Electronic Supplementary information for:

Boron-containing Electron Transport Materials Based on Naphthalene Diimide for Organic Solar Cells: a Theoretical Study

Shu-Pu Yao, [a] Jie Yang, *[a] Qian Guo, [a] Xiao-Juan Yang, [b] and Quan-Song Li *[a]

[a] Key Laboratory of Cluster Science of Ministry of Education, Beijing Key Laboratory of Photoelectronic/ Electrophotonic Conversion Materials, School of Chemistry and Chemical Engineering, Beijing Institute of Technology, Beijing 100081, China

[b] Key Laboratory of Medicinal Molecule Science and Pharmaceutics Engineering, Ministry of Industry and Information Technology, School of Chemistry and Chemical Engineering, Beijing Institute of Technology, Beijing 100081, China.

*E-mail: jieyang24@bit.edu.cn, liquansong@bit.edu.cn

Contents

Section S1 Calculation details on electron mobility

The electron hopping rate (k) is expressed as:

$$k = \frac{2\pi^2}{h} v^2 \frac{1}{\sqrt{\pi \lambda k_B T}} exp[\frac{-\lambda}{4k_B T}]$$

where h is the Planck constant, k_B is the Boltzmann constant, v is the transfer integral, T is the temperature (298.15 K in our calculation), and λ is the reorganization energy. In this work, we consider only the internal reorganization energy which mainly reflects the geometric relaxation during the charge transfer process and the barriers to another molecule. It can be expressed as follows:

$$\lambda = \left(E_0^* - E_0\right) + \left(E_-^* - E_-\right)$$

where E_0^* is the anion energy in the stable configuration of the neutral molecule; E_0 is the energy of neutral molecule; E_-^* is the energy of the neutral molecule in the anionic stable configuration; E_- is the energy of the anion molecule.[1]

The transfer integral v was computed as follows:

$$v = < \psi_i^{LUMO} | SC\varepsilon C^{-1} | \psi_f^{LUMO} >$$

where ψ_i^{LUMO} and ψ_f^{LUMO} represent the LUMOs of the isolated molecules i and f, respectively. S denotes the overlap matrix between the molecules. C is the Kohn-Sham molecular orbital coefficient, and ε is the intrinsic energy of the dimer without interaction.[2] The electron mobility (μ) of the investigated molecules was calculated using the Einstein relation.[3]

$$\mu = \frac{1}{2dk_B T} \frac{e}{\Sigma} r_i^2 k_i P_i$$

where d is the spatial dimension, and generally $d = 3$ represents the three-dimensional system, e is the number of elementary charge (1.6×10^{-19} C), r_i is the distance for each carrier hopping step, typically replaced by the mass center of the dimer. k_i represents the probability of carrier hopping along the i path. P_i is defined as the hopping probability, which can be obtained using:

$$P_i = \frac{k_i}{\Sigma k_i}$$

Section S2 Calculation details on net transferred charge

The net transferred electrons (Δq) from donor (D) to acceptor (A) can be obtained by using the following formula:

$$\Delta q = Q_{D,A} - Q_{A,D}$$

where $Q_{D,A}$($Q_{A,D}$) corresponds to the electron transfer from D(A) to A (D) during the excitation, which can be calculated from:

$$Q_{D,A} = \Sigma_i^{OCC}\Sigma_a^{vir}\left[\left(\omega_i^a\right)^2 - \left(\omega'^a_i\right)^2\right]\Sigma_{R\in D}\Theta_{R,i}\Sigma_{S\in A}\Theta_{S,a}$$

where ω_i^a and ω'^a_i are the configuration coefficients of the excitation molecular orbital i to a and the de-excitation molecular orbital a to i, respectively; $\Theta_{R,i}$ ($\Theta_{S,a}$) is the contribution of atom R (S) to the molecular orbital i (a).

The distance from the hole centroid to the electron centroid can be expressed from the following equation.[4]

$$D = \sqrt{D_X^2 + D_Y^2 + D_Z^2}$$

The charge transfer (CT) length in X/Y/Z can be measured by the centroid distances between the hole and the electron in corresponding directions:

$$D_{X,Y,Z} = \left|N_{ele} - N_{hole}\right|$$

The electron centroid (N_{ele}) and hole centroid (N_{hole}) can be calculated from the following equation:

$$N_{ele/hole} = \int n\rho^{ele/hole}(r)dr$$

where n is the X (Y or Z) component of position vector r. $\rho^{ele/hole}$ presents the spatial charge distribution.

Section S3 Calculation details on interfacial binding energy

The binding energy of E/A interface is calculated by the following formula:

$$E_{inter} = E_{E/A} - E_E - E_A + E_{BSSE}$$

where $E_{E/A}$, E_E, E_A, and E_{BSSE} represent the energy of the optimized E/A interface system, the electron transport material, the acceptor, and the basis set superposition error (BSSE)[38], respectively. The larger the E_{inter}, the stronger the combination of the interface.

References

1. H.-Y. Chen and I. Chao, *Chem. Phys. Lett.*, 2005, **401**, 539-545.
2. X. Yang, Q. Li and Z. Shuai, *Nanotechnology*, 2007, **18**, 424029.
3. V. Coropceanu, J. Cornil, D. A. da Silva Filho, Y. Olivier, R. Silbey and J.-L. Brédas, *Chem. Rev.*, 2007, **107**, 926-952.
4. C. Yao, Y. Yang, L. Li, M. Bo, J. Zhang, C. Peng, Z. Huang and J. Wang, *J. Phys. Chem. C*, 2020, **124**, 23059-23068.
5. M. Frisch, G. Trucks, H. Schlegel, G. Scuseria, M. Robb, J. Cheeseman, G. Scalmani, V. Barone, G. Petersson and H. Nakatsuji, *Gaussian16 (Revision A. 03)*, 2016, **3**.

Benchmark of the used functionals

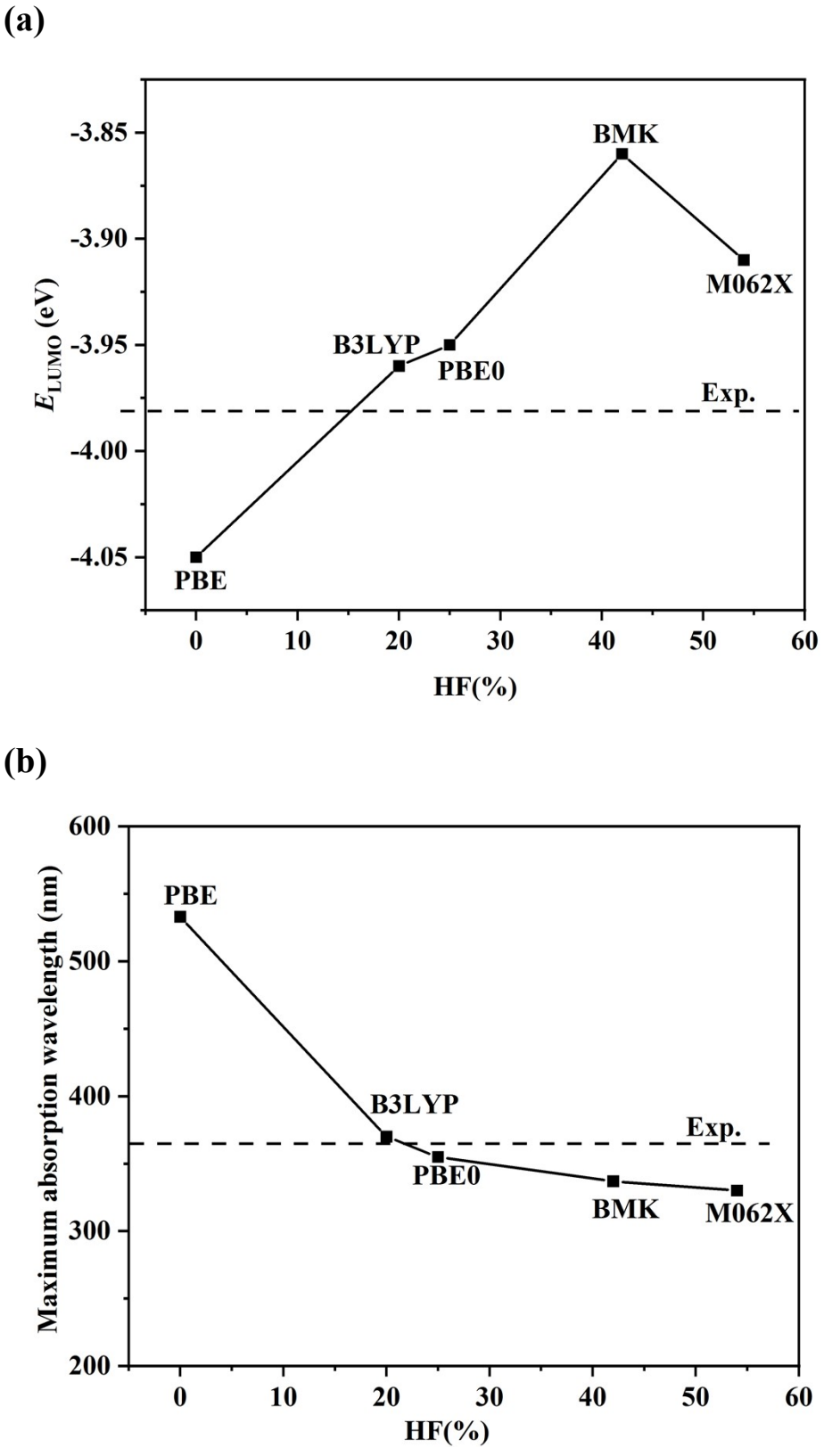
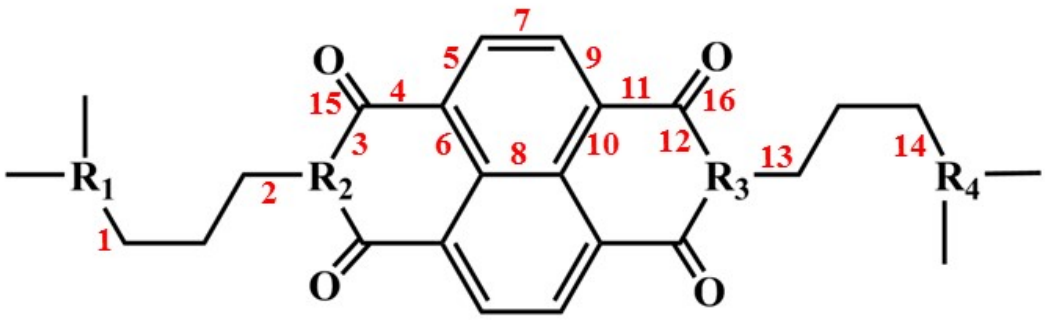


Figure S1. (a) The lowest unoccupied orbital (LUMO) energy and (b) maximum absorption wavelength of NDIN with different functionals. The dashed lines indicate the experimental values.

Details of the single-molecule structure

Table S1. The bond length changes (BLC, in Å) between NDIN and designed molecules.

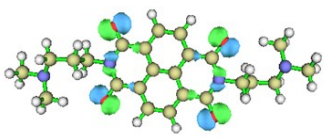


	NDIN	E1	E2	E3	E4	E5	E6
1	0	-0.006	-0.006	0.119	0.120	0.119	-0.006
2	0	0.060	0.060	0.000	0.000	0.062	0.060
3	0	0.186	0.182	0.001	0.001	0.188	0.186
4	0	0.013	0.013	-0.001	-0.001	0.013	0.013
5	0	0.000	-0.001	0.000	0.000	0.001	0.000
6	0	0.019	0.021	0.000	0.000	0.019	0.019
7	0	-0.004	-0.008	0.000	0.000	-0.004	-0.004
8	0	0.010	0.020	0.000	0.000	0.010	0.010
9	0	-0.001	0.000	0.000	0.000	-0.001	-0.001
10	0	0.003	0.022	0.000	0.000	0.003	0.003
11	0	0.001	0.015	0.000	0.000	0.001	0.000
12	0	-0.002	0.188	0.000	0.000	-0.003	-0.002
13	0	0.000	0.060	0.000	0.000	0.000	0.000
14	0	0.000	-0.006	0.000	0.120	0.000	0.120
15	0	0.009	0.009	0.000	0.000	0.009	0.009
16	0	0.000	0.008	0.000	0.000	0.000	0.000

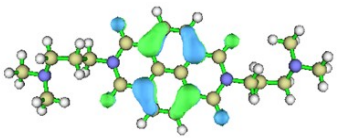
Details of molecular orbitals

Table S2. Relative TD-B3LYP vertical excitation energy (ΔE) and wavelength (λ) at **NDIN**-S_0 together with the electronic configuration (weight in the parenthesis, orbital below the Table) and oscillation strength (f).

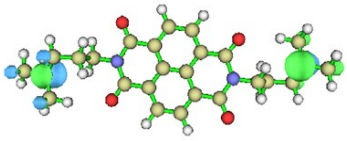
State	Electronic configuration (weight)	ΔE/eV	λ/nm	f
S_0	-	0.00	-	-
S_1	HOMO→LUMO(0.71)	1.96	631	0.0000
S_2	HOMO-1→LUMO(0.71)	1.97	630	0.0006
S_3	HOMO-3→LUMO(0.70)	3.24	383	0.0000
S_4	HOMO-2→LUMO(0.66)	3.35	370	0.3108



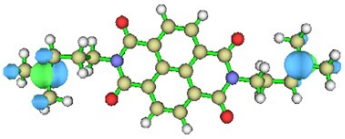
HOMO-3



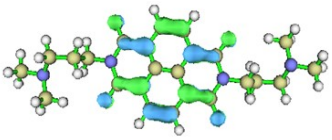
HOMO-2



HOMO-1



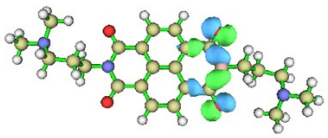
HOMO



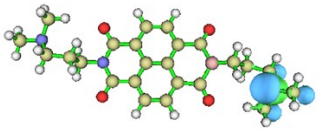
LUMO

Table S3. Relative TD-B3LYP vertical excitation energy (ΔE) and wavelength (λ) at **E1**-S_0 together with the electronic configuration (weight in the parenthesis, orbital below the Table) and oscillation strength (f).

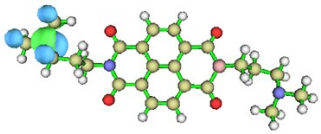
State	Electronic configuration (weight)	ΔE/eV	λ/nm	f
S_0	-	0.00	-	-
S_1	HOMO-1→LUMO(0.65)	1.97	628	0.0303
S_2	HOMO-2→LUMO(0.63)	2.06	603	0.0061
S_3	HOMO→LUMO+1(0.68)	2.12	585	0.0006
S_4	HOMO→LUMO(0.68)	2.13	581	0.0028



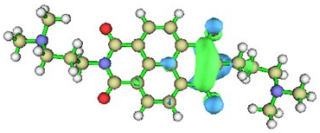
HOMO-2



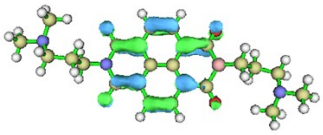
HOMO-1



HOMO



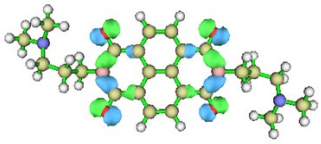
LUMO



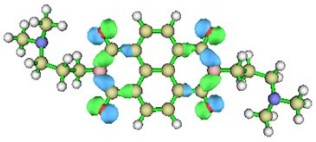
LUMO+1

Table S4. Relative TD-B3LYP vertical excitation energy (ΔE) and wavelength (λ) at **E2**-S_0 together with the electronic configuration (weight in the parenthesis, orbital below the Table) and oscillation strength (f).

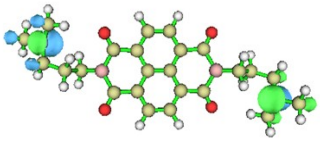
State	Electronic configuration (weight)	ΔE/eV	λ/nm	f
S_0	-	0.00	-	-
S_1	HOMO→LUMO(0.66)	1.85	672	0.0487
S_2	HOMO-1→LUMO(0.68)	1.86	667	0.0000
S_3	HOMO-2→LUMO(0.62)	1.94	638	0.0061
S_4	HOMO-3→LUMO(0.60)	2.02	613	0.0000



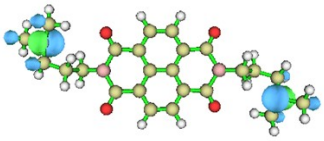
HOMO-3



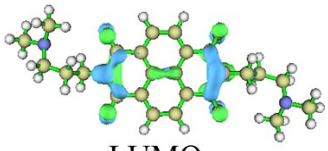
HOMO-2



HOMO-1



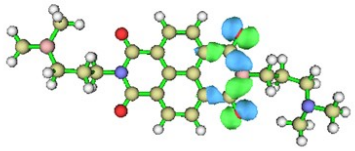
HOMO



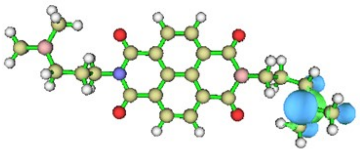
LUMO

Table S5. Relative TD-B3LYP vertical excitation energy (ΔE) and wavelength (λ) at **E6**-S_0 together with the electronic configuration (weight in the parenthesis, orbital below the Table) and oscillation strength (f).

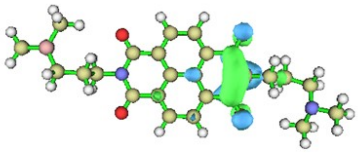
State	Electronic configuration (weight)	ΔE/eV	λ/nm	f
S_0	-	0.00	-	-
S_1	HOMO→LUMO(0.66)	1.97	630	0.0309
S_2	HOMO-1→LUMO(0.64)	2.06	603	0.0053
S_3	HOMO→LUMO+1(0.70)	2.24	553	0.0017
S_4	HOMO-1→LUMO+1(0.53)	2.44	508	0.0004



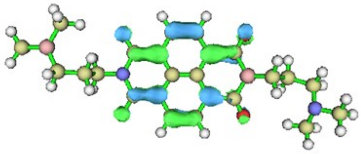
HOMO -1



HOMO

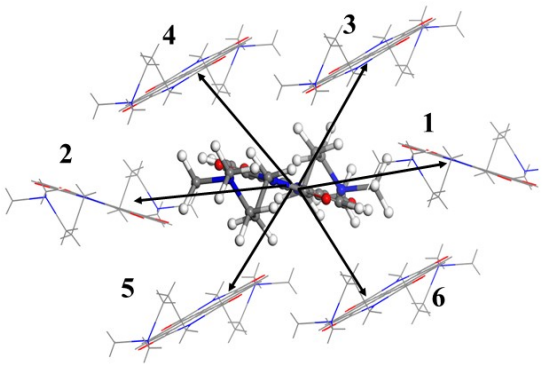


LUMO

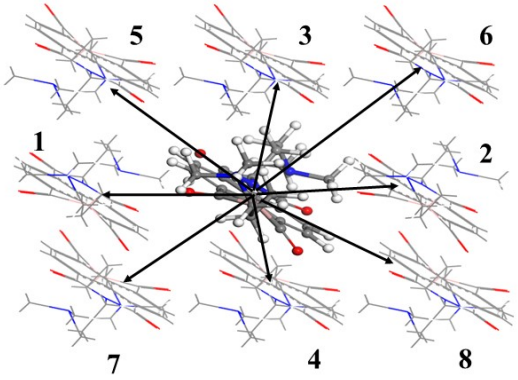


LUMO+1

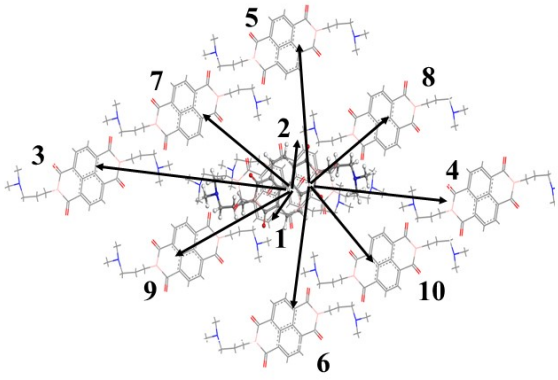
Paths of electron transfer



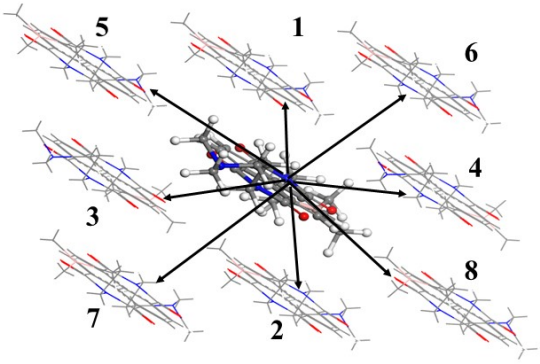
NDIN



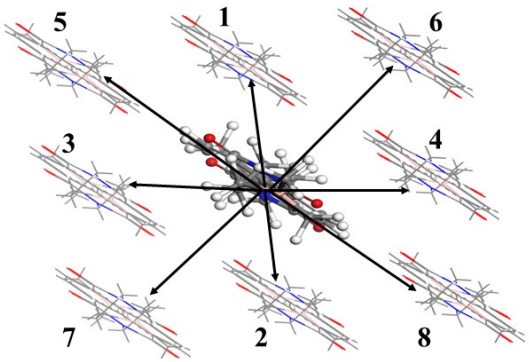
E1



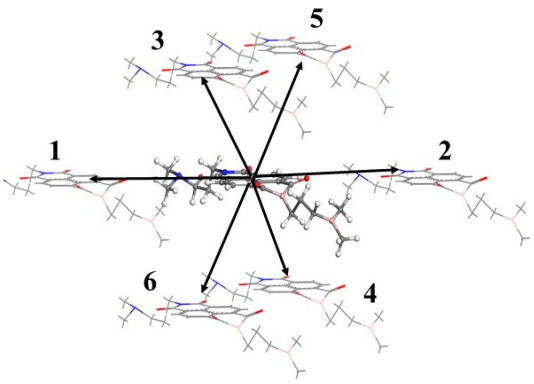
E2



E3



E4



E5

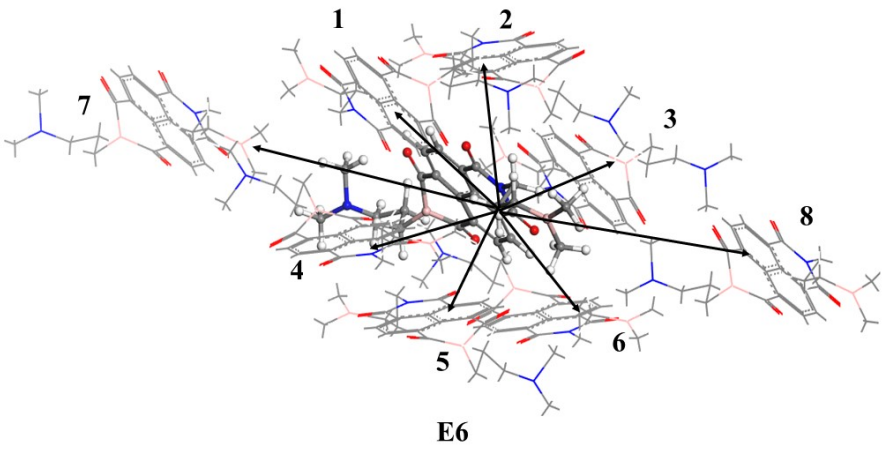


Figure S2. The predicted crystal structures and the main electron hopping pathways of the investigated molecules.

Analysis of non-covalent interaction

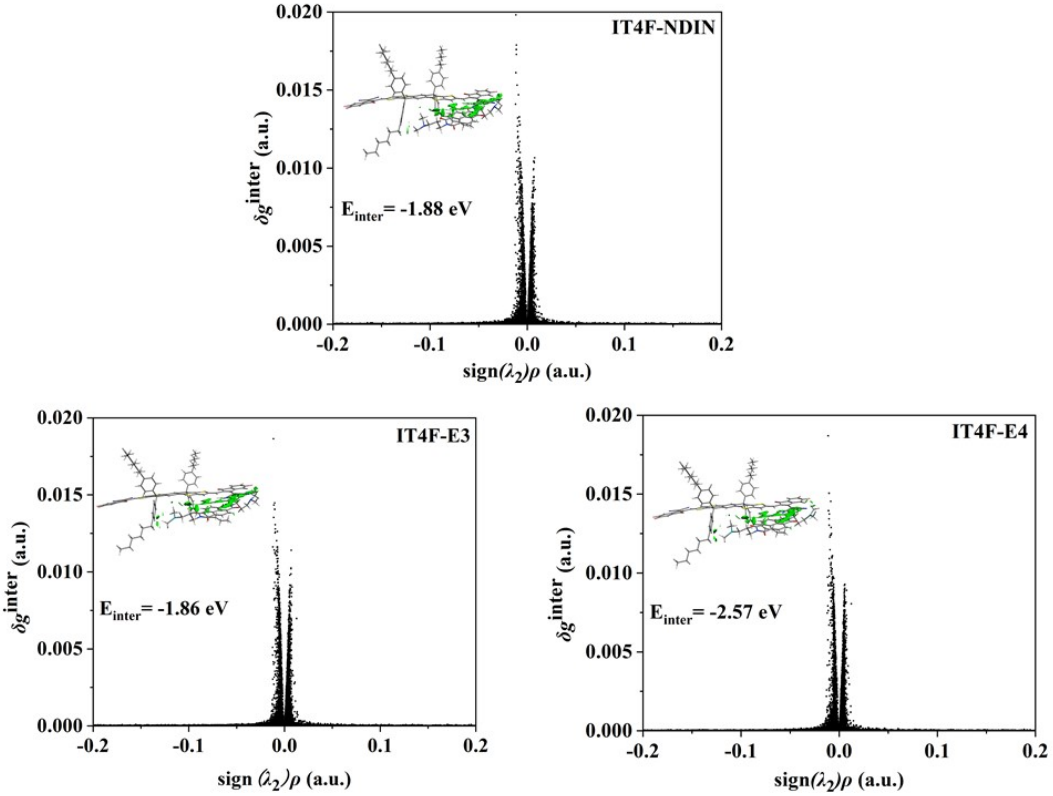


Figure S3. Intermolecular interaction (δg^{inter}/sign(λ_2)ρ 2D plot and δg^{inter} 3D map) between the electron transport layer and the acceptor IT-4F for (a) IT-4F/NDIN, (b) IT-4F/E3, and (c) IT-4F/E4. The green area indicates weak interaction, and the scatter plot shows the interaction distribution between electron transport layer and acceptor, sign(λ_2)ρ = -0.1 ~ 0.10 a.u. represents the weak interaction region.

Details of electron transfer and excitation

Table S6. Details for the reorganization energy λ (eV), centroid to centroid distance d (Å), the electron transfer integral v (eV), the charge hopping rate (k_i) and electron mobility μ ($cm^2\ V^{-1}\ s^{-1}$) of the studied molecules calculated by B3LYP/6-311G(d,p).

Compounds	λ	Path	d	v	k_i	μ
NDIN	0.39	1	7.58	-5.81×10^{-2}	2.04×10^{12}	5.1×10^{-2}
		2	7.58	5.81×10^{-2}	2.04×10^{12}	
		3	5.54	-3.39×10^{-2}	6.93×10^{11}	
		4	5.54	-3.41×10^{-2}	7.01×10^{11}	
		5	5.54	-3.39×10^{-2}	6.93×10^{11}	
		6	5.54	-3.40×10^{-2}	6.97×10^{11}	
E1	0.78	1	6.00	4.49×10^{-3}	1.93×10^{8}	4.3×10^{-4}
		2	6.00	4.49×10^{-3}	1.93×10^{8}	
		3	6.34	2.76×10^{-2}	7.28×10^{9}	
		4	6.99	-4.27×10^{-2}	1.74×10^{10}	
		5	8.70	-1.83×10^{-3}	3.20×10^{7}	
		6	8.75	-2.77×10^{-5}	7.33×10^{3}	
		7	8.77	7.38×10^{-5}	5.21×10^{4}	
		8	9.62	4.71×10^{-3}	2.12×10^{8}	
E2	0.54	1	4.53	3.76×10^{-2}	1.68×10^{11}	1.2×10^{-2}
		2	4.53	9.26×10^{-2}	1.02×10^{12}	
		3	22.85	4.48×10^{-6}	2.39×10^{3}	
		4	22.85	4.49×10^{-6}	2.40×10^{3}	
		5	12.35	9.95×10^{-6}	1.18×10^{4}	
		6	12.35	9.95×10^{-6}	1.18×10^{4}	
		7	12.99	5.61×10^{-4}	3.74×10^{3}	
		8	12.99	-4.98×10^{-5}	2.95×10^{5}	
		9	12.99	-4.97×10^{-5}	2.94×10^{5}	
		10	12.99	5.60×10^{-4}	3.73×10^{7}	
E3	0.39	1	5.24	-7.68×10^{-2}	3.56×10^{12}	5.4×10^{-2}
		2	5.32	-3.23×10^{-2}	6.29×10^{11}	
		3	7.59	-1.09×10^{-2}	7.17×10^{10}	
		4	7.59	-1.09×10^{-2}	7.17×10^{10}	
		5	9.62	-2.89×10^{-3}	5.04×10^{9}	
		6	8.81	-6.17×10^{-5}	2.30×10^{6}	
		7	8.58	-2.78×10^{-5}	4.66×10^{5}	
		8	9.90	-1.60×10^{-3}	1.54×10^{9}	
E4	0.39	1	5.36	-0.1	6.03×10^{12}	1.1×10^{-1}
		2	5.36	0.1	6.03×10^{12}	

		3	7.71	2.67×10^{-4}	4.30×10^{7}	
		4	7.71	-2.74×10^{-4}	4.53×10^{7}	
		5	9.39	4.25×10^{-3}	1.09×10^{10}	
		6	9.39	4.71×10^{-7}	1.34×10^{2}	
		7	9.39	4.79×10^{-7}	1.38×10^{2}	
		8	9.12	4.25×10^{-3}	1.09×10^{10}	
E5	0.78	1	14.24	-3.44×10^{-5}	1.13×10^{4}	4.8×10^{-4}
		2	14.24	-3.24×10^{-5}	1.00×10^{4}	
		3	8.80	1.18×10^{-3}	1.33×10^{7}	
		4	7.75	3.77×10^{-2}	1.36×10^{10}	
		5	8.41	-1.36×10^{-3}	1.77×10^{7}	
		6	8.98	2.76×10^{-2}	7.28×10^{9}	
E6	0.78	1	8.88	1.57×10^{-2}	2.36×10^{9}	1.8×10^{-3}
		2	6.91	1.54×10^{-2}	2.27×10^{9}	
		3	5.81	9.78×10^{-2}	9.14×10^{10}	
		4	6.30	1.23×10^{-2}	1.45×10^{9}	
		5	6.91	1.54×10^{-2}	2.27×10^{9}	
		6	6.30	1.23×10^{-2}	1.45×10^{9}	
		7	20.38	4.31×10^{-8}	1.78×10^{-2}	
		8	20.38	4.09×10^{-8}	1.59×10^{-2}	

Table S7. Excitation energies (E and λ), oscillation strength (f), D index, Sr index, and the amount of charge (Δq) transferring from the D/A/E for the lowest 40 excited states of the studied interfaces calculated by CAM-B3LYP/6-311G(d,p).

PBDB-T-2F/IT-4F						
Excited states	E/eV	λ/nm	f	$\Delta q/e$	D index	Sr index
S_1	2.226	557	2.195	0.054	0.389	0.751
S_2	2.536	489	0.641	0.597	2.209	0.550
S_3	2.650	468	0.168	0.370	1.401	0.688
S_4	2.831	438	0.560	0.109	0.486	0.763
S_5	3.065	404	0.042	0.039	2.131	0.675
S_6	3.197	388	0.021	0.684	2.703	0.553
S_7	3.239	383	0.091	0.182	0.958	0.696
S_8	3.297	376	0.060	0.002	3.108	0.646
S_9	3.344	371	0.051	0.506	2.066	0.677
S_{10}	3.387	366	0.022	0.102	0.984	0.717
S_{11}	3.428	362	0.120	-0.023	1.594	0.758
S_{12}	3.471	357	0.050	0.337	5.713	0.699
S_{13}	3.500	354	0.018	0.518	5.211	0.644
S_{14}	3.539	350	0.061	0.225	1.747	0.701
S_{15}	3.549	349	0.042	-0.061	0.588	0.635
S_{16}	3.597	345	0.010	0.247	2.676	0.648
S_{17}	3.614	343	0.001	-0.006	0.652	0.576
S_{18}	3.628	342	0.036	0.034	0.315	0.625
S_{19}	3.629	342	0.008	0.002	0.539	0.555
S_{20}	3.661	339	0.149	-0.055	0.992	0.743
S_{21}	3.695	336	0.051	0.517	1.965	0.637
S_{22}	3.780	328	0.038	0.457	1.952	0.686
S_{23}	3.868	321	0.124	0.197	1.675	0.780

S_{24}	3.914	317	0.016	0.011	1.681	0.472
S_{25}	3.917	317	0.018	0.441	4.227	0.686
S_{26}	3.961	313	0.024	0.121	0.940	0.784
S_{27}	3.982	311	0.054	-0.116	0.762	0.775
S_{28}	3.994	310	0.008	0.098	1.772	0.457
S_{29}	4.010	309	0.156	0.091	1.051	0.738
S_{30}	4.038	307	0.013	-0.023	0.532	0.786
S_{31}	4.084	303	0.165	0.256	1.466	0.771
S_{32}	4.090	303	0.012	0.018	1.088	0.752
S_{33}	4.115	301	0.073	0.034	0.944	0.776
S_{34}	4.123	301	0.053	0.425	1.391	0.556
S_{35}	4.148	299	0.091	-0.348	2.671	0.695
S_{36}	4.191	296	0.015	0.056	0.431	0.817
S_{37}	4.207	295	0.067	0.010	0.672	0.720
S_{38}	4.209	295	0.017	-0.012	1.763	0.448
S_{39}	4.229	293	0.014	0.639	5.816	0.599
S_{40}	4.232	293	0.009	0.166	1.112	0.516

PBDB-T-2F/IT-4F/NDIN						
Excited states	*E*/eV	*λ*/nm	*f*	Δ*q*/*e*	*D* index	*Sr* index
S_1	2.223	558	2.155	0.007	0.253	0.754
S_2	2.438	508	0.071	0.893	3.076	0.306
S_3	2.602	476	0.785	0.058	0.641	0.740
S_4	2.698	459	0.083	-0.099	3.842	0.347
S_5	2.757	450	0.204	0.024	0.921	0.735
S_6	3.009	412	0.024	0.071	6.077	0.198
S_7	3.082	402	0.040	0.529	2.168	0.621
S_8	3.100	400	0.027	0.111	2.016	0.709
S_9	3.263	380	0.077	0.649	2.440	0.588
S_{10}	3.283	378	0.056	0.244	0.918	0.689
S_{11}	3.304	375	0.064	0.012	1.552	0.692
S_{12}	3.326	373	0.004	0.229	0.886	0.621
S_{13}	3.407	364	0.010	0.681	7.108	0.460
S_{14}	3.420	363	0.035	0.250	3.805	0.643
S_{15}	3.487	356	0.119	0.004	1.786	0.714
S_{16}	3.498	354	0.013	0.108	1.840	0.773
S_{17}	3.536	351	0.008	0.096	0.750	0.679
S_{18}	3.553	349	0.112	0.071	2.545	0.596
S_{19}	3.577	347	0.032	-0.144	0.846	0.631
S_{20}	3.589	345	0.047	-0.039	0.605	0.695
S_{21}	3.600	344	0.084	-0.011	0.639	0.675
S_{22}	3.613	343	0.029	0.053	2.460	0.509
S_{23}	3.619	343	0.029	-0.047	0.853	0.610
S_{24}	3.628	342	0.001	0.001	0.700	0.524
S_{25}	3.628	342	0.015	0.010	0.765	0.580
S_{26}	3.639	341	0.092	0.034	2.471	0.666
S_{27}	3.645	340	0.043	0.162	2.708	0.494

S_{28}	3.705	335	0.008	0.157	1.637	0.414
S_{29}	3.710	334	0.035	0.024	1.276	0.292
S_{30}	3.716	334	0.072	0.188	0.744	0.655
S_{31}	3.749	331	0.026	0.357	1.869	0.580
S_{32}	3.849	322	0.021	-0.096	3.532	0.700
S_{33}	3.863	321	0.150	0.030	1.689	0.750
S_{34}	3.878	320	0.024	0.290	1.750	0.725
S_{35}	3.898	318	0.012	0.356	3.927	0.681
S_{36}	3.924	316	0.049	0.010	1.390	0.508
S_{37}	3.942	315	0.042	0.162	1.194	0.716
S_{38}	3.957	313	0.023	0.193	1.268	0.666
S_{39}	3.963	313	0.005	0.017	0.643	0.658
S_{40}	3.974	312	0.023	0.127	3.349	0.563

PBDB-T-2F/IT-4F/E3						
Excited states	*E*/eV	*λ*/nm	*f*	Δ*q*/*e*	*D* index	*Sr* index
S_1	2.211	561	2.113	0.015	0.382	0.755
S_2	2.466	503	0.080	0.895	3.116	0.296
S_3	2.580	481	0.556	-0.011	1.710	0.601
S_4	2.644	469	0.264	-0.076	2.591	0.543
S_5	2.771	447	0.302	0.071	0.619	0.757
S_6	2.980	416	0.003	0.035	6.388	0.109
S_7	3.074	403	0.024	0.237	1.746	0.690
S_8	3.100	400	0.028	0.496	2.145	0.644
S_9	3.265	380	0.097	0.610	2.117	0.579
S_{10}	3.272	379	0.063	0.260	1.203	0.682
S_{11}	3.298	376	0.060	0.016	2.105	0.672
S_{12}	3.323	373	0.004	0.210	1.064	0.613
S_{13}	3.411	343	0.027	0.435	3.990	0.611
S_{14}	3.425	362	0.017	0.344	4.337	0.664
S_{15}	3.484	356	0.111	0.074	2.346	0.681
S_{16}	3.492	355	0.033	0.165	1.931	0.756
S_{17}	3.512	353	0.037	0.088	3.444	0.548
S_{18}	3.550	349	0.043	0.047	0.601	0.702
S_{19}	3.576	347	0.004	-0.206	1.038	0.581
S_{20}	3.589	345	0.044	-0.017	1.806	0.698
S_{21}	3.600	344	0.162	0.043	2.041	0.648
S_{22}	3.613	343	0.050	0.165	2.710	0.622
S_{23}	3.626	342	0.010	0.012	0.859	0.564
S_{24}	3.628	342	0.025	-0.016	0.691	0.569
S_{25}	3.629	342	0.001	0.001	0.712	0.521
S_{26}	3.650	340	0.101	0.008	0.609	0.805
S_{27}	3.697	335	0.073	0.031	4.471	0.475

S_{28}	3.724	333	0.077	0.144	1.914	0.620
S_{29}	3.735	332	0.010	0.567	3.283	0.489
S_{30}	3.767	329	0.064	0.024	4.310	0.662
S_{31}	3.856	322	0.140	0.317	2.347	0.733
S_{32}	3.882	319	0.024	0.371	3.096	0.709
S_{33}	3.896	318	0.027	0.294	2.353	0.731
S_{34}	3.919	316	0.033	0.008	0.763	0.531
S_{35}	3.948	314	0.031	0.099	1.357	0.720
S_{36}	3.958	313	0.002	0.001	1.163	0.505
S_{37}	3.982	311	0.025	0.024	1.386	0.688
S_{38}	3.984	311	0.027	0.055	1.996	0.658
S_{39}	4.002	310	0.041	0.088	0.898	0.684
S_{40}	4.012	309	0.115	0.235	0.889	0.697

PBDB-T-2F/IT-4F/E4						
Excited states	*E*/eV	*λ*/nm	*f*	Δ*q*/*e*	*D* index	*Sr* index
S_1	2.208	562	2.075	0.015	0.445	0.754
S_2	2.443	508	0.093	0.902	3.112	0.296
S_3	2.593	478	0.744	0.024	0.944	0.703
S_4	2.670	464	0.118	-0.092	3.599	0.396
S_5	2.770	448	0.274	0.064	0.687	0.751
S_6	3.007	412	0.005	0.039	6.369	0.125
S_7	3.062	405	0.048	0.608	2.280	0.603
S_8	3.098	400	0.008	0.137	2.306	0.705
S_9	3.244	382	0.110	0.736	2.748	0.511
S_{10}	3.270	379	0.051	0.123	1.217	0.716
S_{11}	3.300	376	0.068	0.056	0.987	0.709
S_{12}	3.311	374	0.009	0.134	1.229	0.640
S_{13}	3.418	363	0.045	0.807	7.858	0.432
S_{14}	3.449	360	0.049	-0.106	0.663	0.752
S_{15}	3.488	355	0.014	0.168	1.822	0.779
S_{16}	3.523	352	0.030	0.232	2.576	0.647
S_{17}	3.536	351	0.093	0.184	3.034	0.616
S_{18}	3.568	348	0.012	-0.135	0.906	0.675
S_{19}	3.589	345	0.004	0.001	0.660	0.721
S_{20}	3.596	345	0.136	-0.047	0.854	0.734
S_{21}	3.616	343	0.028	0.129	2.070	0.590
S_{22}	3.622	342	0.024	0.013	0.741	0.593
S_{23}	3.624	342	0.075	0.004	0.625	0.643
S_{24}	3.629	342	0.002	0.000	0.706	0.498
S_{25}	3.651	340	0.075	0.018	0.863	0.793
S_{26}	3.705	335	0.050	0.565	2.775	0.614
S_{27}	3.716	334	0.170	0.167	0.994	0.729

S_{28}	3.786	327	0.021	0.006	5.921	0.505
S_{29}	3.851	322	0.151	0.342	2.756	0.734
S_{30}	3.880	320	0.015	0.405	3.575	0.687
S_{31}	3.899	318	0.045	0.106	1.126	0.625
S_{32}	3.910	317	0.055	0.199	0.629	0.690
S_{33}	3.959	313	0.001	0.000	0.957	0.499
S_{34}	3.974	312	0.024	-0.042	1.409	0.739
S_{35}	3.981	311	0.049	0.204	0.586	0.692
S_{36}	3.987	311	0.041	0.118	2.761	0.631
S_{37}	3.993	310	0.031	0.012	1.489	0.721
S_{38}	4.011	309	0.154	0.016	1.463	0.618
S_{39}	4.031	308	0.013	0.172	1.048	0.691
S_{40}	4.047	306	0.003	0.615	3.281	0.467