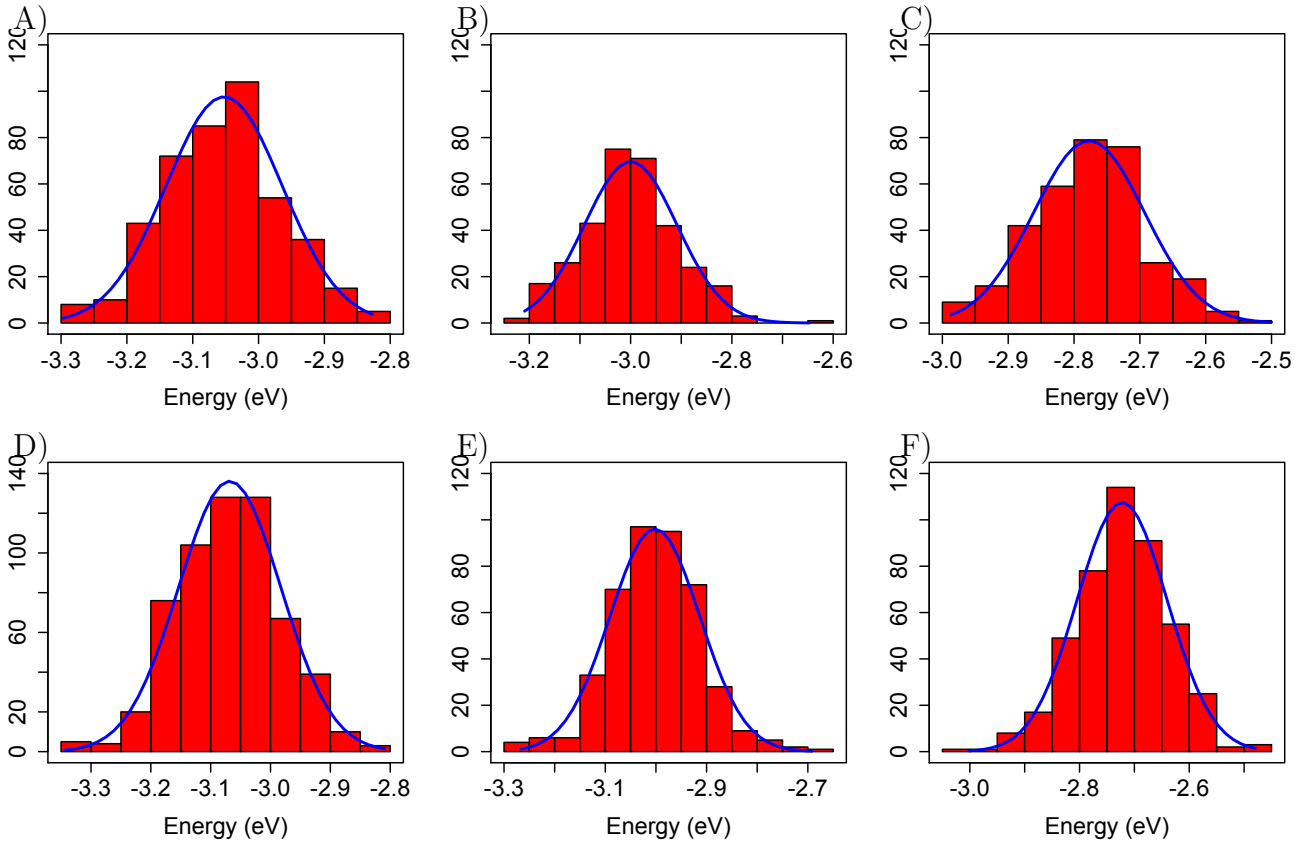

Figure S2: Distribution of LUMO energy levels. A) LUMOs of DRCN5T molecules in DRCN5T/$PC_{71}BM$ film; B) LUMOs of DRCN7T molecules in DRCN7T/$PC_{71}BM$ film; C) LUMOs of DERHD7T molecules in DERHD7T/$PC_{71}BM$ film; D) LUMOs of DRCN5T molecules in DRCN5T film; E) LUMOs of DRCN7T molecules in DRCN7T film; F) LUMOs of DERHD7T molecules in DERHD7T film. Blue lines are the fitted Gaussian distributions.

Table S4: Distributions of LUMO energy levels of DRCN5T, DRCN7T, DERHD7T molecules in blend and single component thin films. The unit is eV.

Molecules	Blend		Pure	
	Average	σ	Average	σ
DRCN5T	-3.05	0.088	-3.07	0.086
DRCN7T	-3.00	0.092	-3.00	0.089
DERHD7T	-2.78	0.084	-2.72	0.082

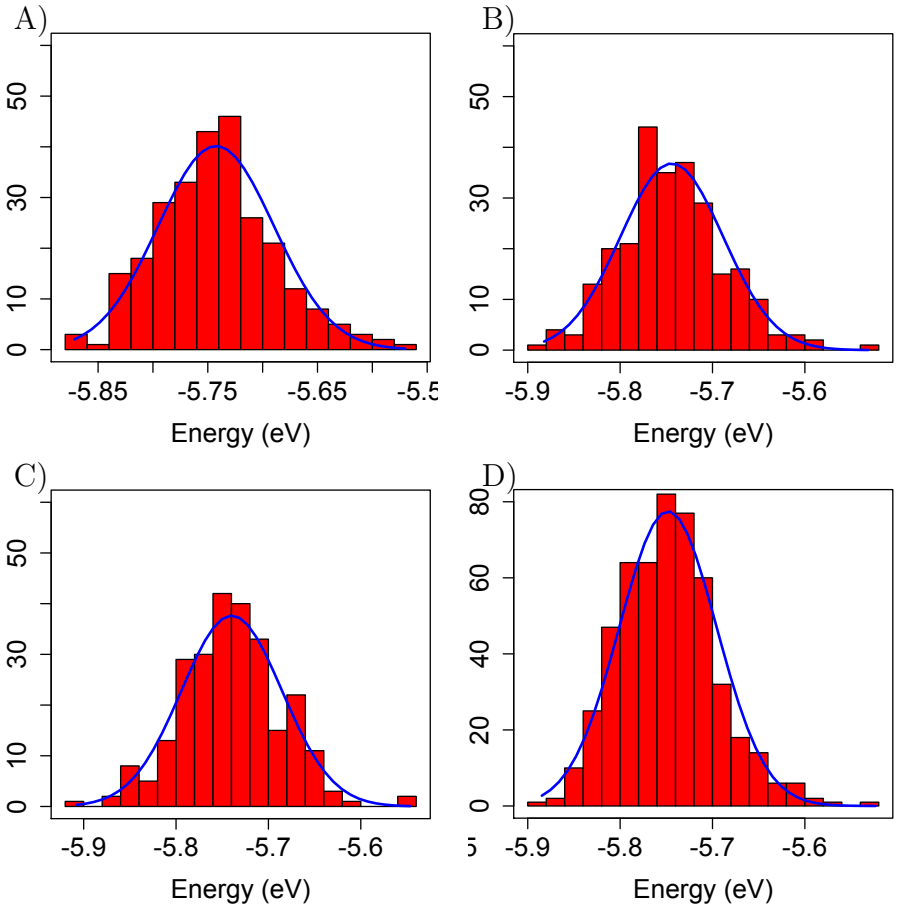

Figure S3: Distribution of HOMO energy levels. A) HOMOs of $PC_{71}BM$ molecules in DRCN5T:$PC_{71}BM$ film; B) HOMOs of $PC_{71}BM$ molecules in DRCN7T:$PC_{71}BM$ film; C) HOMOs of $PC_{71}BM$ molecules in DERHD7T:$PC_{71}BM$ film; D) HOMOs of $PC_{71}BM$ molecules in $PC_{71}BM$ film; Blue lines are the fitted Gaussian distributions.

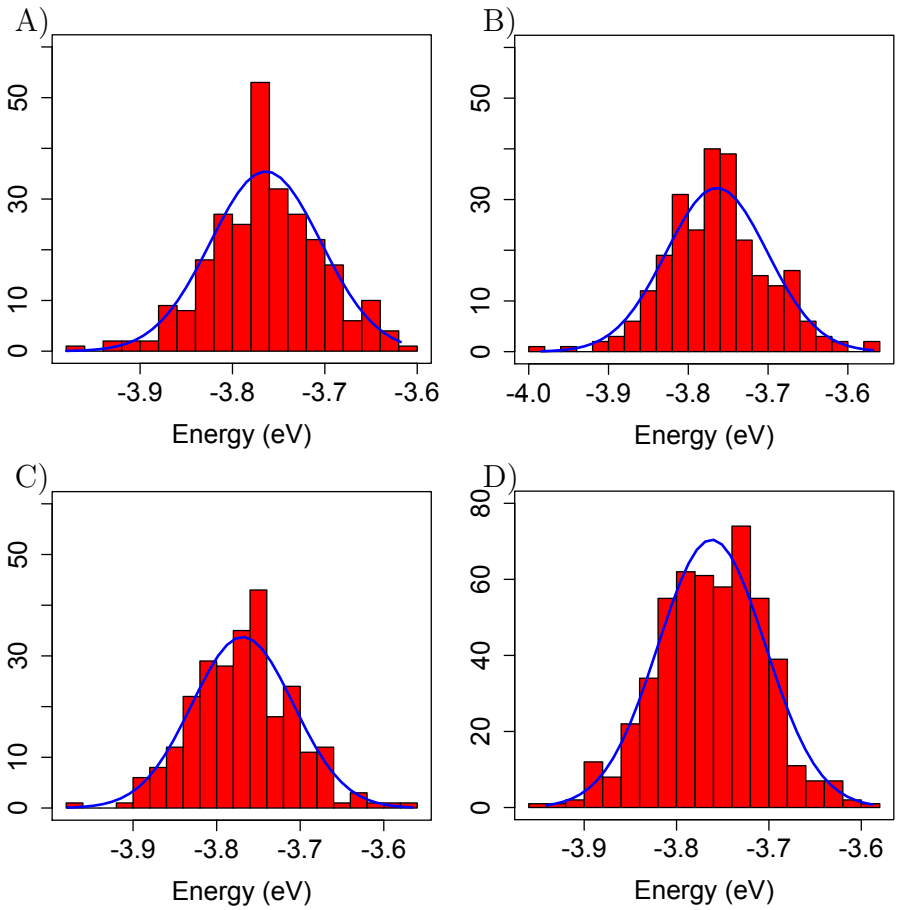

Figure S4: Distribution of LUMO energy levels. A) LUMOs of $PC_{71}BM$ molecules in DRCN5T:$PC_{71}BM$ film; B) LUMOs of $PC_{71}BM$ molecules in DRCN7T:$PC_{71}BM$ film; C) LUMOs of $PC_{71}BM$ molecules in DERHD7T:$PC_{71}BM$ film; D) LUMOs of $PC_{71}BM$ molecules in $PC_{71}BM$ film; Blue lines are the fitted Gaussian distributions.

Table S5: Distributions of HOMO and LUMO energy levels of $PC_{71}BM$ in DRCN5T:$PC_{71}BM$, DRCN7T:$PC_{71}BM$, DERHD7T:$PC_{71}BM$ and single-component $PC_{71}BM$ thin films.

Orbitals	HOMO(eV)		LUMO(eV)	
Molecules	Average	σ	Average	σ
DRCN5T	-5.74	0.053	-3.76	0.060
DRCN7T	-5.74	0.056	-3.76	0.063
DERHD7T	-5.74	0.054	-3.77	0.061
PC71BM	-5.75	0.053	-3.76	0.058

Electronic Coupling

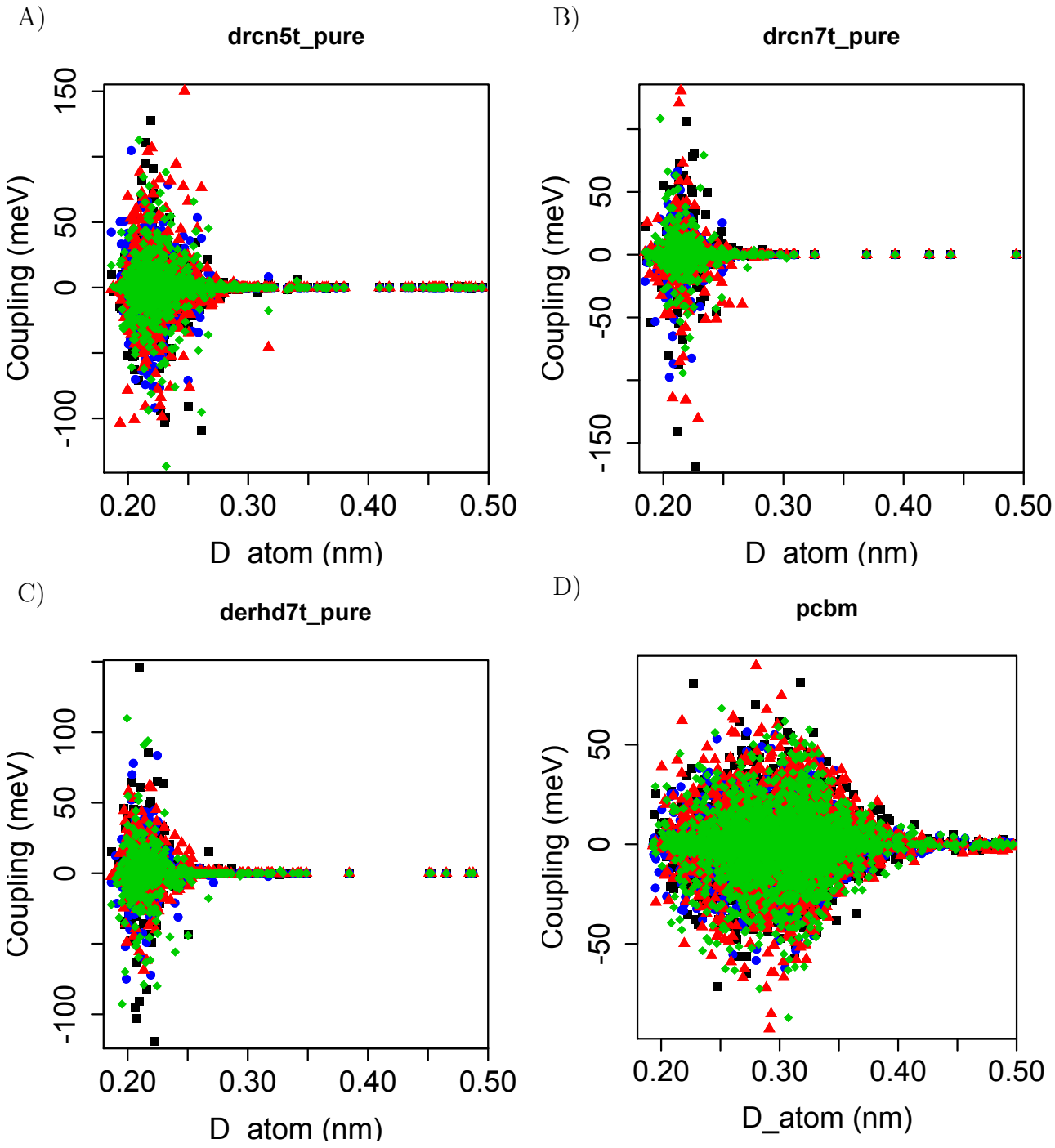

Figure S5: Couplings in single-component donor and $PC_{71}BM$ thin films.

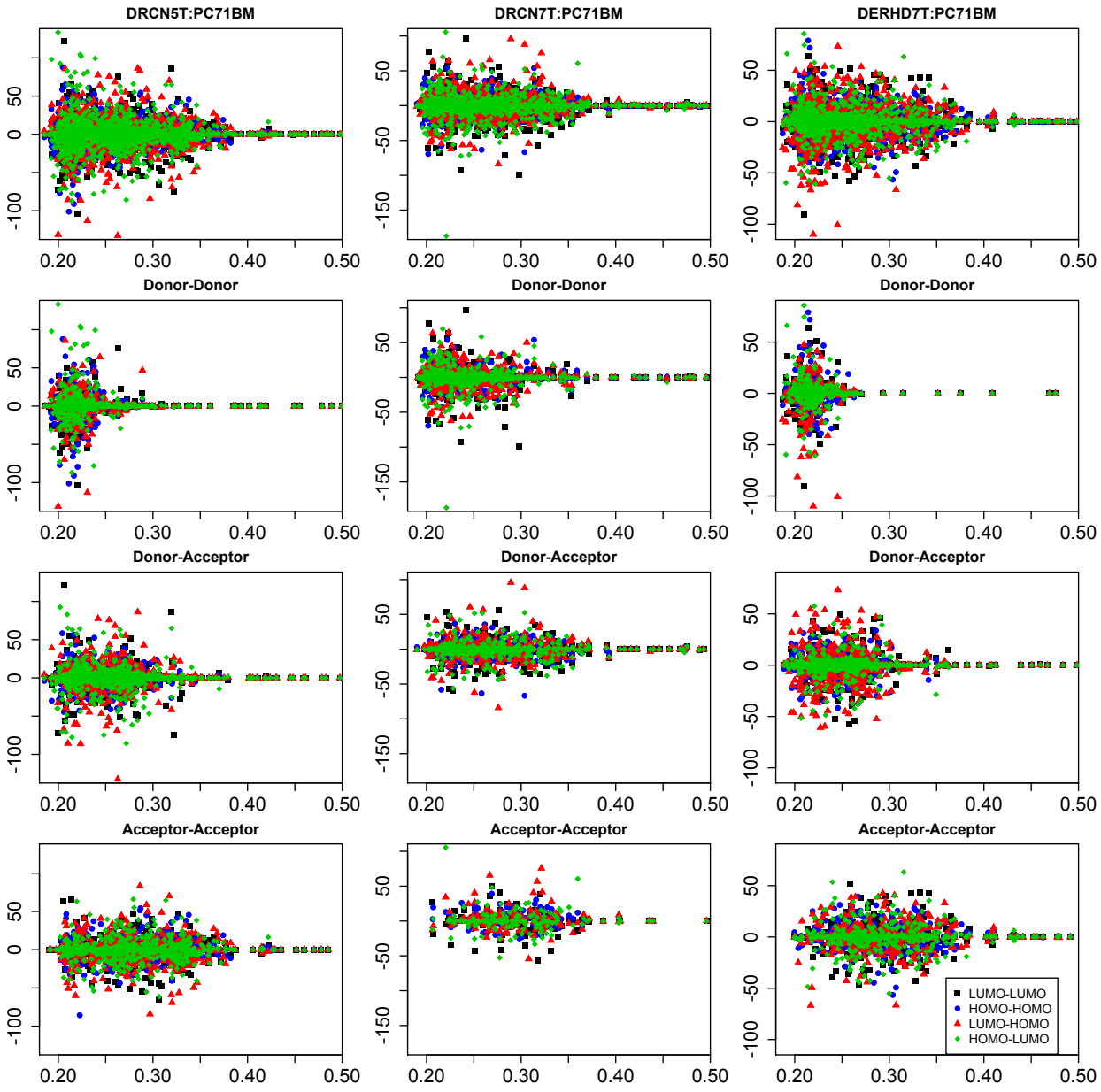

Figure S6: Couplings between different components of blend films. The first column is couplings in DRCN5T:$PC_{71}BM$ film; the second column are that of DRCN7T:$PC_{71}BM$ film; the last column is that of DERHD7T:$PC_{71}BM$ film. The topmost are overall couplings of all components of blend films. From the second to the fourth row are couplings of donor-donor, donor-acceptor and acceptor-acceptor respectively. For the convenience of view, labels are removed. The x-lab is "D_atom", which is the distance of nearest atom of two molecules. The y-lab is "Couplings (meV)"

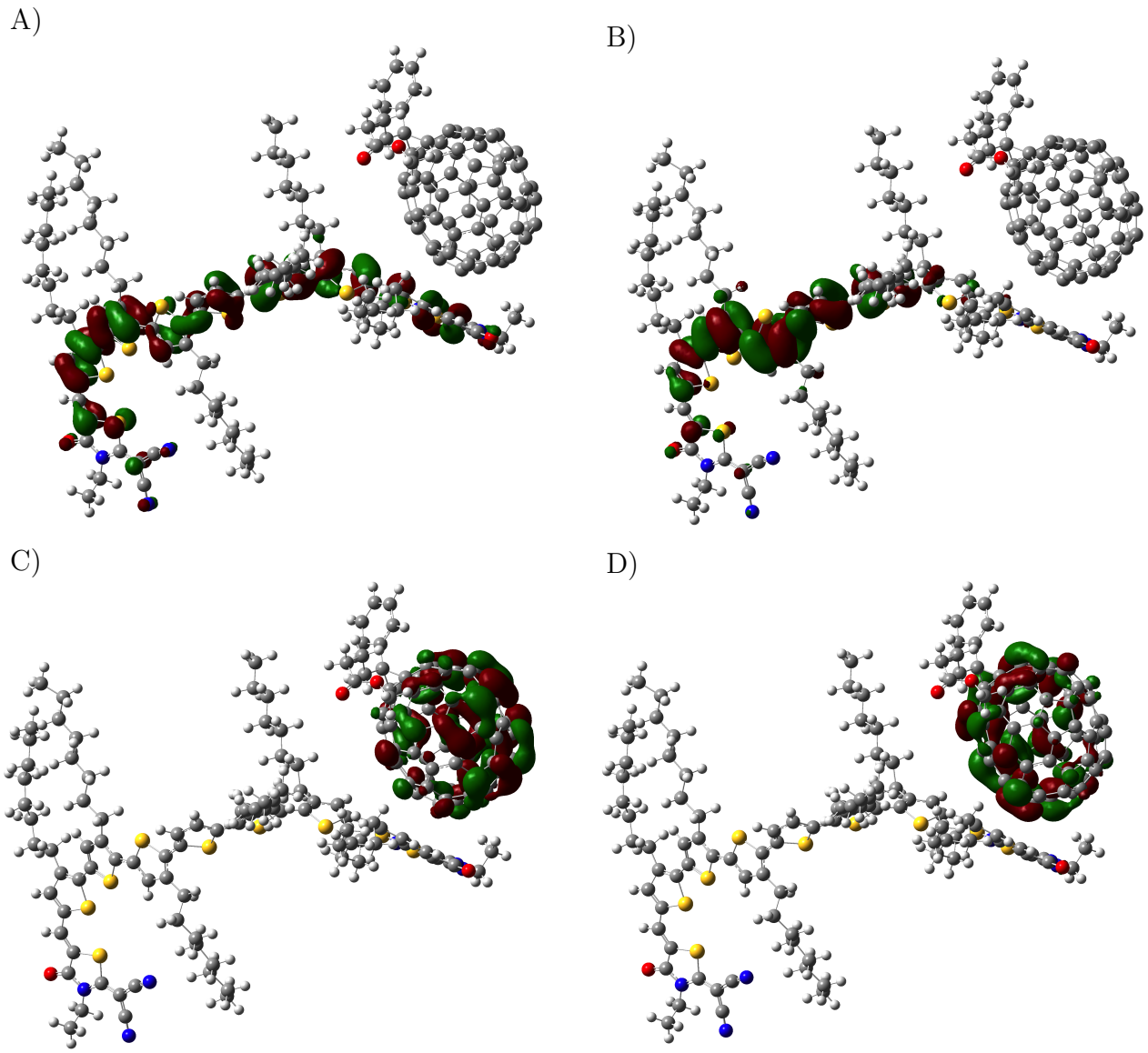

Figure S7: Frontier orbitals of dimer 240-374 in DRCN7T:$PC_{71}BM$. Molecule 240 is DRCN7T and molecule 374 is PC71BM. They show a LUMO-LUMO coupling of 99.47 meV, but a small HOMO-HOMO coupling of 0.01 meV. A), B), C) and D) are the HOMO-2, HOMO-1, LUMO-2 and LUMO-1 of dimer, respectivily.

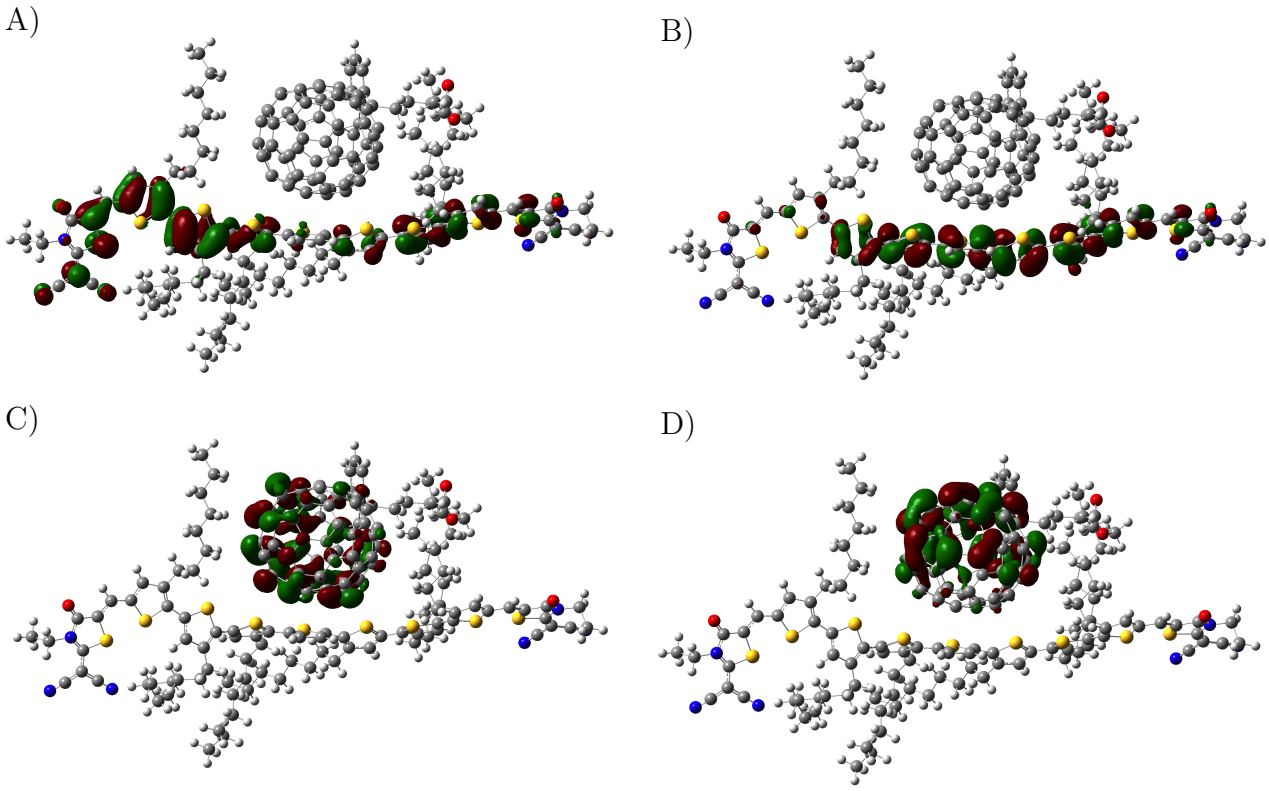

Figure S8: Frontier orbitals of dimer 18-549 in DRCN7T:$PC_{71}BM$. Molecule 18 is DRCN7T and molecule 549 is PC71BM. They show a small LUMO-LUMO coupling of 2.3meV meV, but a large HOMO-HOMO coupling of 63.4 meV. A), B), C) and D) are the HOMO-2, HOMO-1, LUMO-2 and LUMO-1 of dimer, respectivily.

Table S6: The mean square coupling of DRCN5T:$PC_{71}BM$ blend and single-component thin films. The unit is meV.

Orbitals	Pure	All of Blend	D-D of Blend	D-A of Blend	A-A of Blend
LUMO-LUMO	174.41	125.47	139.30	99.81	156.68
HOMO-HOMO	164.68	121.85	176.64	69.00	126.10
LUMO-HOMO	246.97	178.28	200.10	142.74	215.40
HOMO-LUMO	189.36	188.85	265.14	119.59	184.23

Table S7: The mean square coupling of DRCN7T:$PC_{71}BM$ blend and single-component thin films. The unit is meV.

Orbitals	Pure	All of Blend	D-D of Blend	D-A of Blend	A-A of Blend
LUMO-LUMO	174.29	118.31	103.98	109.35	155.36
HOMO-HOMO	104.20	76.60	72.23	62.66	110.41
LUMO-HOMO	176.46	128.05	87.16	131.50	175.53
HOMO-LUMO	113.35	139.51	160.89	96.20	198.00

Table S8: The mean square coupling of DERHD7T:$PC_{71}BM$ blend and single-component thin films. The unit is meV.

Orbitals	Pure	All of Blend	D-D of Blend	D-A of Blend	A-A of Blend
LUMO-LUMO	157.97	91.43	80.98	75.12	142.72
HOMO-HOMO	110.09	87.00	95.15	74.85	100.83
LUMO-HOMO	84.54	162.60	153.82	184.29	129.09
HOMO-LUMO	137.60	105.89	103.96	76.95	171.45

Table S9: The mean square coupling of all blend and single-component thin films. The unit is meV.

Orbitals	DERHD7T		DRCN5T		DRCN7T		$PC_{71}BM$
	Pure	Blend	Pure	Blend	Pure	Blend	single-component
LUMO-LUMO	157.97	91.43	174.41	125.47	174.29	118.31	164.99
HOMO-HOMO	110.09	87.00	164.68	121.85	104.20	76.60	132.82
LUMO-HOMO	84.54	162.60	246.97	178.28	176.46	128.05	220.42
HOMO-LUMO	137.60	105.89	189.36	188.85	113.35	139.51	191.79

Parameters in numerical simulations

Table S10: Parameters of DRCN5T:$PC_{71}BM$ solar cell.

Parameters	Value	Source
N_c(acceptor)	3.20 $\times 10^{18}$ cm^{-3}	DFT
N_v(donor)	3.39 $\times 10^{18}$ cm^{-3}	DFT
Min(E^{donor}_{LUMO})	-3.298 eV	DFT
Max(E^{donor}_{HOMO})	-5.177 eV	DFT
Min($E^{acceptor}_{LUMO}$)	-3.980 eV	DFT
$E^{absorption}_{gap}$	1.880 eV	Min(E^{donor}_{LUMO}) - Max(E^{donor}_{HOMO})
E^{V}_{gap}	1.197 eV	Min($E^{acceptor}_{LUMO}$) - Max(E^{donor}_{HOMO})
D_e	1.49 $\times 10^{-4} cm^2 s^{-1}$	DFT & RW simulation
D_h	1.59 $\times 10^{-4} cm^2 s^{-1}$	DFT & RW simulation
ϵ	4	Ref. 1,2
α	1.5 $\times 10^{6}$ cm^{-1}	Ref. 3
τ	3 μs	Ref. 4
Thickness	120 nm	Ref. 5

Table S11: Parameters of DRCN7T:$PC_{71}BM$ solar cell.

Parameters	Value	Source
N_c(acceptor)	2.93 $\times 10^{18}$ cm^{-3}	DFT
N_v(donor)	9.38 $\times 10^{18}$ cm^{-3}	DFT
Min(E^{donor}_{LUMO})	-3.209 eV	DFT
Max(E^{donor}_{HOMO})	-4.954 eV	DFT
Min($E^{acceptor}_{LUMO}$)	-3.984 eV	DFT
$E^{absorption}_{gap}$	1.745 eV	Min(E^{donor}_{LUMO}) - Max(E^{donor}_{HOMO})
E^{V}_{gap}	0.970 eV	Min($E^{acceptor}_{LUMO}$) - Max(E^{donor}_{HOMO})
D_e	6.88 $\times 10^{-6} cm^2 s^{-1}$	DFT & RW simulation
D_h	1.72 $\times 10^{-5} cm^2 s^{-1}$	DFT & RW simulation
ϵ	4	Ref. 1,2
α	1.5 $\times 10^{6}$ cm^{-1}	Ref. 3
τ	3 μs	Ref. 4
Thickness	120 nm	Ref. 5

Table S12: Parameters of DERHD7T:$PC_{71}BM$ solar cell.

Parameters	Value	Source
N_c(acceptor)	2.95 $\times 10^{18}$ cm^{-3}	DFT
N_v(donor)	3.71 $\times 10^{18}$ cm^{-3}	DFT
Min(E^{donor}_{LUMO})	-2.987 eV	DFT
Max(E^{donor}_{HOMO})	-4.870 eV	DFT
Min($E^{acceptor}_{LUMO}$)	-3.978 eV	DFT
$E^{absorption}_{gap}$	1.883 eV	Min(E^{donor}_{LUMO}) - Max(E^{donor}_{HOMO})
E^{V}_{gap}	0.892 eV	Min($E^{acceptor}_{LUMO}$) - Max(E^{donor}_{HOMO})
D_e	1.90 $\times 10^{-4} cm^2 s^{-1}$	DFT & RW simulation
D_h	2.95 $\times 10^{-5} cm^2 s^{-1}$	DFT & RW simulation
ϵ	4	Ref. 1,2
α	1.5 $\times 10^{6}$ cm^{-1}	Ref. 3
τ	3 μs	Ref. 4
Thickness	120 nm	Ref. 5

References

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