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Supporting Information

Singlet-Triplet Energy Gap as a Critical Molecular Descriptor for Predicting Organic Photovoltaic Efficiency

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Determination of the Film ΔE_{ST}

Because the active layers are in the form of thin films, the values of the three descriptors of E_g, ΔE_{DA}, and ΔE_{ST} should be obtained with the consideration of the impact of intermolecular aggregation. This is critical for correctly describing the electronic processes in OPV devices. The E_g can be obtained from the onset of the absorption spectrum and determined as the intersection of the abscissa axis with the straight line tangent to the inflection point in the absorption edge. The HOMO and LUMO energies can be measured by cyclic voltammetry. With respect to E_g and ΔE_{DA}, the solid-state ΔE_{ST} for most of donors and acceptors are lacking because the T_1 energies (E_T) are rarely available in experiments. Janssen et al. assumed that the E_T in the films can be estimated by: $E_T = E_{T,sol}*(E_g/E_{g,sol})$, where $E_{T,sol}$ and $E_{g,sol}$ represent the T_1 and S_1 energies of isolated molecules or polymer chains in the solution, respectively.[1] Nevertheless, this is inapplicable to the ITIC-like and Y6-like small-molecule acceptors (SMAs). According to our previous theoretical studies, such SMAs are inclined to interact with each other by end-group π-π stacking due to sterically hindered side chains on the central unit.[2-4] Such end-group π-π stacking can lead to the formation of J-type (or X-type) dimers, which was further proved to substantially decrease the S_1 energies (corresponding to the experimental observations of large bathochromic shift from the solution to the film) but slightly change the T_1 energies (~ 0.05 eV or smaller). Thus, the E_T for the ITIC-like and Y6-like SMAs can be reasonably acquired by: $E_T = E_{T,sol} –$ 0.05 eV. The $E_{T,sol}$ can be estimated by: $E_{T,sol} = E_{g,sol} – \Delta E_{ST,cal}$, where $\Delta E_{ST,cal}$ denotes the ΔE_{ST} of isolated molecules or polymer chains obtained by quantum chemical calculations. Combining the $\Delta E_{ST,cal}$ with the experimentally measured E_g and $E_{g,sol}$, we can estimate the film E_T and ΔE_{ST} (= $E_g – E_T$). The obtained results for the chosen 183 donors and 190 acceptors are listed in **Table S1** and **S2**. For some of polymer donors with strong self-aggregation or interchain aggregation in the solution (e.g., PTB7 and PffBT4T-2OD), the second absorption peaks were used to estimate the $E_{g,sol}$ values.[5-6] The ΔE_{ST} values of the systems with very similar chemical structures are approximated to be same. Note that the experimentally determined E_T for P3HT (~ 1.40 eV[1]), PCPDTBT (~ 1.0 eV[7]) and H1 (analogue of Y6, ~ 1.06 eV[8]) are consistent with our estimates (P3HT ~ 1.36; PCPDTBT ~ 0.95 eV; Y6 ~ 1.10 eV), demonstrating that the method used here is reliable. Moreover, the calculated adiabatic T_1 energies for fullerene acceptors ($PC_{61}BM$/$PC_{71}BM$ ~ 1.5 eV) are equal to their experimental E_T.[1, 9-10] As shown in **Figure S5**, the comparison between the $\Delta E_{ST,cal}$ and ΔE_{ST} reflects the aggregation effects. Although close aggregation can also reduce the ΔE_{ST} to some extent, end-group π-π stacking in ITIC-like and Y6-like SMAs have greater potential owing to the weak impact on the T_1 energies.

Database Construction and Machine Learning

To ensure the reliability of the experimental data, we built the database by searching the OPV related literatures in 10 highly prestigious journals (including Angew. Chem. Int. Ed., Adv. Mater., J. Am. Chem. Soc., ACS Energy Lett., Energy Environ. Sci., Joule, Nat. Commun., Nat. Mater., Nat. Energy, and Nat. Photon.) with the keyword “organic solar cell” or “organic photovoltaic” (until July 31, 2022). All the solution processed binary OPV devices were considered. To minimize the influence of inferior phase separation morphologies of the active layers, the devices should be well working and hence the PCEs need to be higher than 4%. When the devices of the same donor/acceptor pairs have multiple reported PCE values, the device with the highest PCE is considered because it more approaches to the efficiency limit. The E_g of the device is determined by the narrower-bandgap material and the ΔE_{DA} is the smaller

one of the HOMO and LUMO energy offsets between donor and acceptor. When all the three values of E_g, ΔE_{DA}, and $E_{g,sol}$ are experimentally available, the devices would be considered. Subsequently, quantum chemical caluclations were carried out to obtain the $\Delta E_{ST,cal}$ for all the related donors and acceptors. Unfortunately, the geometry optimization of 25 donor and acceptor molecules (twisted dendritic or multi-armed large molecules) failed to converge for the S_1 and/or T_1 states, thus the corresponding devices had to be removed. Because the narrower-bandgap material usually has lower E_T, the ΔE_{ST} of all the blends is determined solely by the narrower-bandgap material except for D18:$PC_{71}BM$, PTO2:$PC_{71}BM$, DRTB-T:$PC_{71}BM$, PBDTTT-E-T:IEIC, PTB7-Th:P-BN-IID, PBDB-T:IDT-T, PSEHTT:DBFI-EDOT, and DPPEZnP-TBO:4TIC; for these eight blending systems, the wider-bandgap material has lower E_T, so the ΔE_{ST} is the difference between the E_g of the narrower-bandgap material and the E_T of the wider-bandgap material. Finally, based on the device E_g, ΔE_{DA}, ΔE_{ST}, and photovoltaic parameters, a database consisting of 515 data points was constructed (**Table S3** and **S4**). Note that, for the chemically similar pairs with almost identical entries but different PCEs, only the one with the highest PCE was considered. **Figure S1** shows the distributions and statistical analyses of all the parameters. For each parameter, the average value is similar to the median one.

Three different ML algorithms (LR: linear regression; KNN: k-nearest neighbors; GBRT: gradient boosting regression tree) with the leave-one-out (LOO) cross validation and 5-fold cross validation with shuffling of the raw data were used for comparisons (**Table S5**). The Python scripts "OPVpredict_loo.py" and "OPVpredict_cv.py" are provided in the supplementary ZIP file, which can reproduce the ML results reported in **Table S5** and **Figure 4** and **5** when combined with the scikit-learn package.

Evidently, the Pearson's correlation coefficients (*r*) are very similar for the two cross validation methods, and in most cases, GBRT performs better than LR and KNN. Further, 460 data points were randomly sampled as the training set and the remaining 55 data points as the testing set. The GBRT model optimized by the LOO cross validation based on the training set is used for the testing set. The *r* values obtained for the testing set are similar to those obtained by the LOO cross validation over all data points (**Table S6**), confirming the prediction reliability of the GBRT model based on our database. The *r* value is estimated by the relation: $r = \frac{\sum_{n=1}^{N}(x_n-\overline{x_n})\times(y_n-\overline{y_n})}{\sqrt{\sum_{n=1}^{N}(x_n-\overline{x_n})^2}\times\sqrt{\sum_{n=1}^{N}(y_n-\overline{y_n})^2}}$, where x_n and y_n are molecular properties and photovoltaic parameters (**Figure 2**, **3**, **S2** and **S3**) or measured and predicted values (**Figure 4**, **5** and **Table S5**, **S6**), respectively, and $\overline{x_n}$ and $\overline{y_n}$ represent the average values. The *r* value is in the range of -1–1 with r = 1/r = -1 corresponding to a perfect positive/negative correlation and r = 0 indicating no relevance.

Quantum Chemical Calculations

Firstly, the ground-state geometries of donors and acceptors were optimized by density functional theory (DFT) at the B3LYP/6-31G* level. To reduce the computational costs, all alkyl chains are shortened by methyl groups. Then, the vertical excitations were calculated by time-dependent DFT (TDDFT) at the B3LYP/6-31G* and ωB97XD/6-31G* levels, which can produce vertical ΔE_{ST} (**Figure S6**a). The vertical ΔE_{ST} calculated by B3LYP and ωB97XD are similar, indicating that B3LYP can reasonably describe the singlet and triplet excitations. Finally, geometry optimizations of the S_1 and T_1 states were performed at the B3LYP/6-31G* level to gain adiabatic ΔE_{ST} ($\Delta E_{ST,cal}$, given in **Table S1** and **S2**) that

involve geometric relaxations. The Cartesian coordinates of the ground-state, S_1 and T_1 geometries are given in the supplementary ZIP file. The distinct difference between vertical ΔE_{ST} and adiabatic ΔE_{ST} for many systems (**Figure S6**b) can be attributed to the different relaxed energies between S_1 and T_1. The Tamm-Dancoff approximation (TDA) scheme within TDDFT was applied to avoid the instabilities of triplet states.[11] All the DFT and TDDFT calculations were carried out by Gaussian 16 with the polarizable continuum model (PCM) to implicitly consider the dielectric environments.[12] The static dielectric constants in the films (3–4, similar to those in common organic solvents) were taken from or estimated according to the literature.[13] The range-separated parameter (ω) of the functional ωB97XD was optimally tuned with the PCM.

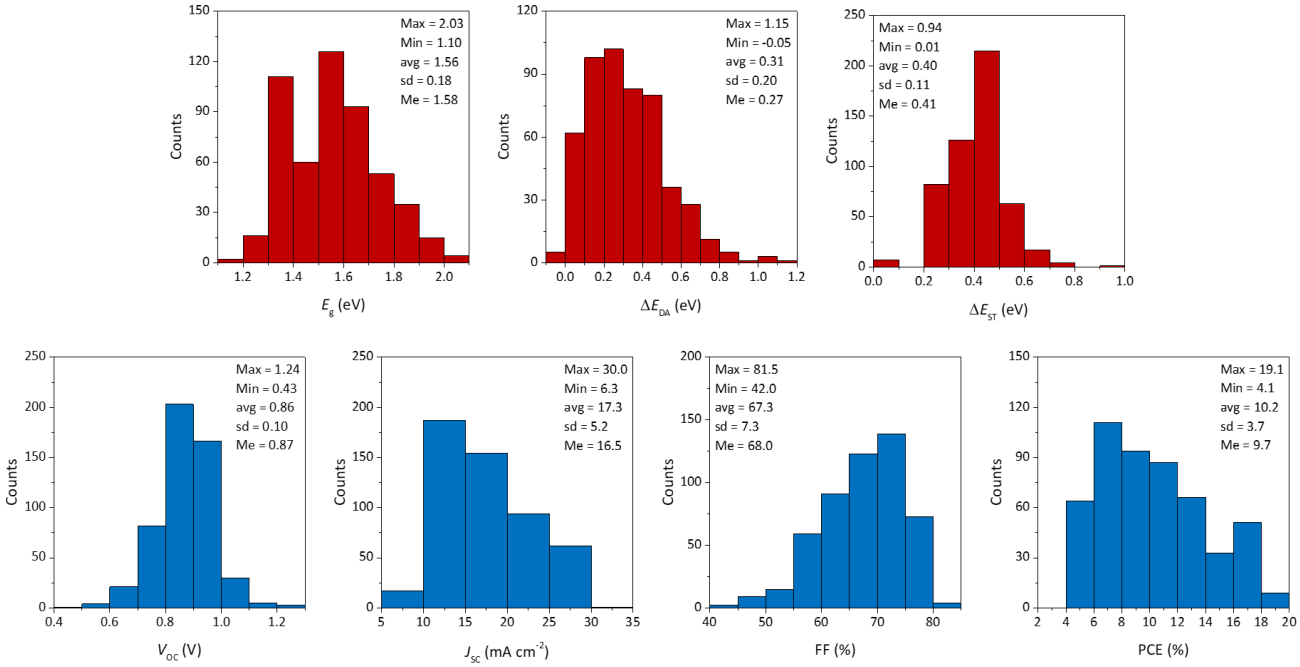

Figure S1. Distributions and statistical analyses of the three molecular properties and four photovoltaic parameters in the data set (Max: maximum; Min: minimum; Me: median value; avg; average value; sd: standard deviation).

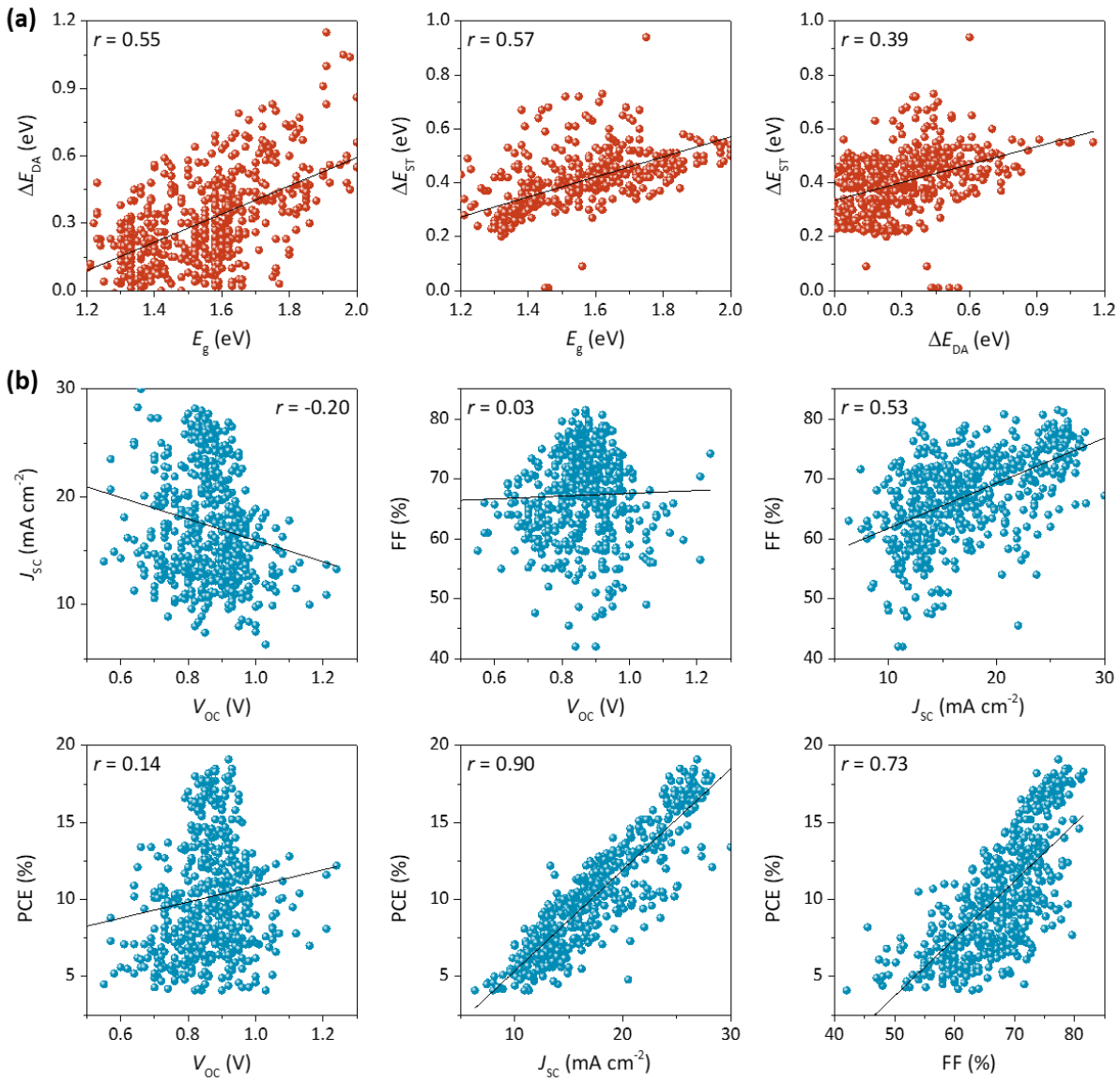

Figure S2. (a) Direct comparisons between each two quantities of the three molecular descriptors. (b) Direct comparisons between each two quantities of the four photovoltaic parameters.

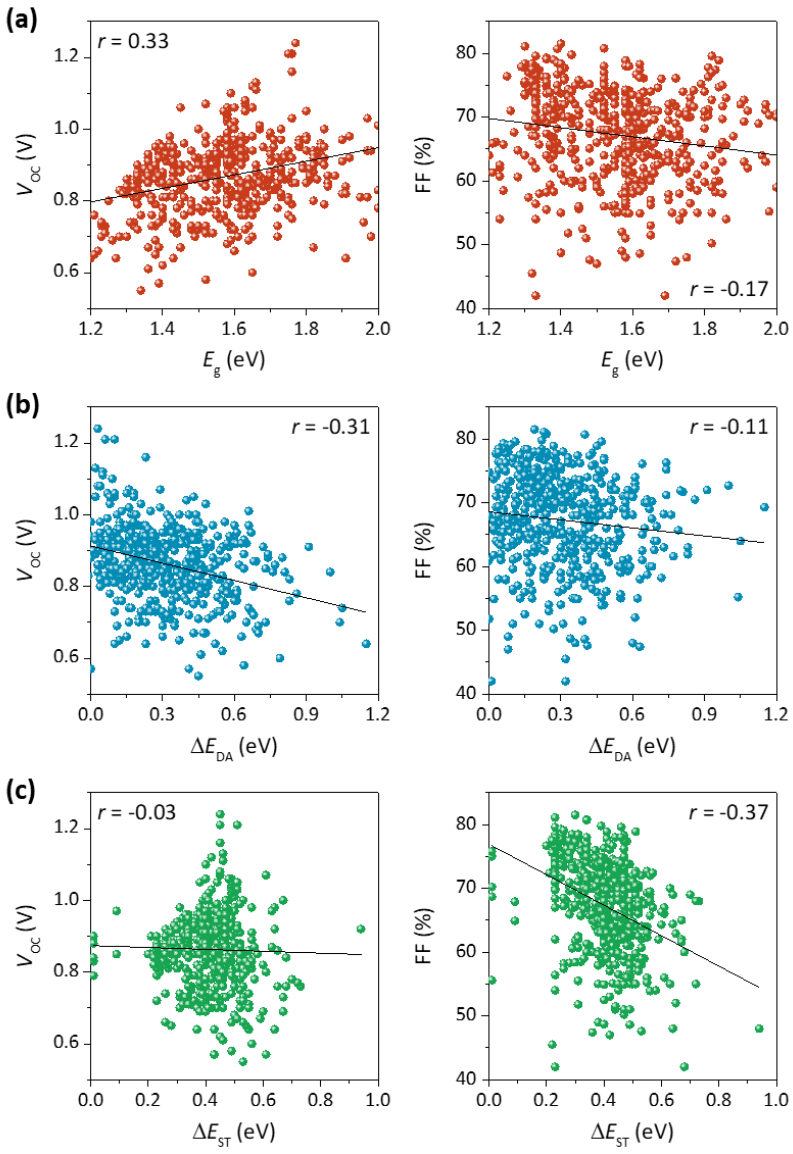

Figure S3. V_{OC} and FF versus E_g (a), ΔE_{DA} (b), and ΔE_{ST} (c), respectively.

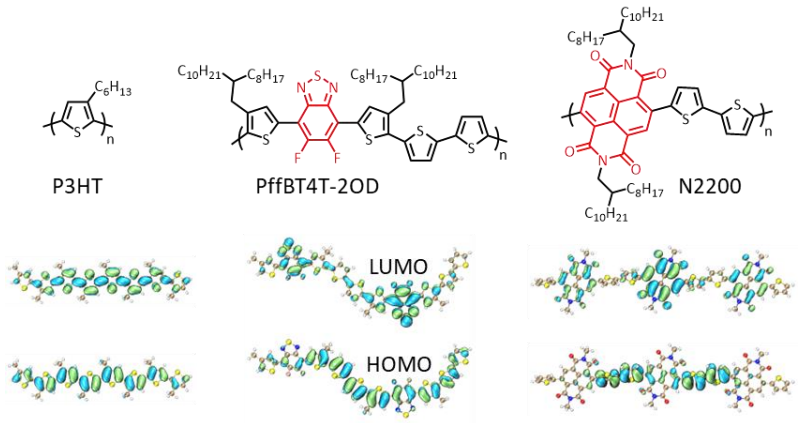

Figure S4. Chemical structures and frontier molecular orbitals of three typical OPV polymers (P3HT, PffBT4T-2OD, and N2200).

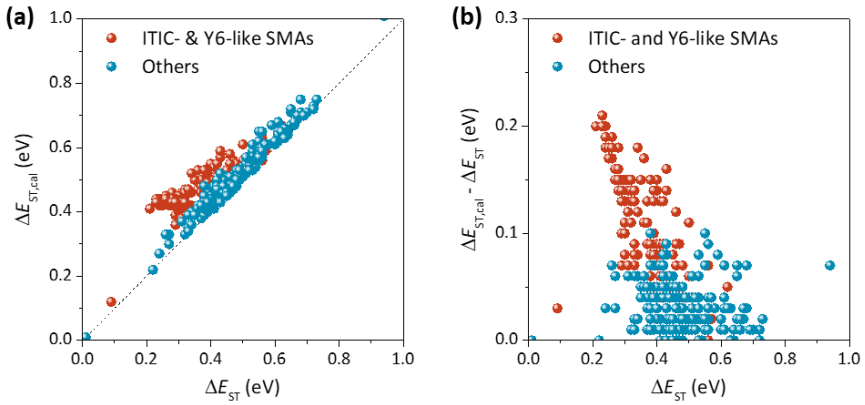

Figure S5. (a) $\Delta E_{ST,cal}$ and (b) $\Delta E_{ST,cal}$ - ΔE_{ST} versus ΔE_{ST} for the donors and acceptors.

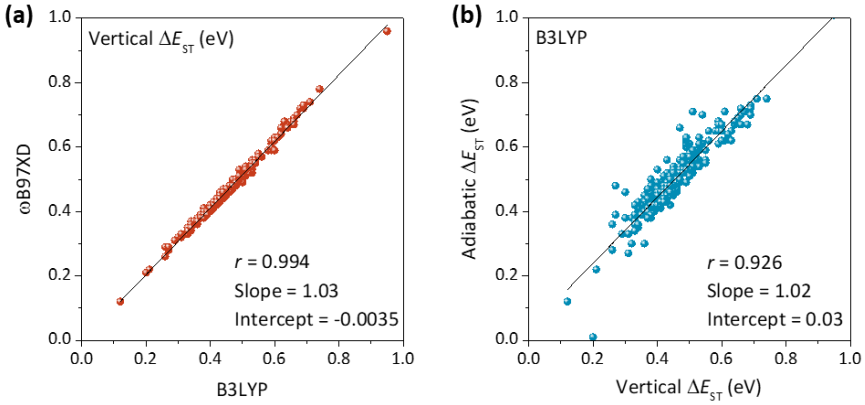

Figure S6. (a) Vertical ΔE_{ST}: B3LYP versus ωB97XD. (b) Vertical ΔE_{ST} versus adiabatic ΔE_{ST} ($\Delta E_{ST,cal}$).

Table S1. $E_{g,sol}$, E_g, $\Delta E_{ST,cal}$, E_T and ΔE_{ST} for 174 donors (the number of repeat units for each polymer model is given in the bracket after the polymer name).

No.	Donor	$E_{g,sol}$ (eV)	E_g (eV)	Ref.	$\Delta E_{ST,cal}$ (eV)	E_T (eV)	ΔE_{ST} (eV)
Homopolymer donors							
1	P3HT (8) P5TCN-F25 (1)	2.25	1.91 1.88	[1, 14]	0.65	1.36 ~ 1.33	0.55
2	PDHTT (3)	2.20	1.96	[15-16]	0.62	1.41	0.55
3	PDCBT (2)	2.19	1.90	[17-18]	0.65	1.34	0.56
4	PTVT-T (2)	1.93	1.76	[19-20]	0.71	1.11	0.65
D-A copolymer donors							
5	PDPP3T (3)	1.43	1.36	[21-22]	0.54	0.85	0.51
6	PDPP2FT (3)	1.42	1.38	[23-25]	0.56	0.84	0.54
7	PDPPTPT (3)	1.57	1.54	[22, 26]	0.62	0.93	0.61
8	PDPP2T-TT (3)	1.41	1.39	[22, 27]	0.52	0.88	0.51
9	PDPPTPyT (3)	1.38	1.34	[28]	0.55	0.81	0.53
10	PDPPTDTPT (3)	1.28	1.23	[28]	0.47	0.78	0.45
11	PDPP-TNT (3)	1.62	1.57	[29]	0.67	0.92	0.65
12	PDTTDPP (3)	1.31	1.22	[30]	0.53	0.73	0.49
13	PDPP2T-DBT (2)	1.66	1.62	[22]	0.75	0.89	0.73
14	PDPP4T (2)	1.43	1.43	[22]	0.64	0.79	0.64
15	PDPP2T-BDT (2)	1.53	1.51	[22]	0.73	0.79	0.72
16	PBDTT-DPP (2)	1.51	1.44	[31]	0.70	0.77	0.67
17	PBDTP-DPP (2)	1.53	1.46	[31]	0.71	0.78	0.68
18	PBDTT-FDPP (2)	1.56	1.55	[31]	0.72	0.83	0.72
19	PBDTT-SeDPP (2)	1.43	1.38	[32]	0.69	0.71	0.67
20	DPPTT-T (2)	1.42	1.39	[33-34]	0.62	0.78	0.61
21	PDPP2PyT (3)	1.81	1.73	[35]	0.70	1.06	0.67
22	PDPP2Py2T (3)	1.73	1.70	[35]	0.65	1.06	0.64
23	PDPP2PyDTP (3)	1.58	1.54	[35]	0.56	0.99	0.55
24	PDPP2Py3T (2)	1.74	1.68	[35]	0.67	1.03	0.65
25	PBnDT-DTPyT (2)	1.77	1.51	[36]	0.46	1.12	0.39
26	PNDT-DTPyT (2)	1.73	1.53	[36]	0.45	1.13	0.40
27	PQDT-DTPyT (2)	1.73	1.56	[36]	0.48	1.13	0.43
28	POD2T-DTBT (2)	1.75	1.59	[37]	0.50	1.14	0.45
29	PTh_4FBT (2)	1.81	1.65	[38]	0.44	1.25	0.40
30	PBT4T-2OD (2)	1.81	1.65	[39-40]	0.50	1.19	0.46
31	PffBT4T-2OD (2) PffBT4T-2DT (2) PffBT4T-C_9C_{13} (2)	1.80	1.65	[41-42]	0.46	1.23	0.42
32	PffBT-T3(1,2)-2 (1.5)	1.78	1.63	[43]	0.42	1.25	0.38
33	PBTff4T-2OD (2)	1.77	1.63	[41]	0.49	1.18	0.45
34	PffBX4T-2DT (2)	1.82	1.66	[44]	0.49	1.21	0.45
35	PffBT2T-TT (2)	1.78	1.64	[45]	0.47	1.21	0.43
36	PBT4T-4Cl (2)	1.83	1.67	[46]	0.47	1.24	0.43
37	PCBT4T-2OD (2)	1.86	1.59	[40]	0.48	1.18	0.41
38	PCCBT4T-2OD (2)	2.04	1.61	[40]	0.48	1.23	0.38
39	PPDTBT (2.5)	1.86	1.72	[47]	0.48	1.28	0.44
40	PPDTFBT (2.5)	1.78	1.72	[47]	0.45	1.29	0.43
41	PPDT2FBT (2.5)	1.80	1.76	[47]	0.43	1.34	0.42

42	PDTBTBz-0F (2.5)	2.14	1.97	[48]	0.51	1.50	0.47
43	PDTBTBz-2F$_{syn}$ (2.5)	1.96	1.92	[48]	0.51	1.42	0.50
44	PDTBTBz-2F$_{anti}$ (2.5)	1.94	1.90	[48]	0.51	1.40	0.50
45	PDTBTBz-4F (2.5)	2.00	1.97	[48]	0.52	1.46	0.51
46	PCPDTBT (3)	1.55	1.40	[49]	0.50	0.95	0.45
47	PSBTBT (3)	1.54	1.52	[50]	0.50	1.03	0.49
48	PBDT-BT (3)	1.77	1.75	[51]	0.46	1.30	0.45
49	PFDCTBT-C8 (2)	1.84	1.71	[52]	0.56	1.19	0.52
50	PIDT-DFBT (2)	1.84	1.78	[53]	0.52	1.28	0.50
51	PIDTT-DFBT (2)	1.84	1.78	[53]	0.46	1.34	0.44
52	PITBT (3)	1.90	1.82	[54]	0.49	1.35	0.47
53	PITFBT (3)	1.91	1.79	[54]	0.46	1.36	0.43
54	PCDTBT (2)	2.00	1.88	[55]	0.61	1.31	0.57
55	HXS-1 (2)	2.03	1.95	[56]	0.58	1.39	0.56
56	EI-PFDTBT (2)	1.92	1.86	[57]	0.61	1.28	0.58
57	PBnDT-DTffBT (2)	1.75	1.73	[58-59]	0.45	1.29	0.44
58	PBDT2FBT-2EHO (2)	1.96	1.83	[60]	0.46	1.40	0.43
59	PBDT$_{TEH}$-DT$_{EH}$BTff (2)	1.77	1.75	[61]	0.45	1.31	0.44
60	PBDTP-DTBT (2) PTFBDT-BZS (2)	1.84	1.70 1.81	[62-63]	0.51	1.23 ~ 1.34	0.47
61	PBDTDTBT-R (2)	1.91	1.72	[64]	0.51	1.26	0.46
62	PBDTDT$_{ff}$BT-H (2)	1.77	1.76	[64]	0.46	1.30	0.46
63	PBDTTS-TTBT (2)	1.75	1.73	[65]	0.52	1.22	0.51
64	PBDTTS-TTDffBT (2)	1.80	1.74	[65]	0.47	1.29	0.45
65	PNDT-DTBT (2)	1.72	1.69	[66]	0.44	1.26	0.43
66	PTFB-P (2)	1.97	1.97	[67]	0.53	1.44	0.53
67	PTFB-O (2)	2.00	2.00	[67]	0.54	1.46	0.54
68	PvBDTTAZ (2)	2.28	2.05	[68]	0.59	1.52	0.53
69	PBnDT-HTAZ (2)	2.00	1.98	[69]	0.56	1.43	0.55
70	PBnDT-FTAZ (2)	2.02	2.00	[69]	0.53	1.48	0.52
71	PBDTFBZO (2)	1.94	1.83	[70]	0.54	1.32	0.51
72	PBDTFBZS (2)	1.97	1.81	[70]	0.54	1.31	0.50
73	PBDT-FBTA/J51 (2) J52 (2) J52-2F (2) J60, J61 or PBFTAZ (2) J71 (2) J91 (2)	1.98	1.91 1.96 1.94 1.93 1.96 1.92	[71-76]	0.51	1.42 ~ 1.47 ~ 1.45 ~ 1.44 ~ 1.47 ~ 1.43	0.49
74	PSiBO (2)	1.68	1.66	[77]	0.56	1.11	0.55
75	PSiNO (2)	1.57	1.51	[77]	0.43	1.10	0.41
76	NT812 (2)	1.57	1.50	[78]	0.40	1.11	0.39
77	PNTz4T (2) PNOz4T (2)	1.58	1.54 1.52	[39, 79]	0.38	1.17 ~ 1.15	0.37
78	PNTz4TF2 (2)	1.63	1.60	[80]	0.38	1.23	0.37
79	PNTz4TF4 (2)	1.65	1.62	[80]	0.42	1.21	0.41
80	PNNT-12DT (2)	1.70	1.66	[81]	0.46	1.21	0.45
81	PTB3 (3)	1.72	1.60	[82-83]	0.57	1.07	0.53
82	PBDTTT-C (3)	1.73	1.61	[84]	0.56	1.09	0.52
83	PBDTTT-E-T (3)	1.70	1.58	[85]	0.54	1.08	0.50
84	PBDTTT-C-T (3)	1.71	1.58	[85]	0.53	1.09	0.49
85	PTB7 (3)	1.76	1.63	[86]	0.57	1.10	0.53

86	PTB7-Th/PCE10 (3)	1.70	1.58	[87]	0.53	1.09	0.49
87	PBDTTT-H (3)	1.74	1.68	[64]	0.56	1.14	0.54
88	PTAT-3 (3)	1.69	1.60	[88]	0.56	1.07	0.53
89	PBT-1F (2)	1.78	1.65	[89]	0.60	1.09	0.56
90	PBT-3F (2)	1.76	1.64	[89]	0.61	1.07	0.57
91	PTBTz-2 (2)	1.72	1.70	[90]	0.57	1.14	0.56
92	PTBTz-5 (2)	1.76	1.73	[90]	0.61	1.13	0.60
93	PBDTDTTT-S-T (2)	1.69	1.64	[91]	0.62	1.04	0.60
94	PDT-S-T (3)	1.65	1.64	[92]	0.53	1.11	0.53
95	PTPD3T (3)	1.84	1.82	[93]	0.47	1.36	0.46
96	PT-ttTPD (2)	1.88	1.75	[94]	0.55	1.24	0.51
97	PBT-ttTPD (2)	1.85	1.72	[94]	0.50	1.26	0.46
98	PDTSTPD (3)	1.77	1.73	[95]	0.53	1.21	0.52
99	PDTG-TPD (3)	1.74	1.70	[96-97]	0.53	1.18	0.52
100	PDTTG-TPD (3)	1.79	1.75	[98]	0.46	1.30	0.45
101	PBDTTPD (3)	2.00	1.80	[99-100]	0.53	1.32	0.48
102	PT8/PBDTTTPD (3) PTP8 (3)	1.88 1.84	1.85 1.78	[101-102]	0.49	1.37 1.31	0.48 0.47
103	PBDT-ttTPD (2)	1.92	1.90	[103]	0.47	1.43	0.47
104	PBDTT-ttTPD (2) PMOT40 (2) TPD-3 or TPD-3F (2)	1.88	1.86 1.89 1.90	[103-105]	0.45	1.41 ~ 1.44 ~ 1.45	0.45
105	PBTI3T (3)	1.81	1.81	[93]	0.41	1.40	0.41
106	PBTISi-C8 (3)	1.77	1.75	[106]	0.45	1.31	0.44
107	BTI-BDT (3)	1.93	1.92	[107]	0.48	1.44	0.48
108	TQ1 (4)	1.84	1.70	[108]	0.49	1.25	0.45
109	PTQ10 (5) PTQ9 (5) PTQ11 (5)	1.94	1.92 1.87 1.95	[109-111]	0.43	1.49 ~ 1.44 ~ 1.52	0.43
110	PIDT-phanQ (2)	1.71	1.67	[9, 112]	0.50	1.18	0.49
111	PBQ-4F (2) PBQ-0F (2) PBQ-QF (2) PBQ-6 (2) TTFQx-T1 (2)	1.75	1.73 1.70 1.72 1.71 1.69	[113-116]	0.47	1.27 ~ 1.24 ~ 1.26 ~ 1.25 ~ 1.23	0.46
112	PIDTDTQx (2)	1.87	1.81	[117]	0.47	1.36	0.45
113	PBDB-T (2) PBT1-EH (2) PFBDB-T (2) PClBDB-T (2)	1.90	1.80 1.84 1.77 1.78	[118-121]	0.50	1.33 ~ 1.37 ~ 1.30 ~ 1.31	0.47
114	PBDF-T1 (2)	1.86	1.83	[122]	0.49	1.35	0.48
115	PBDT-T1 (2) PBT1-C (2) PBT1-O (2)	1.85	1.81 1.84 1.82	[122-123]	0.52	1.30 ~ 1.33 ~ 1.31	0.51
116	PM6 (2)	1.89	1.80	[124]	0.49	1.33	0.47
117	PDBT-T1 (2)	1.86	1.85	[125]	0.47	1.38	0.47
118	P3TI (2)	1.63	1.50	[126]	0.56	0.98	0.52
119	PiITVT (2.5)	1.65	1.61	[127]	0.53	1.09	0.52
120	P(IID-DTC) (2)	1.64	1.61	[128]	0.71	0.91	0.70
121	P(IID2F-DTC) (2)	1.67	1.59	[128]	0.66	0.96	0.63
122	PThTPTI (3)	1.89	1.86	[129]	0.49	1.38	0.48
123	PCPDTTTz (2)	1.82	1.76	[130]	0.54	1.24	0.52

124	PSEHTT (2)	1.88	1.82	[131]	0.53	1.31	0.51
125	PBDTS-TDZ (2) PBDT-TDZ (2) PBDT-ODZ (2)	2.09	2.09 2.07 2.12	[132-133]	0.53	1.56 ~ 1.54 ~ 1.59	0.53
126	BBTI-1 (2)	1.50	1.48	[134]	0.46	1.03	0.45
127	PTzBI (2) PTzBI-*d*F (2)	1.93	1.81 1.72	[135-137]	0.49	1.35 ~ 1.26	0.46
128	P2F-EHp (2)	1.95	1.85	[138]	0.51	1.37	0.48
129	D18 (2) PBQx-TCl (2) PQM-Cl (2) pBDTT-DPI-Me (2)	2.00	1.98 2.05 2.00 1.97	[139-142]	0.45	1.53 ~ 1.60 ~ 1.55 ~ 1.52	0.45
130	PTZ1 (2)	2.07	1.97	[143-144]	0.51	1.48	0.49
131	PIPCP (1)	1.53	1.47	[145-146]	0.49	1.00	0.47
132	P3TEA (1)	1.66	1.66	[147]	0.46	1.20	0.46
133	PDTB-EF-T (2) PB3T (2)	1.95	1.93 1.96	[148-149]	0.57	1.37 ~ 1.40	0.56
134	PTO2 (3)	2.08	2.03	[150]	0.53	1.51	0.52
Small-molecule donors							
135	DPP(TBFu)$_2$	1.89	1.75	[151-152]	1.01	0.81	0.94
136	NDT(TDPP)$_2$	1.87	1.69	[153]	0.75	1.01	0.68
137	DPPEZnP-TBO A1	1.53	1.37	[154-156]	0.51	0.91	0.46
138	CNDPP	1.71	1.48	[157]	0.61	0.95	0.53
139	*p*-DTS(PTTh$_2$)$_2$	1.69	1.50	[158-159]	0.51	1.05	0.45
140	*d*-DTS(PTTh$_2$)$_2$	1.70	1.50	[159]	0.50	1.06	0.44
141	*p*-DTS(FBTTh$_2$)$_2$	1.85	1.55	[160]	0.51	1.12	0.43
142	*p*-SIDT(FBTTh$_2$)$_2$	1.94	1.84	[161]	0.49	1.38	0.46
143	X1	1.64	1.44	[162]	0.40	1.09	0.35
144	X4	1.59	1.40	[163]	0.40	1.05	0.35
145	X5	1.66	1.43	[163]	0.42	1.07	0.36
146	BIT4F	1.91	1.81	[164-165]	0.42	1.41	0.40
147	BIT6F	1.85	1.79	[165]	0.38	1.42	0.37
148	DCAO7T	2.07	1.74	[166-167]	0.45	1.36	0.38
149	T2	2.04	1.77	[168]	0.41	1.41	0.36
150	T3	2.01	1.72	[168]	0.40	1.38	0.34
151	DCAO3TBDT DCAO3T(BDT)3T	2.10 2.12	1.84 1.83	[167, 169]	0.50	1.40	0.44 0.43
152	DCAO3TBDTT/SM1 SM1-F or H31 H22	2.10	1.84 1.88 1.89	[170-173]	0.48	1.42 ~ 1.46 ~ 1.47	0.42
153	DR3TBDT	2.05	1.74	[169]	0.49	1.32	0.42
154	DR3TSBDT	2.05	1.74	[174]	0.50	1.32	0.42
155	DR3TBDTT BDTT-S-TR H21	1.98 2.05	1.72 1.73 1.81	[172, 175-176]	0.48	1.30 1.32 ~ 1.39	0.42 0.41
156	BTR BTR-Cl or BM-Cl BSFTR B1 L2	2.01	1.82 1.76 1.83 1.75 1.77	[177-181]	0.46	1.40 ~ 1.34 ~ 1.41 ~ 1.33 ~ 1.35	0.42
157	BTTzR	2.04	1.88	[182]	0.40	1.51	0.37

158	ZR1 ZR-SiO-EH or M-PhS	2.03	1.84 1.82	[183-185]	0.51	1.38 ~ 1.36	0.46
159	DRTB-T	2.09	2.00	[186]	0.42	1.60	0.40
160	DERHD7T	2.02	1.72	[187-188]	0.42	1.36	0.36
161	DRCN5T	1.95	1.60	[189]	0.52	1.17	0.43
162	DRCN6T	1.91	1.60	[189]	0.45	1.22	0.38
163	DRCN7T	1.91	1.62	[188-189]	0.39	1.29	0.33
164	DRCN8T	1.94	1.61	[189]	0.37	1.30	0.31
165	DRCN9T	1.94	1.59	[189]	0.33	1.32	0.27
166	BTID-0F	1.94	1.71	[190]	0.43	1.33	0.38
167	BTID-1F	1.91	1.70	[190]	0.41	1.34	0.36
168	BTID-2F	1.88	1.68	[190]	0.41	1.31	0.37
169	H11	-	1.87	[191]	0.39	> 1.48	-
170	H12	-	1.87	[191]	0.41	> 1.46	-
171	M-1	1.97	1.75	[192]	0.47	1.33	0.42
172	M-2	1.97	1.76	[192]	0.39	1.41	0.35
173	CS1	1.97	1.85	[193]	0.40	1.47	0.38
174	D1	1.78	1.66	[156]	0.65	1.05	0.61

Table S2. $E_{g,sol}$, E_g, $\Delta E_{ST,cal}$, E_T, and ΔE_{ST} for 182 acceptors (the number of repeat units for each polymer model is given in the bracket after the polymer name).

No.	Acceptor	$E_{g,sol}$ (eV)	E_g (eV)	Ref.	$\Delta E_{ST,cal}$ (eV)	E_T (eV)	ΔE_{ST} (eV)
Perylene diimide derivatives							
1	di-PBI	2.11	2.07	[194-195]	0.67	1.41	0.66
2	SdiPBI-S	2.36	2.20	[196]	0.65	1.59	0.61
3	SdiPBI-Se	2.34	2.22	[197]	0.64	1.61	0.61
4	SF-PDI_2	2.10	2.00	[147, 198]	0.65	1.38	0.62
5	Helical PDI 1	2.18	2.14	[199]	0.62	1.53	0.61
6	FPDI-T	2.30	2.22	[200]	0.68	1.56	0.66
7	BFPTP	2.20	2.12	[201]	0.57	1.57	0.55
8	FTTB-PDI4	2.16	2.10	[202]	0.49	1.62	0.48
9	FIDTT-2PDI	1.75	1.73	[203-204]	0.22	1.51	0.22
10	DBFI-T	1.80	1.73	[131]	0.46	1.29	0.44
11	DBFI-DMT	2.02	1.91	[205]	0.36	1.57	0.34
12	DBFI-EDOT	1.75	1.70	[206]	0.39	1.32	0.38
ITIC-like A-D-A small-molecule acceptors (SMAs)							
13	IDT-T	2.01	1.91	[207]	0.67	1.29	0.62
14	IDTT-T	1.89	1.82	[208-209]	0.59	1.25	0.57
15	6TBA	1.64	1.52	[210]	0.63	0.96	0.56
16	IDIC IDIC-C4Ph	1.76	1.62	[211-212]	0.56	1.15	0.47
17	IDTI/IDIC-PhC6	1.79	1.70	[213]	0.56	1.18	0.52
18	IDTN	1.71	1.59	[213]	0.53	1.13	0.46
19	IDT-2B	1.78	1.73	[214]	0.56	1.17	0.56
20	IDT-OB	1.77	1.66	[214]	0.56	1.16	0.50
21	IDT-2O	1.75	1.64	[214]	0.57	1.13	0.51
22	IDIC-4F	1.76	1.64	[215]	0.55	1.16	0.48
23	IDIC-4Cl	1.72	1.53	[183]	0.54	1.13	0.40
24	MO-IDIC	1.74	1.60	[216]	0.55	1.14	0.46
25	MO-IDIC-2F	1.75	1.55	[216]	0.55	1.15	0.40
26	MO-IDIC-Cl-2	1.72	1.54	[217]	0.54	1.13	0.41
27	SiOTIC	1.74	1.55	[218]	0.53	1.16	0.39
28	ITIC *m*-ITIC	1.73 1.74	1.59 1.58	[219-220]	0.49	1.19 1.20	0.40 0.38
29	C8-ITIC	1.70	1.55	[120]	0.49	1.16	0.39
30	IT-M	1.73	1.60	[221]	0.49	1.19	0.41
31	IT-DM	1.74	1.63	[221]	0.49	1.20	0.43
32	IDT6CN-M	1.73	1.63	[222]	0.52	1.16	0.47
33	IDT8CN-M	1.67	1.58	[222]	0.45	1.17	0.41
34	ITIC-Th	1.72	1.60	[223]	0.47	1.20	0.40
35	ITIC-Th1	1.71	1.55	[224]	0.47	1.19	0.36
36	ITCC	1.80	1.67	[225]	0.48	1.27	0.40
37	IDTCN	1.76	1.67	[226]	0.56	1.15	0.52
38	IDT6CN	1.72	1.63	[226]	0.52	1.15	0.48
39	IDT6CN-Th	1.74	1.61	[226]	0.51	1.18	0.43
40	ITCPTC	1.68	1.58	[227-228]	0.49	1.14	0.44
41	MeIC	1.68	1.58	[227]	0.49	1.15	0.44
42	MeIC1	1.69	1.54	[229-230]	0.48	1.17	0.37

43	ITIC3	1.69	1.55	[231]	0.47	1.17	0.38
44	IT-4F	1.69	1.52	[232]	0.46	1.18	0.34
45	IT-2Cl	1.69	1.55	[233]	0.46	1.18	0.37
46	IT-4Cl	1.65	1.48	[233]	0.46	1.14	0.34
47	SeTIC	1.69	1.58	[234]	0.50	1.14	0.44
48	SeTIC4Cl	1.63	1.44	[234]	0.47	1.11	0.33
49	ITIC1/NFBDT	1.65	1.55	[235-236]	0.52	1.08	0.47
50	ITIC2	1.63	1.53	[235]	0.51	1.07	0.46
51	NCBDT	1.59	1.45	[237]	0.49	1.05	0.40
52	BDCPDT-FIC	1.63	1.49	[238]	0.50	1.08	0.41
53	BDCPDT-TTC	1.71	1.58	[238]	0.38	1.28	0.30
54	NNBDT	1.55	1.43	[239-240]	0.48	1.02	0.41
55	BT-IC	1.57	1.43	[241]	0.47	1.05	0.38
56	FNIC1	1.58	1.48	[242]	0.43	1.10	0.38
57	FNIC2	1.52	1.38	[242]	0.42	1.05	0.33
58	INIC 3TP3T-IC	1.66	1.57 1.63	[243-244]	0.42	1.19	0.38 0.44
59	INIC1	1.63	1.56	[243]	0.40	1.18	0.38
60	INIC2	1.64	1.52	[243]	0.40	1.19	0.33
61	INIC3 3TP3T-4F	1.63	1.48 1.50	[243-244]	0.39	1.19	0.29 0.31
62	FINIC	1.66	1.51	[245]	0.40	1.21	0.30
63	INPIC	1.55	1.46	[246]	0.44	1.06	0.40
64	INPIC-4F	1.52	1.39	[246]	0.42	1.05	0.34
65	IPIC-4Cl	1.48	1.32	[247]	0.41	1.02	0.30
66	IHIC2	1.77	1.66	[248]	0.48	1.24	0.42
67	IOIC2	1.65	1.55	[248]	0.45	1.15	0.40
68	NOIC	1.69	1.55	[249]	0.42	1.22	0.33
69	NOIC1	1.50	1.38	[249]	0.36	1.09	0.29
70	NOIC2	1.65	1.49	[249]	0.43	1.17	0.32
71	NOIC3	1.80	1.62	[249]	0.43	1.32	0.30
72	NOIC4	1.67	1.55	[249]	0.38	1.24	0.31
73	AOIC	1.52	1.39	[250]	0.46	1.01	0.38
74	DICTF	1.93	1.82	[251]	0.47	1.41	0.41
75	FDICTF	1.76	1.63	[251]	0.47	1.24	0.39
76	ZITI	1.62	1.53	[252]	0.42	1.15	0.38
77	IHIC/4TIC	1.56	1.40	[253-254]	0.61	0.90	0.50
78	F6IC/4TIC-4F	1.53	1.36	[255-256]	0.58	0.90	0.46
79	6TIC	1.50	1.37	[257-258]	0.53	0.92	0.45
80	FOIC	1.46	1.32	[231]	0.51	0.90	0.42
81	F8IC/6TIC-4F	1.45	1.27	[255-256]	0.50	0.90	0.37
82	CO_i8DFIC	1.40	1.26	[259]	0.47	0.88	0.38
83	M3	1.57	1.41	[260]	0.43	1.14	0.27
84	M8	1.47	1.28	[261]	0.43	0.99	0.29
85	DTPC-DFIC	1.34	1.21	[262]	0.42	0.87	0.34
86	IEIC	1.60	1.50	[263]	0.44	1.11	0.39
87	IDSe-T-IC	1.61	1.52	[264]	0.46	1.10	0.42
88	IEICO	1.44	1.34	[263]	0.47	0.92	0.42
89	IEICO-4F	1.42	1.24	[265]	0.45	0.92	0.32
90	i-IEICO-4F	1.64	1.56	[266]	0.12	1.47	0.09
91	IDTT2F	1.59	1.46	[267]	0.41	1.13	0.33

92	IDTOT2F	1.58	1.44	[267]	0.42	1.11	0.33
93	IEICO-4Cl	1.42	1.23	[268]	0.45	0.92	0.31
94	PTIC	1.75	1.53	[215]	0.53	1.17	0.36
95	PTB4F	1.76	1.65	[269]	0.50	1.21	0.44
96	PTB4Cl	1.73	1.58	[269]	0.49	1.19	0.39
97	*o*-4TBC-2F	1.54	1.34	[270]	0.50	0.99	0.35
98	A4T-16	1.61	1.43	[271]	0.52	1.04	0.39
99	DF-PCIC	1.71	1.59	[272]	0.49	1.17	0.42
100	HC-PCIC	1.66	1.48	[273]	0.46	1.15	0.33
101	DOC2C6-IC	1.57	1.44	[274]	0.47	1.05	0.39
102	DOC2C6-2F	1.53	1.42	[274]	0.44	1.04	0.38
103	BN-0F	1.50	1.41	[275]	0.44	1.01	0.40
104	BN-2F	1.49	1.40	[275]	0.42	1.02	0.38
105	BN-4F	1.49	1.38	[275]	0.42	1.02	0.36
106	CTIC-4F	1.48	1.30	[276]	0.55	0.88	0.42
107	CO1-4F	1.39	1.20	[276]	0.57	0.77	0.43
108	COTIC-4F	1.31	1.10	[276]	0.59	0.67	0.43
Y6-like SMAs							
109	BZ4F-O-3	1.60	1.40	[277]	0.53	1.02	0.38
110	Y1	1.55	1.36	[278]	0.45	1.05	0.31
111	Y2	1.53	1.34	[278]	0.45	1.03	0.31
112	Y11 Y1-4F	1.53	1.31	[279-280]	0.43	1.05	0.26
113	mBzS-4F	1.50	1.25	[281]	0.44	1.01	0.24
114	Y5	1.61	1.38	[116]	0.46	1.10	0.28
115	BTP-M	1.62	1.42	[282]	0.46	1.11	0.31
116	L8-BO-F Y6-F	1.60	1.41 1.36	[283-285]	0.45	1.10	0.31 0.26
117	Y6 L8-BO N3	1.59	1.33 1.40 1.32	[286-288]	0.44	1.10	0.23 0.30 0.22
118	*p*-BTP-PhC6 *m*-BTP-PhC6	1.58	1.35 1.36	[289]	0.42	1.11	0.24 0.25
119	BTP-Th BTP-FTh *m*-TEH	1.58	1.33 1.32 1.38	[290-291]	0.41	1.12	0.21 0.20 0.26
120	BTPV-4F	1.40	1.21	[292]	0.42	0.93	0.28
121	Y6Se	1.57	1.32	[293]	0.44	1.08	0.24
122	CH1007	1.54	1.30	[294]	0.45	1.04	0.26
123	BPF-4F	1.56	1.36	[295]	0.45	1.06	0.30
124	BPT-4F	1.58	1.36	[295]	0.43	1.10	0.26
125	BPS-4F	1.55	1.29	[295]	0.44	1.06	0.23
126	BTP-2ThCl	1.55	1.35	[296]	0.44	1.06	0.29
127	BTP-2F-ThCl	1.57	1.34	[296]	0.44	1.08	0.26
128	LY-Cl-2 L8-BO-Cl	1.57	1.36 1.39	[217, 284]	0.44	1.08	0.28 0.33
129	BTP-4Cl BTP-eC9 or BO-4Cl	1.55	1.30	[297-298]	0.43	1.07	0.25
130	Y-BO-FCl	1.57	1.33	[299]	0.43	1.09	0.24
131	A-WSSe-Cl	1.53	1.33	[300]	0.43	1.05	0.28
132	S-WSeSe-Cl	1.52	1.30	[300]	0.43	1.04	0.26

133	BTP-S1	1.63	1.43	[301]	0.47	1.11	0.32
134	BTP-S2	1.60	1.41	[301]	0.46	1.09	0.32
135	BT-BO-L4F/BTP-S7	1.53	1.33	[302-303]	0.42	1.06	0.27
136	BTP-S9	1.54	1.32	[302]	0.42	1.07	0.25
137	BO-5Cl	1.61	1.42	[304]	0.47	1.09	0.33
138	BTIC-2Cl-γCF_3	1.55	1.31	[305]	0.43	1.07	0.24
139	BTF	1.50	1.31	[306]	0.42	1.03	0.28
140	BTFM	1.51	1.33	[306]	0.42	1.04	0.29
141	TPT10 BTP-H2	1.59	1.36 1.39	[111, 284]	0.44	1.10	0.26 0.29
142	AQx-1	1.55	1.37	[307]	0.43	1.07	0.30
143	AQx-2	1.60	1.35	[307]	0.43	1.12	0.23
144	CH4	1.54	1.37	[308]	0.43	1.06	0.31
145	CH6	1.57	1.40	[308]	0.43	1.09	0.31
146	CH-4Cl	1.55	1.39	[309]	0.43	1.07	0.32
147	CH-6Cl	1.54	1.36	[309]	0.42	1.07	0.29
148	Qx-1	1.56	1.36	[310]	0.43	1.08	0.28
149	Qx-2	1.55	1.36	[310]	0.43	1.07	0.29
150	NoCA-5	1.50	1.41	[311]	0.47	0.98	0.43
151	ZY-4Cl	1.82	1.59	[312-313]	0.52	1.25	0.34
A-A'-D-A'-A SMAs							
152	CDTBM	1.65	1.45	[314-315]	0.67	0.86	0.59
153	FBR	2.26	2.14	[316]	0.59	1.58	0.56
154	IDT-2BR	1.77	1.68	[317]	0.47	1.23	0.45
155	O-IDTBR EH-IDTBR	1.72	1.63 1.68	[318]	0.47	1.18 ~ 1.23	0.45
156	SFBRCN	2.23	2.05	[319]	0.41	1.67	0.38
157	BTA3	1.85	1.76	[320-321]	0.47	1.31	0.45
158	GS-ISO	1.96	1.75	[322]	0.57	1.24	0.51
159	MPU3	1.68	1.52	[193, 323]	0.68	0.90	0.61
160	ATT-1	1.68	1.54	[324]	0.53	1.05	0.49
161	ATT-2	1.45	1.32	[325]	0.48	0.88	0.44
162	NITI	1.61	1.49	[326]	0.43	1.09	0.40
163	ATT-9	1.40	1.15	[327]	0.33	0.89	0.26
164	NIDCS-MO NIDCS-HO	2.23	2.01 2.04	[328-329]	0.72	1.36 ~ 1.39	0.65
D-A copolymer acceptors							
165	PDI-V (2)	1.80	1.74	[330]	0.62	1.14	0.60
166	NDP-V (2)	1.97	1.91	[331]	0.46	1.46	0.45
167	PNDIT-HD (3)	2.04	1.85	[332]	0.27	1.61	0.24
168	PNDIS-HD (3)	1.86	1.65	[333]	0.30	1.38	0.27
169	N2200 (3) NOE10 (3)	1.45	1.45 1.46	[334-335]	0.01	1.44 ~ 1.45	0.01
170	f-BTI2-FT (2)	1.90	1.84	[336]	0.50	1.36	0.48
171	f-FBTI2-T (2)	1.77	1.74	[337]	0.48	1.27	0.47
172	DCNBT-IDT (2)	1.57	1.43	[338]	0.43	1.04	0.39
173	DCNBT-TPIC (2) DCNBT-TPC (2)	1.44	1.28 1.38	[339]	0.42 ~ 0.42	0.91 0.98	0.37 0.40
174	P-BN-IID (2)	1.65	1.63	[340]	0.70	0.94	0.69
175	BN-2fT (2)	1.64	1.61	[341]	0.46	1.16	0.45
176	PIID[2F]T (3)	1.71	1.71	[75]	0.63	1.08	0.63

Polymerized SMAs							
177	PZ1 (2)	1.55	1.55	[342]	0.45	1.10	0.45
178	PY-V-*γ* (2)	1.47	1.41	[343]	0.33	1.09	0.32
179	PY-IT (2) PY-DT (2)	1.46	1.39 1.42	[344-345]	0.36	1.05 ~ 1.08	0.34
180	PYF-T-*o* (2)	1.45	1.38	[346]	0.35	1.05	0.33
181	PZT-*γ* (2)	1.42	1.36	[347]	0.34	1.03	0.33
182	L15 (2)	1.46	1.38	[348]	0.36	1.04	0.34

Table S3. Four photovoltaic parameters (V_{OC}, J_{SC}, FF, and PCE) and the three chosen molecular properties (E_g, ΔE_{DA}, and ΔE_{ST}) for 165 fullerene-based OPVs. The LUMO energies of $PC_{61}BM$ and $PC_{71}BM$ adopt 3.91 eV, if not specified.[349]

No.	Donor:Acceptor	V_{OC} (V)	J_{SC} (mA cm^{-2})	FF (%)	PCE (%)	E_g (eV)	ΔE_{DA} (eV)	ΔE_{ST} (eV)	Ref.
1	P3HT:$PC_{61}BM$	0.64	11.3	69.3	5.2	1.91	1.15	0.55	[350-351]
2	P3HT:$IC_{60}BA$	0.84	10.6	72.7	6.5	1.91	1.00	0.55	[352]
3	PDHTT:$PC_{71}BM$	0.74	8.9	64.0	4.2	1.96	1.05	0.55	[16]
4	PDCBT:$PC_{71}BM$	0.91	11.0	72.0	7.2	1.90	0.91	0.56	[17, 351]
5	PDPP3T:$PC_{71}BM$	0.67	15.4	69.0	7.1	1.36	0.43	0.51	[22, 353]
6	PDPP2FT:$PC_{71}BM$	0.65	14.8	64.0	6.2	1.38	0.37	0.54	[24-25]
7	PDPPTPT:$PC_{71}BM$	0.80	13.8	67.0	7.5	1.54	0.44	0.61	[22, 26]
8	PDPP2T-TT:$PC_{71}BM$	0.67	20.1	70.0	9.4	1.39	0.48	0.51	[22, 354]
9	PDPPTPyT:$PC_{61}BM$	0.55	14.0	58.0	4.5	1.34	0.45	0.53	[28]
10	PDPPTDTPT:$PC_{71}BM$	0.43	20.5	54.0	4.8	1.23	0.48	0.45	[28]
11	PDPP-TNT:$PC_{71}BM$	0.76	11.8	52.0	4.7	1.57	0.61	0.65	[29]
12	PDTTDPP:$PC_{71}BM$	0.66	13.7	66.1	6.1	1.22	0.30	0.49	[30]
13	PDPP2T-DBT:$PC_{71}BM$	0.76	10.2	68.0	5.3	1.62	0.44	0.73	[22]
14	PDPP4T:$PC_{71}BM$	0.64	16.0	69.0	7.1	1.43	0.52	0.64	[22]
15	PDPP2T-BDT:$PC_{71}BM$	0.77	13.2	68.0	6.9	1.51	0.35	0.72	[22]
16	PBDTT-DPP:$PC_{71}BM$	0.73	14.0	65.0	6.6	1.44	0.37	0.67	[31]
17	PBDTP-DPP:$PC_{71}BM$	0.76	13.6	60.0	6.2	1.46	0.44	0.68	[31]
18	PBDTT-FDPP:$PC_{71}BM$	0.77	13.8	55.0	5.8	1.55	0.36	0.72	[31]
19	PBDTT-SeDPP:$PC_{71}BM$	0.69	16.8	62.0	7.2	1.38	0.30	0.67	[32]
20	DPPTT-T:$PC_{71}BM$	0.57	23.5	66.0	8.8	1.39	0.41	0.61	[34]
21	PDPP2PyT:$PC_{61}BM$	1.00	7.5	61.6	4.6	1.73	0.41	0.67	[35]
22	PDPP2Py2T:$PC_{61}BM$	0.98	11.3	64.4	7.1	1.70	0.44	0.64	[35]
23	PDPP2PyDTP:$PC_{71}BM$	0.71	12.6	56.0	5.0	1.54	0.45	0.55	[35]
24	PDPP2Py3T:$PC_{61}BM$	0.86	11.1	62.9	6.0	1.68	0.52	0.65	[35]
25	PBnDT-DTPyT:$PC_{61}BM$	0.85	12.8	58.2	6.3	1.51	0.47	0.39	[36]
26	PNDT-DTPyT:$PC_{61}BM$	0.71	14.2	61.7	6.2	1.53	0.49	0.40	[36]
27	PQDT-DTPyT:$PC_{61}BM$	0.75	13.5	55.1	5.6	1.56	0.47	0.43	[36]
28	POD2T-DTBT:$PC_{71}BM$	0.72	12.3	70.5	6.3	1.59	0.51	0.45	[37]
29	PTh_4FBT:$PC_{71}BM$	0.76	14.4	71.0	7.8	1.65	0.27	0.40	[38, 355]
30	PBT4T-2OD:$PC_{71}BM$	0.70	10.6	65.5	4.9	1.65	0.23	0.46	[40]
31	PffBT4T-C_9C_{13}:$PC_{71}BM$	0.79	20.2	74.0	11.7	1.65	0.41	0.42	[41-42]
32	PffBT-T3(1,2)-2:$PC_{71}BM$	0.82	18.9	68.8	10.7	1.63	0.42	0.38	[43]
33	PBTff4T-2OD:$PC_{71}BM$	0.77	18.2	74.0	10.4	1.63	0.53	0.45	[41]
34	PffBX4T-2DT:$PC_{71}BM$	0.88	15.8	66.0	9.1	1.66	0.25	0.45	[44]
35	PffBT2T-TT:$PC_{71}BM$	0.80	17.7	69.0	9.8	1.64	0.39	0.43	[45]
36	PBT4T-Cl:$PC_{71}BM$	0.80	18.7	74.6	11.2	1.67	0.26	0.43	[46]
37	PCBT4T-2OD:$PC_{71}BM$	0.73	16.2	69.0	8.2	1.59	0.27	0.41	[40]
38	PCCBT4T-2OD:$PC_{71}BM$	0.85	11.9	60.1	6.1	1.61	0.24	0.38	[40]
39	PPDTBT:$PC_{71}BM$	0.70	11.7	63.0	5.2	1.72	0.73	0.44	[47]
40	PPDTFBT:$PC_{71}BM$	0.73	13.3	69.0	6.6	1.72	0.67	0.43	[47]
41	PPDT2FBT:$PC_{71}BM$	0.79	16.3	73.0	9.4	1.76	0.61	0.42	[47]
42	PDTBTBz-0F:$PC_{71}BM$	0.94	11.0	71.0	7.3	1.97	0.60	0.47	[48]
43	PDTBTBz-2F_{syn}:$PC_{71}BM$	0.98	11.7	71.0	8.1	1.92	0.56	0.50	[48]
44	PDTBTBz-2F_{anti}:$PC_{71}BM$	0.97	14.0	72.0	9.8	1.90	0.51	0.50	[48]

45	PDTBTBz-4F:$PC_{71}BM$	1.03	6.3	63.0	4.1	1.97	0.48	0.51	[48]
46	PCPDTBT:$PC_{71}BM$	0.62	16.2	55.0	5.5	1.40	0.55	0.45	[49, 356]
47	PSBTBT:$PC_{61}BM$	0.58	14.9	61.0	5.2	1.52	0.64	0.49	[50, 357]
48	PBDT-BT:$PC_{71}BM$	0.92	15.4	66.0	9.4	1.75	0.65	0.45	[51]
49	PFDCTBT-C8:$PC_{71}BM$	0.83	12.6	66.8	7.0	1.71	0.40	0.52	[52]
50	PIDT-DFBT:$PC_{71}BM$	0.97	11.2	55.0	6.0	1.78	0.35	0.50	[53]
51	PIDTT-DFBT:$PC_{71}BM$	0.95	12.2	61.0	7.0	1.78	0.41	0.44	[53]
52	PITBT:$PC_{71}BM$	0.94	12.5	50.2	5.9	1.82	0.27	0.47	[54]
53	PITFBT:$PC_{71}BM$	0.90	15.4	65.9	9.1	1.79	0.23	0.43	[54]
54	PCDTBT:$PC_{71}BM$	0.87	11.0	67.0	6.4	1.88	0.40	0.57	[358]
55	HXS-1:$PC_{71}BM$	0.81	9.6	69.0	5.4	1.95	0.56	0.56	[56]
56	EI-PFDTBT:$PC_{71}BM$	0.85	11.0	54.0	5.1	1.86	0.30	0.58	[57]
57	PBnDT-DTffBT:$PC_{61}BM$	0.91	12.9	61.2	7.2	1.73	0.58	0.44	[58]
58	PBDT2FBT-2EHO:$PC_{71}BM$	0.86	15.4	61.6	8.2	1.83	0.77	0.43	[60]
59	$PBDT_{TEH}$-DT_{EH}BTff:$PC_{71}BM$	0.76	13.2	61.9	6.2	1.75	0.83	0.44	[61]
60	PBDTP-DTBT:$PC_{71}BM$	0.88	12.9	70.9	8.1	1.70	0.57	0.47	[62]
61	PBDTDTBT-R:$PC_{71}BM$	0.84	13.6	71.7	8.2	1.72	0.81	0.46	[64]
62	$PBDTDT_{ff}$BT-H:$PC_{71}BM$	0.88	14.9	71.9	9.4	1.76	0.80	0.46	[64]
63	PBDTTS-TTBT:$PC_{71}BM$	0.81	12.5	67.0	6.8	1.73	0.41	0.51	[65]
64	PBDTTS-TTDffBT:$PC_{71}BM$	0.85	15.4	72.0	9.4	1.76	0.43	0.45	[65]
65	PNDT-DTBT:$PC_{71}BM$	0.81	10.9	63.6	5.6	1.69	0.36	0.43	[66, 359]
66	PTFB-P:$PC_{71}BM$	0.81	12.9	72.0	7.4	1.97	0.58	0.53	[67]
67	PTFB-O:$PC_{71}BM$	0.83	13.1	59.0	6.4	2.00	0.55	0.54	[67]
68	PBnDT-HTAZ:$PC_{61}BM$	0.70	11.1	55.2	4.3	1.98	1.04	0.55	[69]
69	PBnDT-FTAZ:$PC_{61}BM$	0.78	13.3	70.5	7.3	2.00	0.86	0.52	[69, 360]
70	PBDTFBZO:$PC_{71}BM$	0.91	11.8	58.2	6.3	1.83	0.72	0.51	[70]
71	PBDTFBZS:$PC_{71}BM$	0.88	12.4	71.2	7.7	1.81	0.74	0.50	[70]
72	PSiBO:$PC_{71}BM$	0.86	10.9	62.3	5.9	1.66	0.36	0.55	[77]
73	PSiNO:$PC_{71}BM$	0.90	13.3	70.2	8.4	1.51	0.18	0.41	[77]
74	NT812:$PC_{71}BM$	0.72	19.1	72.9	10.3	1.50	0.51	0.39	[78]
75	PNTz4T:$PC_{71}BM$	0.71	19.4	73.4	10.1	1.54	0.31	0.37	[79, 361]
76	PNOz4T:$PC_{71}BM$	0.96	14.5	64.0	8.9	1.52	0.12	0.37	[79]
77	PNTz4TF2:$PC_{71}BM$	0.82	19.3	67.0	10.5	1.60	0.24	0.37	[79-80]
78	PNTz4TF4:$PC_{71}BM$	0.93	10.5	66.0	6.5	1.62	0.21	0.41	[79-80]
79	PNNT-12DT:$PC_{71}BM$	0.82	15.6	64.0	8.2	1.66	0.54	0.45	[81]
80	PTB3:$PC_{61}BM$	0.72	13.9	58.5	5.9	1.60	0.41	0.53	[83]
81	PBDTTT-C:$PC_{71}BM$	0.70	14.7	70.0	6.6	1.61	0.65	0.52	[84]
82	PBDTTT-E-T:$PC_{71}BM$	0.68	14.6	62.6	6.2	1.58	0.69	0.50	[85]
83	PBDTTT-C-T:$PC_{71}BM$	0.74	17.5	58.7	7.6	1.58	0.66	0.49	[85]
84	PTB7:$PC_{71}BM$	0.76	19.3	68.1	10.0	1.63	0.60	0.53	[362]
85	PTB7-Th:$PC_{71}BM$	0.83	17.4	73.8	10.6	1.58	0.46	0.49	[363]
86	PBDTTT-H:$PC_{71}BM$	0.80	17.4	67.5	9.4	1.68	0.68	0.54	[64]
87	PTAT-3:$PC_{61}BM$	0.66	15.0	58.0	5.6	1.60	0.63	0.53	[88]
88	PBT-1F:$PC_{71}BM$	0.60	14.3	65.7	5.6	1.65	0.79	0.56	[89]
89	PBT-3F:$PC_{71}BM$	0.78	15.2	72.4	8.6	1.64	0.61	0.57	[89]
90	PTBTz-2:$PC_{71}BM$	0.83	16.8	69.5	9.7	1.70	0.26	0.56	[90]
91	PTBTz-5:$PC_{71}BM$	0.82	13.1	64.3	6.9	1.73	0.40	0.60	[90]
92	PBDTDTTT-S-T:$PC_{71}BM$	0.69	16.4	66.3	7.5	1.64	0.70	0.60	[91]
93	PDT-S-T:$PC_{71}BM$	0.73	16.6	64.1	7.8	1.64	0.53	0.53	[92]
94	PTPD3T:$PC_{71}BM$	0.80	12.5	79.6	7.7	1.82	0.47	0.46	[93]
95	PT-ttTPD:$PC_{71}BM$	0.86	15.3	70.0	9.2	1.75	0.40	0.51	[94]

96	PBT-ttTPD:$PC_{71}BM$	0.78	10.6	62.0	5.1	1.72	0.48	0.46	[94]
97	PDTSTPD:$PC_{71}BM$	0.88	12.2	68.0	7.3	1.73	0.41	0.52	[95-96]
98	PDTG-TPD:$PC_{71}BM$	0.86	14.0	67.3	8.1	1.70	0.41	0.52	[96, 364]
99	PDTTG-TPD:$PC_{71}BM$	0.81	13.9	64.0	7.2	1.75	0.42	0.45	[98]
100	PBDTTPD:$PC_{71}BM$	0.97	12.6	70.0	8.5	1.80	0.16	0.48	[99, 365]
101	PT8:$PC_{71}BM$	1.00	9.8	63.0	6.2	1.85	0.44	0.48	[102]
102	PTP8:$PC_{71}BM$	0.96	11.0	58.5	6.2	1.78	0.38	0.47	[101]
103	PBDT-ttTPD:$PC_{71}BM$	0.82	10.3	72.0	6.1	1.90	0.53	0.47	[103]
104	PBDTT-ttTPD:$PC_{71}BM$	0.84	11.1	73.0	6.8	1.86	0.47	0.45	[103]
105	PBTI3T:$PC_{71}BM$	0.86	12.9	77.8	8.7	1.81	0.43	0.41	[93]
106	PBTISi-C8:$PC_{71}BM$	0.80	12.8	62.3	6.4	1.75	0.42	0.44	[106]
107	BTI-BDT:$PC_{71}BM$	0.92	9.6	62.0	5.5	1.92	0.48	0.48	[107]
108	TQ1:$PC_{71}BM$	0.91	12.2	64.0	7.1	1.70	0.50	0.45	[366]
109	PIDT-phanQ:$PC_{71}BM$	0.87	11.2	64.0	6.2	1.67	0.69	0.49	[9, 112]
110	PIDTDTQx:$PC_{71}BM$	0.87	12.3	70.2	7.5	1.81	0.68	0.45	[117]
111	PBDB-T:$PC_{71}BM$	0.85	12.8	68.2	7.5	1.80	0.73	0.47	[367]
112	PBT1-EH:$PC_{71}BM$	0.96	14.1	74.7	10.1	1.84	0.47	0.47	[119]
113	PBDF-T1:$PC_{71}BM$	0.92	13.3	77.4	9.4	1.83	0.37	0.48	[122]
114	PBT1-C:$PC_{71}BM$	0.93	13.1	78.9	9.7	1.84	0.45	0.51	[123]
115	PBT1-O:$PC_{71}BM$	0.88	11.1	72.7	7.1	1.82	0.51	0.51	[123]
116	PM6:$PC_{71}BM$	0.98	12.7	74.0	9.2	1.80	0.45	0.47	[124]
117	PDBT-T1:$PC_{71}BM$	0.92	14.1	75.0	9.7	1.85	0.48	0.47	[125]
118	P3TI:$PC_{71}BM$	0.72	14.6	66.0	6.9	1.50	0.30	0.52	[126, 368]
119	PiITVT:$PC_{61}BM$	0.91	13.2	59.0	7.1	1.61	0.30	0.52	[127]
120	P(IID-DTC):$PC_{71}BM$	0.78	15.2	69.0	8.2	1.61	0.46	0.70	[128]
121	P(IID2F-DTC):$PC_{71}BM$	0.87	12.4	70.0	7.6	1.59	0.26	0.63	[128]
122	PThTPTI:$PC_{71}BM$	0.87	13.7	65.6	7.8	1.86	0.54	0.48	[129]
123	PCPDTTTz:$PC_{71}BM$	0.75	12.2	59.0	5.4	1.76	0.43	0.52	[130]
124	PSEHTT:$PC_{71}BM$	0.67	13.2	64.0	5.6	1.82	0.70	0.51	[206]
125	BBTI-1:$PC_{71}BM$	0.80	16.5	63.0	8.3	1.48	0.40	0.45	[134]
126	D18:$PC_{71}BM$	0.94	11.8	70.3	7.8	1.98	0.45	0.48	[369-370]
127	PIPCP:$PC_{61}BM$	0.90	14.8	51.0	6.9	1.47	0.21	0.47	[145-146]
128	P3TEA:$PC_{71}BM$	0.90	12.4	69.6	7.7	1.66	0.35	0.46	[202]
129	PTO2:$PC_{71}BM$	1.00	8.1	62.0	5.0	2.03	0.32	0.53	[150]
130	$DPP(TBFu)_2$:$PC_{71}BM$	0.92	10.0	48.0	4.4	1.75	0.60	0.94	[151, 371]
131	$NDT(TDPP)_2$:$PC_{61}BM$	0.84	11.3	42.0	4.1	1.69	0.32	0.68	[153]
132	DPPEZnP-TBO:$PC_{61}BM$	0.73	19.6	63.4	9.1	1.37	0.10	0.46	[155]
133	CNDPP:$PC_{71}BM$	0.72	13.6	47.6	4.7	1.48	0.41	0.53	[157]
134	*p*-$DTS(PTTh_2)_2$:$PC_{71}BM$	0.78	14.4	59.3	6.7	1.50	0.58	0.45	[158-159]
135	*d*-$DTS(PTTh_2)_2$:$PC_{71}BM$	0.73	12.7	60.0	5.6	1.50	0.54	0.44	[159]
136	*p*-$DTS(FBTTh_2)_2$:$PC_{71}BM$	0.80	14.5	69.0	8.0	1.55	0.57	0.43	[372]
137	*p*-$SIDT(FBTTh_2)_2$:$PC_{71}BM$	0.91	11.0	65.0	6.4	1.84	0.55	0.46	[161]
138	X1:$PC_{61}BM$	0.71	13.6	60.0	5.8	1.44	0.57	0.35	[162]
139	X4:$PC_{61}BM$	0.75	12.6	61.0	5.7	1.40	0.56	0.35	[163]
140	X5:$PC_{61}BM$	0.72	12.7	60.0	5.5	1.43	0.59	0.36	[163]
141	BIT4F:$PC_{71}BM$	0.89	12.3	76.3	8.3	1.81	0.74	0.40	[165]
142	BIT6F:$PC_{71}BM$	0.89	13.4	75.2	8.9	1.79	0.74	0.37	[165]
143	DCAO7T:$PC_{61}BM$	0.86	10.7	55.0	5.1	1.74	0.62	0.38	[166-167]
144	T2:$PC_{71}BM$	0.85	7.4	71.6	4.5	1.77	0.44	0.36	[168]
145	T3:$PC_{71}BM$	0.85	10.8	67.1	6.2	1.72	0.42	0.34	[168]
146	DCAO3TBDT:$PC_{61}BM$	0.95	8.0	60.0	4.6	1.84	0.67	0.44	[169]

147	DR3TBDT:$PC_{71}BM$	0.93	12.2	65.0	7.4	1.74	0.64	0.42	[169]
148	DCAO3T(BDT)3T:$PC_{61}BM$	0.93	9.8	59.9	5.4	1.83	0.37	0.43	[167]
149	DR3TSBDT:$PC_{71}BM$	0.92	14.6	74.0	9.9	1.74	0.61	0.42	[174]
150	DR3TBDTT:$PC_{71}BM$	0.89	14.2	76.1	9.6	1.72	0.64	0.42	[373]
151	BDTT-S-TR:$PC_{71}BM$	0.97	13.5	70.5	9.2	1.73	0.66	0.41	[176]
152	BTR:$PC_{71}BM$	0.90	13.4	77.0	9.3	1.82	0.48	0.42	[177]
153	DRTB-T:$PC_{71}BM$	1.01	10.0	70.0	7.1	2.00	0.66	0.50	[374-375]
154	DERHD7T:$PC_{61}BM$	0.92	14.0	47.4	6.1	1.72	0.63	0.36	[187-188]
155	DRCN5T:$PC_{71}BM$	0.92	15.7	68.0	9.8	1.60	0.50	0.43	[189]
156	DRCN6T:$PC_{71}BM$	0.92	11.5	58.0	6.1	1.60	0.35	0.38	[189]
157	DRCN7T:$PC_{71}BM$	0.90	14.8	68.0	9.1	1.62	0.47	0.33	[189]
158	DRCN8T:$PC_{71}BM$	0.86	10.8	68.0	6.4	1.61	0.46	0.31	[189]
159	DRCN9T:$PC_{71}BM$	0.81	13.8	68.0	7.6	1.59	0.47	0.27	[189]
160	BTID-0F:$PC_{71}BM$	0.95	14.5	72.2	10.0	1.71	0.61	0.38	[190, 376]
161	BTID-1F:$PC_{71}BM$	0.94	15.3	72.0	10.4	1.70	0.53	0.36	[190]
162	BTID-2F:$PC_{71}BM$	0.95	15.7	76.0	11.3	1.68	0.44	0.37	[190]
163	M-1:$PC_{71}BM$	0.94	13.5	71.0	9.0	1.75	0.58	0.42	[192]
164	M-2:$PC_{71}BM$	0.92	13.3	70.0	8.6	1.76	0.57	0.35	[192]
165	CS1:$PC_{71}BM$	0.79	10.5	58.0	4.8	1.85	0.40	0.38	[193]

Table S4. Four photovoltaic parameters and the three chosen molecular properties for 350 NF OPVs.

No.	Donor:Acceptor	V_{OC} (V)	J_{SC} (mA cm^{-2})	FF (%)	PCE (%)	E_g (eV)	ΔE_{DA} (eV)	ΔE_{ST} (eV)	Ref.
1	P3HT:ZY-4Cl	0.90	17.1	66.0	10.2	1.59	0.54	0.34	[312-313]
2	P3HT:FBR	0.82	8.0	63.0	4.1	1.91	0.83	0.55	[316, 349]
3	P3HT:IDT-2BR	0.84	8.9	68.1	5.1	1.68	0.76	0.45	[317]
4	P3HT:O-IDTBR	0.72	13.9	60.0	6.3	1.63	0.68	0.45	[318]
5	P5TCN-F25:Y6	0.79	27.1	77.1	16.6	1.33	0.33	0.23	[14]
6	PDCBT:IDIC	0.81	11.3	64.1	6.3	1.62	0.37	0.47	[63]
7	PDCBT:ITIC	0.94	16.5	65.7	10.2	1.59	0.27	0.40	[351]
8	PDCBT-Cl:ITIC-Th1	0.94	18.3	70.0	12.1	1.55	0.40	0.36	[18, 377]
9	PTVT-T:*m*-BTP-PhC6	0.82	23.8	71.6	14.0	1.36	0.14	0.25	[19]
10	PffBT4T-2DT:di-PBI	0.84	11.4	53.0	5.1	1.65	0.25	0.42	[378]
11	PffBT4T-2DT:SF-PDI$_2$	0.98	10.7	57.0	6.0	1.65	0.12	0.42	[378]
12	PffBT4T-2DT:FBR	1.12	11.5	61.0	7.8	1.65	0.05	0.42	[379]
13	PffBT4T-2DT:O-IDTBR	1.07	15.0	62.0	10.0	1.63	0.16	0.45	[379]
14	PffBT2T-TT:O-IDTBR	1.08	14.7	64.0	10.1	1.63	0.03	0.45	[45]
15	PPDT2FBT:NIDCS-HO	1.03	11.9	63.0	7.6	1.76	0.08	0.42	[380]
16	PTFBDT-BZS:IDIC	0.91	17.3	70.8	11.0	1.62	0.26	0.47	[63]
17	PTFB-P:ITIC	0.92	12.8	65.0	7.6	1.59	0.31	0.40	[67, 221]
18	PTFB-O:ITIC	0.92	15.5	70.0	9.9	1.59	0.25	0.40	[67, 221]
19	PTFB-O:ITIC-Th	0.92	17.1	67.0	10.5	1.60	0.30	0.40	[67, 223]
20	PffT2-FTAZ-2DT:IEIC	1.00	12.2	59.0	7.2	1.50	0.17	0.39	[381]
21	PvBDTTAZ:O-IDTBR	1.08	16.3	63.6	11.2	1.63	0.04	0.45	[68]
22	PBnDT-FTAZ:IDIC	0.84	20.8	71.8	12.5	1.62	0.31	0.47	[382]
23	PBnDT-FTAZ:IT-M	0.95	16.8	66.1	10.6	1.60	0.22	0.41	[383]
24	PBnDT-FTAZ:ITIC-Th	0.92	15.8	61.3	8.9	1.60	0.28	0.40	[224]
25	PBnDT-FTAZ:ITIC-Th1	0.85	19.3	73.7	12.1	1.55	0.36	0.36	[224]
26	PBnDT-FTAZ:ITIC1	0.92	16.1	56.2	8.3	1.55	0.10	0.47	[235]
27	PBnDT-FTAZ:ITIC2	0.92	18.6	62.0	10.6	1.53	0.05	0.46	[235]
28	PBnDT-FTAZ:INIC	0.96	13.5	57.9	7.5	1.57	0.07	0.38	[243]
29	PBnDT-FTAZ:INIC1	0.93	16.6	64.3	9.9	1.56	0.16	0.38	[243]
30	PBnDT-FTAZ:INIC2	0.90	17.6	66.8	10.6	1.52	0.14	0.33	[243]
31	PBnDT-FTAZ:INIC3	0.86	19.4	67.4	11.2	1.48	0.14	0.29	[243]
32	PBnDT-FTAZ:IHIC2	0.78	15.7	61.2	7.5	1.66	0.31	0.42	[248]
33	PBnDT-FTAZ:IOIC2	0.90	19.7	69.3	12.3	1.55	0.03	0.40	[248]
34	J51:IDIC	0.80	12.2	66.0	6.9	1.62	0.49	0.47	[63]
35	J51:ITIC	0.82	16.5	69.0	9.3	1.59	0.22	0.40	[384]
36	J51:IDSe-T-IC	0.91	15.2	62.0	8.6	1.52	0.16	0.42	[264]
37	J51:N2200	0.83	14.2	70.2	8.3	1.45	0.51	0.01	[385]
38	J52:IEICO-4F	0.73	21.9	58.5	9.4	1.24	0.23	0.32	[265]
39	J52:i-IEICO-4F	0.85	22.9	67.9	13.2	1.56	0.41	0.09	[266]
40	J52:IEICO-4Cl	0.70	23.8	60.7	10.1	1.23	0.35	0.31	[72, 268]
41	J52:BN-0F	0.84	21.9	60.0	11.0	1.41	0.26	0.40	[275]
42	J52:BN-2F	0.81	25.3	70.8	14.5	1.40	0.30	0.38	[275]
43	J52:BN-4F	0.79	25.8	64.9	13.2	1.38	0.35	0.36	[275]
44	J52:NoCA-5	0.81	26.0	70.0	14.8	1.41	0.34	0.43	[311]
45	J52-2F:IT-M	0.97	17.8	71.0	12.2	1.60	0.22	0.41	[386]
46	J52-2F:ITCC	1.00	15.5	67.0	10.4	1.67	0.11	0.40	[386]
47	J52-2F:IT-4F	0.73	20.2	72.0	10.6	1.52	0.30	0.34	[386]

48	J52-2F:A4T-16	0.82	18.1	69.9	10.4	1.43	0.31	0.39	[76, 271]
49	J61:*m*-ITIC	0.91	18.3	70.6	11.8	1.58	0.20	0.38	[72, 220]
50	J61:BT-IC	0.87	16.4	67.1	9.4	1.43	0.10	0.38	[241]
51	J61:Y5	0.90	21.1	58.3	11.0	1.38	0.23	0.28	[116]
52	J71:ITIC	0.94	17.3	69.8	11.4	1.59	0.11	0.40	[73]
53	J71:ITCPTC	0.88	17.7	72.3	11.2	1.58	0.22	0.44	[227]
54	J71:MeIC	0.92	18.4	74.2	12.5	1.58	0.17	0.44	[227]
55	J71:ZITI	0.93	20.4	69.5	13.2	1.53	0.11	0.38	[252]
56	J91:*m*-ITIC	0.98	18.0	65.5	11.6	1.58	0.04	0.38	[74]
57	PBDT-TAZ:NOE10	0.84	12.9	75.0	8.1	1.46	0.46	0.01	[335]
58	PBFTAZ:PIID[2F]T	0.97	13.2	55.0	7.1	1.71	0.18	0.63	[75]
59	PTB7:Helical PDI 1	0.79	11.0	59.0	5.1	1.63	0.46	0.53	[199]
60	PTB7:SFBRCN	0.85	13.9	60.7	7.3	1.63	0.50	0.53	[319]
61	PBDTTT-E-T:IEIC	0.90	11.7	47.0	4.9	1.50	0.08	0.42	[263]
62	PBDTTT-E-T:IEICO	0.82	17.7	58.0	8.4	1.34	0.23	0.42	[263]
63	PBDTTT-E-T:DCNBT-TPIC	0.70	22.5	64.8	10.2	1.28	0.20	0.37	[339]
64	PBDTTT-E-T:DCNBT-TPC	0.73	19.4	65.8	9.3	1.38	0.23	0.40	[339]
65	PTB7-Th:di-PBI	0.80	12.0	59.0	5.9	1.58	0.23	0.49	[194]
66	PTB7-Th:Helical PDI 1	0.80	13.5	55.0	5.9	1.58	0.13	0.49	[199]
67	PTB7-Th:FPDI-T	0.93	12.0	58.0	6.5	1.58	0.04	0.49	[200]
68	PTB7-Th:FIDTT-2PDI	1.06	12.7	58.0	7.8	1.58	0.07	0.49	[203]
69	PTB7-Th:DBFI-EDOT	0.95	14.0	51.0	6.7	1.58	0.31	0.49	[206]
70	PTB7-Th:IDTT-T	1.02	18.0	65.0	11.8	1.58	0.29	0.49	[208]
71	PTB7-Th:6TBA	0.98	15.2	68.0	10.1	1.52	0.04	0.56	[210]
72	PTB7-Th:IDIC	0.81	10.9	56.1	5.2	1.58	0.49	0.49	[63]
73	PTB7-Th:ITIC	0.83	14.4	66.0	7.8	1.58	0.24	0.49	[208, 219]
74	PTB7-Th:ITIC-Th	0.80	15.9	68.0	8.7	1.58	0.37	0.49	[223]
75	PTB7-Th:ITIC3	0.76	16.8	63.1	8.1	1.55	0.34	0.38	[231]
76	PTB7-Th:BT-IC	0.81	17.5	59.6	8.3	1.43	0.10	0.38	[387]
77	PTB7-Th:FNIC1	0.77	19.8	65.1	10.0	1.48	0.39	0.38	[242]
78	PTB7-Th:FNIC2	0.73	23.8	72.7	12.7	1.38	0.34	0.33	[242]
79	PTB7-Th:AOIC	0.74	24.5	75.0	13.7	1.39	0.28	0.38	[250]
80	PTB7-Th:4TIC	0.78	18.8	72.0	10.4	1.40	0.08	0.50	[253-254]
81	PTB7-Th:F6IC	0.61	18.1	64.0	7.1	1.36	0.46	0.46	[255]
82	PTB7-Th:FOIC	0.74	24.0	67.1	12.0	1.32	0.16	0.42	[231]
83	PTB7-Th:F8IC	0.64	25.1	67.6	10.9	1.27	0.23	0.37	[255]
84	PTB7-Th:CO$_i$8DFIC	0.69	27.3	71.0	13.4	1.26	0.11	0.38	[388]
85	PTB7-Th:DTPC-DFIC	0.76	21.9	61.3	10.2	1.21	0.11	0.34	[262]
86	PTB7-Th:IEICO-4F	0.71	27.3	65.7	12.8	1.24	0.20	0.32	[265, 389]
87	PTB7-Th:IEICO-4Cl	0.73	22.8	62.0	10.3	1.23	0.34	0.31	[87, 268]
88	PTB7-Th:CTIC-4F	0.70	23.4	64.0	10.5	1.30	0.20	0.42	[276]
89	PTB7-Th:CO1-4F	0.64	24.8	64.0	10.2	1.20	0.10	0.43	[276]
90	PTB7-Th:COTIC-4F	0.57	20.7	61.0	7.3	1.10	0.00	0.43	[276]
91	PTB7-Th:BTPV-4F	0.65	28.3	65.9	12.1	1.21	0.12	0.28	[292]
92	PTB7-Th:CDTBM	0.67	12.7	62.0	5.6	1.45	0.47	0.59	[314-315]
93	PTB7-Th:EH-IDTBR	1.03	18.5	63.0	12.0	1.58	0.21	0.49	[390]
94	PTB7-Th:IDT-2BR	1.05	12.8	61.1	8.2	1.58	0.10	0.49	[391]
95	PTB7-Th:SFBRCN	0.90	17.3	65.2	10.1	1.58	0.31	0.49	[319]
96	PTB7-Th:ATT-1	0.87	16.5	70.0	10.0	1.54	0.20	0.49	[324]
97	PTB7-Th:ATT-2	0.73	20.8	63.0	9.6	1.32	0.30	0.44	[325]
98	PTB7-Th:ATT-9	0.66	30.0	67.2	13.4	1.15	0.15	0.26	[327]

99	PTB7-Th:PDI-V	0.74	15.4	64.0	7.4	1.58	0.24	0.49	[330-331]
100	PTB7-Th:NDP-V	0.74	17.1	67.0	8.6	1.58	0.24	0.49	[331]
101	PTB7-Th:N2200	0.79	13.0	55.6	5.7	1.45	0.55	0.01	[385, 392]
102	PTB7-Th:PNDIT-HD	0.79	13.5	56.0	6.0	1.58	0.15	0.49	[332]
103	PTB7-Th:f-BTI2-FT	1.04	11.6	57.0	6.9	1.58	0.40	0.49	[336]
104	PTB7-Th:f-FBTI2-T	1.05	13.6	56.5	8.1	1.58	0.43	0.49	[337]
105	PTB7-Th:P-BN-IID	0.92	11.4	48.0	5.0	1.58	0.36	0.64	[340]
106	PBDTT-FTTE:Ph(PDI)$_3$	0.85	14.3	48.6	5.9	1.62	0.40	0.49	[393-394]
107	PBDTTF-FTTE:Ph(PDI)$_3$	1.06	15.3	56.2	9.1	1.65	0.18	0.49	[393-394]
108	PTPD3T:ITIC	0.92	13.5	68.0	8.4	1.59	-0.03	0.40	[395]
109	PBDTTTPD:PNDIT-HD	1.06	11.2	56.0	6.6	1.45	0.15	0.48	[396]
110	PMOT40:IDIC	0.97	17.4	72.7	12.2	1.62	0.32	0.47	[104]
111	PMOT40:i-IEICO-4F	0.97	20.6	64.9	13.0	1.56	0.14	0.09	[104]
112	TPD-3:IT-4F	0.80	20.1	75.3	12.1	1.52	0.17	0.34	[105]
113	TPD-3F:IT-4F	0.92	21.6	72.3	14.4	1.52	0.04	0.34	[105]
114	PBTI3T:ITIC	0.93	11.2	54.9	5.7	1.59	0.02	0.40	[395]
115	PTQ10:IDIC	0.97	17.8	73.6	12.7	1.62	0.20	0.47	[109]
116	PTQ10:MO-IDIC	0.97	16.9	68.1	11.2	1.60	0.15	0.46	[216]
117	PTQ10:MO-IDIC-2F	0.91	19.9	74.8	13.5	1.55	0.26	0.40	[216]
118	PTQ10:MO-IDIC-Cl-2	0.88	19.2	73.9	12.5	1.54	0.25	0.41	[397]
119	PTQ10:HC-PCIC	0.94	16.0	68.0	10.4	1.48	0.00	0.33	[273]
120	PTQ10:Y6	0.83	26.6	79.6	17.5	1.33	0.11	0.23	[110, 398]
121	PTQ10:*m*-BTP-PhC6	0.88	25.3	79.3	17.7	1.36	0.06	0.25	[289]
122	PTQ10:BTP-Th	0.90	24.4	72.4	15.9	1.33	0.18	0.21	[290]
123	PTQ10:BTP-FTh	0.85	26.3	76.7	17.2	1.32	0.23	0.20	[290]
124	PTQ10:TPT10	0.92	17.3	58.2	9.2	1.36	-0.03	0.26	[111]
125	PTQ10:PY-IT	0.96	18.5	68.2	12.1	1.39	0.11	0.34	[399]
126	PTQ9:Y6	0.82	23.7	54.0	10.5	1.33	0.25	0.23	[110]
127	PTQ11:TPT10	0.88	24.8	74.8	16.3	1.36	0.00	0.26	[111]
128	PBQ-0F:ITIC	0.69	16.2	59.9	6.7	1.59	0.35	0.40	[113]
129	PBQ-QF:ITIC	0.83	17.2	62.5	8.9	1.59	0.19	0.40	[113]
130	PBQ-4F:ITIC	0.95	17.9	66.8	11.3	1.59	0.04	0.40	[113]
131	PBQ5:Y6	0.84	26.0	70.8	15.6	1.33	0.17	0.23	[115]
132	PBQ6:Y6	0.85	26.6	77.9	17.6	1.33	0.08	0.23	[115]
133	PBQ6:*m*-TEH	0.88	26.6	79.0	18.5	1.38	0.08	0.26	[291]
134	TTFQx-T1:Y5	0.89	21.2	69.6	13.1	1.38	0.23	0.28	[116]
135	PBDB-T:BFPTP	0.94	12.8	62.4	7.5	1.80	0.35	0.47	[201]
136	PBDB-T:IDT-T	1.05	11.8	59.8	7.4	1.80	0.18	0.51	[207]
137	PBDB-T:IDIC-C4Ph	0.82	18.1	77.4	11.5	1.62	0.42	0.47	[212]
138	PBDB-T:IDIC-PhC6	0.87	12.2	57.9	6.1	1.70	0.44	0.52	[212]
139	PBDB-T:IDT-2B	0.89	13.3	53.9	6.4	1.73	0.47	0.56	[214]
140	PBDB-T:IDT-OB	0.88	16.2	71.1	10.1	1.66	0.44	0.50	[214]
141	PBDB-T:IDT-2O	0.86	15.6	72.3	9.7	1.64	0.40	0.51	[214]
142	PBDB-T:ITIC	0.90	16.8	74.2	11.2	1.59	0.28	0.40	[221, 367]
143	PBDB-T:C8-ITIC	0.87	19.7	73.0	12.4	1.55	0.30	0.39	[120]
144	PBDB-T:IT-M	0.94	17.4	73.5	12.1	1.60	0.25	0.41	[221]
145	PBDB-T:IT-DM	0.97	16.5	70.6	11.3	1.63	0.23	0.43	[221]
146	PBDB-T:IDT6CN-M	0.92	16.0	76.1	11.2	1.63	0.35	0.47	[222]
147	PBDB-T:IDT8CN-M	0.92	17.1	78.9	12.4	1.58	0.27	0.41	[222]
148	PBDB-T:ITCC	1.01	15.9	71.0	11.4	1.67	0.25	0.40	[225]
149	PBDB-T:IDTCN	0.85	12.1	62.5	6.4	1.67	0.64	0.52	[226]

150	PBDB-T:IDT6CN	0.83	15.1	73.8	9.3	1.63	0.45	0.48	[226]
151	PBDB-T:IDT6CN-Th	0.81	16.8	76.7	10.4	1.61	0.48	0.43	[226]
152	PBDB-T:ITCPTC	0.84	17.5	72.8	10.7	1.58	0.38	0.44	[226]
153	PBDB-T:MeIC1	0.93	18.3	74.1	12.6	1.54	0.26	0.37	[229-230]
154	PBDB-T:IT-4F	0.71	20.1	70.7	10.1	1.52	0.33	0.34	[121, 400]
155	PBDB-T:NFBDT	0.87	17.9	67.2	10.4	1.55	0.07	0.47	[236]
156	PBDB-T:NCBDT	0.84	20.3	71.0	12.1	1.45	0.03	0.40	[237]
157	PBDB-T:BDCPDT-FIC	0.70	19.2	60.7	8.1	1.49	0.16	0.41	[238]
158	PBDB-T:BDCPDT-TTC	0.94	17.7	61.8	10.3	1.58	0.02	0.30	[238]
159	PBDB-T:NNBDT	0.86	20.1	69.7	12.0	1.43	0.20	0.41	[239-240]
160	PBDB-T:INPIC	0.96	8.6	52.5	4.3	1.46	0.15	0.40	[246]
161	PBDB-T:INPIC-4F	0.85	21.6	71.5	13.1	1.39	0.21	0.34	[246, 401]
162	PBDB-T:IPIC-4Cl	0.81	22.2	74.0	13.4	1.32	0.18	0.30	[247]
163	PBDB-T:DICTF	0.93	10.3	59.0	5.7	1.82	0.34	0.41	[251]
164	PBDB-T:FDICTF	0.94	15.8	66.0	9.8	1.63	0.10	0.39	[251]
165	PBDB-T:ZITI	0.89	19.8	74.0	13.0	1.53	0.21	0.38	[252]
166	PBDB-T:4TIC	0.76	19.8	64.8	9.7	1.40	0.13	0.50	[402-403]
167	PBDB-T:6TIC	0.81	23.5	65.4	12.5	1.37	0.06	0.45	[402-403]
168	PBDB-T:IDTT2F	0.81	18.5	59.0	8.9	1.46	0.24	0.33	[267]
169	PBDB-T:IDTOT2F	0.85	20.9	72.0	12.8	1.44	0.21	0.33	[267]
170	PBDB-T:IEICO-4Cl	0.74	20.8	62.5	9.7	1.23	0.23	0.31	[268]
171	PBDB-T:*o*-4TBC-2F	0.76	20.5	65.7	10.3	1.34	0.40	0.35	[270]
172	PBDB-T:A4T-16	0.74	20.9	64.3	9.9	1.43	0.34	0.39	[271]
173	PBDB-T:DF-PCIC	0.91	15.7	72.0	10.1	1.59	0.16	0.42	[272]
174	PBDB-T:HC-PCIC	0.73	17.5	69.1	9.0	1.48	0.21	0.33	[273]
175	PBDB-T:DOC2C6-IC	0.93	18.9	63.3	11.1	1.44	0.05	0.39	[274]
176	PBDB-T:DOC2C6-2F	0.85	21.4	73.2	13.2	1.42	0.16	0.38	[274]
177	PBDB-T:Y1	0.87	22.4	69.1	13.4	1.36	0.06	0.31	[278]
178	PBDB-T:Y2	0.82	23.6	69.4	13.4	1.34	0.04	0.31	[278]
179	PBDB-T:Y1-4F	0.74	22.7	57.4	9.6	1.31	0.17	0.26	[280]
180	PBDB-T:Y5	0.88	22.8	70.2	14.1	1.38	0.17	0.28	[116]
181	PBDB-T:Y6	0.72	25.0	62.0	10.8	1.33	0.32	0.23	[280]
182	PBDB-T:SFBRCN	0.97	13.7	70.9	9.4	1.80	0.60	0.47	[404]
183	PBDB-T:BTA3	1.16	10.0	59.8	7.0	1.76	0.23	0.45	[320]
184	PBDB-T:NITI	0.86	20.7	71.0	12.7	1.49	0.35	0.40	[326]
185	PBDB-T:N2200	0.90	15.3	68.7	9.5	1.45	0.44	0.01	[405-406]
186	PBDB-T:DCNBT-IDT	0.90	14.2	65.0	8.3	1.43	0.26	0.39	[338]
187	PBDB-T:BN-2fT	0.93	13.0	69.8	8.4	1.61	0.38	0.45	[341]
188	PBDB-T:PZ1	0.83	16.1	69.0	9.2	1.55	0.31	0.45	[342]
189	PBDB-T:PZT-γ	0.90	24.7	71.3	15.8	1.36	0.27	0.33	[347]
190	PBT1-EH:ITIC-Th	0.97	15.5	68.1	10.3	1.60	0.19	0.40	[119]
191	PFBDB-T:ITIC	0.95	18.5	66.0	11.7	1.59	0.17	0.40	[120]
192	PFBDB-T:C8-ITIC	0.94	19.6	72.0	13.2	1.55	0.16	0.39	[120]
193	PCl(4)BDB-T:IT-4F	0.84	20.6	71.1	12.3	1.52	0.24	0.34	[121]
194	PBT1-C:ITCPTC	0.94	17.0	78.0	12.5	1.58	0.19	0.44	[123]
195	PBT1-C:IT-2Cl	0.86	18.0	70.3	10.9	1.55	0.27	0.37	[407]
196	PBT1-C:BTA3	1.21	10.9	56.5	8.1	1.76	0.10	0.45	[320]
197	PBT1-O:ITCPTC	0.91	12.6	64.0	7.3	1.58	0.32	0.44	[123]
198	PM6:IDIC	0.97	17.8	69.0	11.9	1.62	0.15	0.47	[408]
199	PM6:IDIC-C4Ph	0.94	19.1	78.3	14.0	1.62	0.22	0.47	[212]
200	PM6:IDTI	0.99	13.0	57.0	7.4	1.70	0.33	0.52	[213]

201	PM6:IDTN	0.95	16.6	78.0	12.2	1.59	0.31	0.46	[213]
202	PM6:IDIC-4F	0.84	13.4	61.0	6.9	1.64	0.36	0.48	[215]
203	PM6:SiOTIC	0.92	14.5	74.9	10.0	1.55	0.07	0.39	[218]
204	PM6:ITIC	1.00	16.4	65.0	10.8	1.59	0.18	0.40	[409-410]
205	PM6:IT-M	1.02	15.8	65.0	10.5	1.60	0.16	0.41	[410-411]
206	PM6:ITCPTC	0.97	17.1	74.3	12.3	1.58	0.12	0.44	[412]
207	PM6:MeIC	0.99	18.5	71.1	13.0	1.58	0.07	0.44	[412]
208	PM6:IT-4F	0.87	20.7	80.8	14.6	1.52	0.24	0.34	[410, 413]
209	PM6:IT-2Cl	0.92	19.1	74.8	13.2	1.55	0.23	0.37	[233]
210	PM6:IT-4Cl	0.79	22.7	75.2	13.5	1.48	0.30	0.34	[233]
211	PM6:SeTIC	0.95	15.5	51.0	7.5	1.58	0.10	0.44	[234]
212	PM6:SeTIC4Cl	0.78	22.9	75.0	13.3	1.44	0.20	0.33	[234]
213	PM6:3TP3T-IC	1.05	13.0	65.6	8.9	1.63	0.02	0.44	[244]
214	PM6:3TP3T-4F	0.92	20.3	73.9	13.7	1.50	0.13	0.31	[244]
215	PM6:NOIC	0.88	17.7	70.3	11.0	1.55	0.31	0.33	[249, 297]
216	PM6:NOIC1	0.86	21.1	66.9	12.2	1.38	-0.04	0.29	[249]
217	PM6:NOIC2	0.92	20.2	73.4	13.6	1.49	0.19	0.32	[249]
218	PM6:NOIC3	0.93	12.6	58.4	6.8	1.62	0.38	0.30	[249]
219	PM6:NOIC4	0.93	16.6	62.2	9.6	1.55	0.19	0.31	[249]
220	PM6:M3	0.91	24.0	76.2	16.7	1.41	0.10	0.27	[260]
221	PM6:M8	0.83	8.4	60.6	4.2	1.28	-0.01	0.29	[261]
222	PM6:PTIC	0.93	16.7	66.0	10.3	1.53	0.12	0.36	[215]
223	PM6:PTB4F	0.94	14.6	51.5	7.0	1.65	0.39	0.44	[269]
224	PM6:PTB4Cl	0.93	19.0	72.2	12.8	1.58	0.43	0.39	[269]
225	PM6:A4T-16	0.88	21.8	79.8	15.2	1.43	0.22	0.39	[271]
226	PM6:HC-PCIC	0.89	18.1	72.1	11.8	1.48	0.06	0.33	[273]
227	PM6:BZ4F-O-3	0.85	23.5	73.7	14.7	1.40	0.18	0.38	[277]
228	PM6:Y1	0.92	12.9	55.5	6.6	1.36	-0.05	0.31	[280]
229	PM6:Y11	0.83	26.7	74.3	16.5	1.31	0.17	0.26	[279]
230	PM6:Y1-4F	0.83	25.2	68.5	14.4	1.31	0.06	0.26	[280]
231	PM6:mBzS-4F	0.80	27.7	76.4	17.0	1.25	0.04	0.24	[281]
232	PM6:BTP-M	0.98	8.4	51.8	4.3	1.42	0.00	0.31	[282]
233	PM6:L8-BO-F	0.93	23.9	77.7	17.2	1.41	0.07	0.31	[414]
234	PM6:Y6-F	0.90	24.1	75.0	16.2	1.36	0.15	0.26	[285]
235	PM6:Y6	0.85	27.6	75.5	17.7	1.33	0.20	0.23	[297, 415]
236	PM6:L8-BO	0.87	25.7	81.5	18.3	1.40	0.19	0.30	[287]
237	PM6:CH1007	0.82	28.2	77.8	18.0	1.30	0.04	0.26	[294, 416]
238	PM6:BTP-2ThCl	0.89	23.5	69.8	14.5	1.35	0.22	0.29	[296-297]
239	PM6:BTP-2F-ThCl	0.87	25.4	77.4	17.1	1.34	0.25	0.26	[296-297]
240	PM6:LY-Cl-2	0.88	24.2	70.9	15.2	1.36	0.16	0.28	[397]
241	PM6:L8-BO-Cl	0.92	24.5	78.5	17.7	1.39	0.06	0.31	[284]
242	PM6:BTP-eC9	0.84	26.2	81.1	17.8	1.30	0.23	0.23	[297-298]
243	PM6:Y-BO-FCl	0.85	26.5	77.9	17.5	1.33	0.24	0.24	[299]
244	PM6:A-WSSe-Cl	0.85	26.6	77.5	17.5	1.33	0.13	0.28	[300]
245	PM6:S-WSeSe-Cl	0.83	26.4	73.4	16.0	1.30	0.09	0.26	[300]
246	PM6:BTP-S1	0.93	22.4	72.7	15.2	1.43	0.07	0.32	[301]
247	PM6:BTP-S2	0.95	24.1	72.0	16.4	1.41	0.17	0.32	[301]
248	PM6:BTP-S7	0.86	25.9	75.1	16.8	1.33	0.04	0.27	[302]
249	PM6:BTP-S9	0.85	26.5	78.4	17.6	1.32	0.15	0.25	[302]
250	PM6:BO-5Cl	0.96	22.6	70.1	15.0	1.42	0.12	0.33	[304]
251	PM6:BTIC-2Cl-γCF_3	0.84	25.1	77.0	16.3	1.31	0.10	0.24	[305]

252	PM6:BTP-H2	0.93	25.3	78.5	18.5	1.39	0.04	0.29	[284]
253	PM6:AQx-1	0.89	22.2	67.1	13.3	1.37	0.02	0.30	[307]
254	PM6:AQx-2	0.86	25.4	76.3	16.6	1.35	0.05	0.23	[307]
255	PM6:CH4	0.89	26.1	71.1	16.5	1.37	0.18	0.31	[308]
256	PM6:CH6	0.88	26.6	78.4	18.3	1.40	0.22	0.31	[308]
257	PM6:CH-4Cl	0.87	26.5	76.7	17.7	1.39	0.28	0.32	[309]
258	PM6:CH-6Cl	0.87	26.1	76.3	17.2	1.36	0.33	0.29	[309]
259	PM6:Qx-1	0.91	26.1	75.5	17.9	1.36	0.06	0.28	[310]
260	PM6:Qx-2	0.93	26.5	73.7	18.2	1.36	0.02	0.29	[310]
261	PM6:GS-ISO	1.21	13.7	70.4	11.6	1.75	0.06	0.51	[297, 322]
262	PM6:PZ1	0.96	17.1	68.2	11.2	1.55	0.24	0.45	[417-418]
263	PM6:PY-V-*γ*	0.91	24.8	75.8	17.1	1.41	0.12	0.32	[343]
264	PM6:PY-IT	0.94	22.8	74.1	15.8	1.39	0.23	0.34	[141, 344]
265	PM6:PY-DT	0.95	23.7	74.4	16.8	1.42	0.26	0.34	[345]
266	PM6:PYF-T-*o*	0.90	23.3	72.4	15.2	1.38	0.21	0.33	[346]
267	PM6:L15	0.95	22.2	71.9	15.2	1.38	0.30	0.34	[348]
268	PBDB-T-SF:IT-4F	0.88	20.9	71.3	13.1	1.52	0.26	0.34	[232]
269	PBDB-T-SF:INIC	1.05	9.9	49.0	5.1	1.57	0.08	0.38	[245]
270	PBDB-T-SF:FINIC	0.87	22.0	73.0	14.0	1.51	0.18	0.30	[245]
271	PBN-S:IT-4F	0.89	21.0	69.9	13.1	1.52	0.18	0.34	[419]
272	PBTT-F:Y6	0.84	24.8	77.1	16.1	1.33	0.17	0.23	[420]
273	PM7:IT-4F	0.86	21.8	77.0	14.4	1.52	0.21	0.34	[410, 421]
274	PM7:A4T-16	0.91	20.8	74.0	14.0	1.43	0.16	0.39	[271]
275	PM7:Y6	0.88	25.6	73.3	16.6	1.33	0.08	0.23	[422-423]
276	PDBT-T1:SdiPBI-S	0.90	12.0	66.1	7.2	1.85	0.42	0.47	[196]
277	PDBT-T1:SdiPBI-Se	0.95	12.5	69.7	8.2	1.85	0.44	0.47	[197]
278	PDBT-T1:TPH-Se	1.00	12.5	71.7	9.0	1.85	0.37	0.47	[394, 424]
279	PDBT-T1:IDIC	0.83	17.0	73.2	10.4	1.62	0.33	0.47	[63]
280	PDBT-T1:ITIC-Th	0.88	16.2	67.1	9.6	1.60	0.30	0.40	[223]
281	PBNT-BDD:Y6-BO	0.88	25.4	72.0	16.1	1.33	0.27	0.23	[425]
282	PSEHTT:DBFI-T	0.86	10.1	58.0	5.0	1.73	0.30	0.44	[131]
283	PSEHTT:DBFI-DMT	0.92	12.6	55.0	6.4	1.82	0.36	0.51	[205]
284	PSEHTT:DBFI-EDOT	0.93	13.8	63.0	8.1	1.70	0.35	0.39	[206]
285	PSEHTT:PNDIS-HD	0.76	10.5	60.0	4.8	1.65	0.55	0.34	[426]
286	PBDTS-TDZ:ITIC	1.10	17.8	65.4	12.8	1.59	0.09	0.40	[132]
287	PBDT-TDZ:ITIC	1.01	17.2	67.7	11.7	1.59	0.13	0.40	[132]
288	PBDT-ODZ:ITIC-Th	1.06	17.1	68.1	12.3	1.60	0.10	0.40	[133]
289	Pt10-PSFTZ:Y6	0.81	26.5	76.3	16.4	1.33	0.07	0.23	[427]
290	PTzBI:ITIC	0.87	18.3	64.3	10.2	1.59	0.17	0.40	[136]
291	PTzBI-DT:ITIC	0.91	16.8	61.5	9.4	1.59	0.12	0.40	[136]
292	PTzBI-*d*F:Y6	0.85	26.3	75.5	16.8	1.33	0.13	0.23	[137]
293	PTzBI-Si:N2200	0.88	17.6	75.8	11.8	1.45	0.43	0.01	[428]
294	P2F-EHp:IT-4F	0.89	19.7	74.1	13.0	1.52	0.26	0.34	[138]
295	P2F-EHp:Y6	0.81	26.7	74.1	16.0	1.33	0.22	0.23	[429-430]
296	D18:Y6	0.86	27.7	76.6	18.2	1.33	0.14	0.23	[139, 293]
297	D18:L8-BO	0.92	26.9	77.3	19.1	1.40	0.17	0.30	[287, 431]
298	D18:Y6Se	0.84	28.0	75.3	17.7	1.32	0.19	0.24	[293]
299	D18:BO-4Cl	0.86	26.3	77.7	17.6	1.30	0.03	0.25	[432]
300	D18-Cl:BTF	0.86	26.9	74.6	17.3	1.31	0.20	0.28	[306]
301	D18-Cl:BTFM	0.88	26.7	73.1	17.1	1.33	0.23	0.29	[306]
302	PBQx-TCl:BTP-eC9	0.82	26.0	75.2	16.0	1.30	0.13	0.23	[140]

303	PBQx-TCl:BTA3	1.24	13.3	74.2	12.2	1.77	0.03	0.45	[140]
304	PQM-Cl:PY-IT	0.92	24.3	80.7	18.0	1.39	0.40	0.34	[141]
305	pBDTT-DPI-Me:Y6	0.83	27.4	72.6	16.6	1.33	0.13	0.23	[142]
306	PNTB6-Cl:N3	0.86	26.6	77.3	17.6	1.32	0.27	0.22	[414]
307	PTZ1:IDIC	0.92	16.4	76.2	11.5	1.62	0.38	0.47	[144]
308	PB2:BTP-eC9	0.86	26.2	78.4	17.7	1.30	0.16	0.23	[433]
309	P3TEA:SF-PDI_2	1.11	13.3	64.3	9.5	1.66	0.05	0.46	[147]
310	P3TEA:FTTB-PDI4	1.13	13.9	65.9	10.4	1.66	0.02	0.46	[202]
311	PDTB-EF-T:IT-4F	0.90	20.7	76.0	14.2	1.52	0.16	0.34	[148]
312	PB3T:IT-M	1.00	18.9	63.0	11.9	1.60	0.19	0.41	[149]
313	PTO2:IT-4F	0.91	21.5	75.0	14.7	1.52	0.07	0.34	[150]
314	PTO2:A4T-16	0.95	18.7	66.5	11.8	1.43	0.08	0.39	[271]
315	PBCT-2F:Y6	0.85	27.2	74.3	17.1	1.33	0.15	0.23	[434]
316	SZ3:N3	0.84	25.6	77.7	16.7	1.32	0.28	0.22	[435]
317	SZ4:N3	0.85	26.0	77.4	17.1	1.32	0.21	0.22	[435]
318	SZ5:BPF-4F	0.85	22.1	67.4	12.6	1.36	0.08	0.30	[295]
319	SZ5:BPT-4F	0.85	24.8	79.1	16.8	1.36	0.09	0.26	[295]
320	SZ5:BPS-4F	0.82	25.4	77.9	16.3	1.29	0.04	0.23	[295]
321	PBDB-TF-T1:IT-4F	0.90	21.5	78.0	15.1	1.52	0.21	0.34	[436]
322	DPPEZnP-TBO:4TIC	0.73	17.2	59.4	7.5	1.37	0.25	0.47	[403]
323	DPPEZnP-TBO:6TIC	0.80	20.4	73.9	12.1	1.37	0.21	0.46	[258]
324	*p*-DTS($FBTTh_2$)$_2$:NIDCS-MO	0.85	9.6	64.0	5.3	1.55	0.32	0.43	[328]
325	SM1:Y6	0.81	23.6	67.0	12.7	1.33	0.40	0.23	[171]
326	SM1-F:Y6	0.87	23.3	69.9	14.1	1.33	0.28	0.23	[171]
327	BTEC-2F:Y6	0.85	21.6	72.4	13.3	1.33	0.26	0.23	[437]
328	H31:Y6	0.83	23.0	71.0	13.6	1.33	0.33	0.23	[173]
329	H21:IDIC	0.90	13.0	65.6	7.6	1.62	0.27	0.47	[172]
330	H22:IDIC	0.94	15.4	71.2	10.3	1.62	0.26	0.47	[172]
331	BTR:Y6	0.85	22.3	56.4	10.7	1.33	0.31	0.23	[178]
332	BTR:NITI	0.95	15.0	48.7	6.8	1.40	0.34	0.40	[438]
333	BTR-Cl:Y6	0.83	23.7	74.7	14.7	1.33	0.19	0.23	[178, 439]
334	BSFTR:Y6	0.85	23.2	69.7	13.7	1.33	0.11	0.23	[179]
335	B1:BTP-eC9	0.83	25.0	75.4	15.7	1.30	0.27	0.25	[440]
336	BM-Cl:BO-4Cl	0.83	25.9	73.6	15.7	1.30	0.38	0.25	[180]
337	L2:Y6	0.83	26.4	72.1	15.8	1.33	0.32	0.23	[181]
338	ZR1:IDIC-4Cl	0.78	18.3	68.0	9.6	1.53	0.57	0.40	[183]
339	ZR1:Y6	0.86	24.3	68.4	14.3	1.33	0.40	0.23	[183]
340	ZR-SiO-EH:Y6	0.87	25.6	73.7	16.4	1.33	0.25	0.23	[184]
341	M-PhS:BTP-eC9	0.84	25.4	75.6	16.2	1.30	0.30	0.23	[185]
342	SM-CA:N3	0.84	24.3	75.6	15.4	1.32	0.25	0.22	[441]
343	SM-CA-Reh:N3	0.84	25.1	77.5	16.3	1.32	0.13	0.22	[441]
344	SM-CA-ID:N3	0.82	22.0	45.5	8.2	1.32	0.32	0.22	[441]
345	DRTB-T:IDIC	0.98	14.3	65.0	9.1	1.62	0.18	0.47	[186]
346	DRTB-T:Y6	0.90	10.9	42.0	4.1	1.33	0.01	0.23	[442]
347	H11:IDIC	0.98	15.2	65.5	9.7	1.62	0.34	0.47	[191]
348	H12:IDIC	0.96	10.5	54.9	5.5	1.62	0.37	0.47	[191]
349	CS1:MPU3	1.07	13.0	56.0	7.8	1.52	0.29	0.61	[193]
350	D1:A1	0.76	14.4	65.7	7.2	1.37	0.25	0.46	[156]

Table S5. Pearson's correlation coefficients (r) for predicting V_{OC}, J_{SC}, FF, and PCE by three different ML algorithms (LR, KNN, and GBRT) with the two cross validations. The hyperparameters of KNN (n_neighbors = 10) and GBRT (max_depth = 3; learning_rate = 0.04) were optimized based on the PCE predictions by combining the three descriptors.

		V_{OC}		J_{SC}		FF		PCE	
		LOO	**5-fold**	**LOO**	**5-fold**	**LOO**	**5-fold**	**LOO**	**5-fold**
E_g	LR	0.315	0.320	0.773	0.774	0.151	0.156	0.582	0.584
	KNN	0.331	0.318	0.805	0.802	0.220	0.182	0.633	0.625
	GBRT	**0.357**	**0.362**	**0.803**	**0.796**	**0.253**	**0.238**	**0.647**	**0.641**
ΔE_{DA}	LR	0.303	0.303	0.464	0.466	0.082	0.096	0.499	0.500
	KNN	0.204	0.177	0.458	0.470	0.107	0.133	0.503	0.518
	GBRT	**0.242**	**0.231**	**0.484**	**0.489**	**0.172**	**0.159**	**0.534**	**0.536**
ΔE_{ST}	LR	-0.090	-0.080	0.630	0.634	0.361	0.363	0.632	0.635
	KNN	0.139	0.192	0.715	0.721	0.324	0.315	0.690	0.697
	GBRT	**0.172**	**0.182**	**0.739**	**0.747**	**0.351**	**0.357**	**0.717**	**0.720**
E_g $+\Delta E_{DA}$	LR	0.673	0.673	0.773	0.774	0.142	0.150	0.619	0.621
	KNN	0.695	0.686	0.821	0.825	0.344	0.331	0.711	0.715
	GBRT	**0.704**	**0.703**	**0.837**	**0.841**	**0.353**	**0.358**	**0.749**	**0.743**
E_g $+\Delta E_{ST}$	LR	0.407	0.408	0.806	0.808	0.360	0.362	0.686	0.689
	KNN	0.493	0.499	0.822	0.828	0.374	0.360	0.747	0.751
	GBRT	**0.536**	**0.512**	**0.844**	**0.845**	**0.405**	**0.395**	**0.770**	**0.764**
ΔE_{DA} $+\Delta E_{ST}$	LR	0.314	0.303	0.674	0.677	0.358	0.361	0.689	0.694
	KNN	0.370	0.363	0.770	0.781	0.371	0.375	0.759	0.770
	GBRT	**0.392**	**0.389**	**0.786**	**0.790**	**0.407**	**0.423**	**0.777**	**0.784**
E_g $+\Delta E_{DA}$ $+\Delta E_{ST}$	LR	0.702	0.702	0.805	0.808	0.356	0.357	0.708	0.712
	KNN	0.717	0.722	0.851	0.854	0.428	0.411	0.790	0.789
	GBRT	**0.746**	**0.740**	**0.866**	**0.868**	**0.435**	**0.436**	**0.807**	**0.806**

Table S6. Pearson's correlation coefficients (r) for predicting V_{OC}, J_{SC}, FF, and PCE by GBRT with the combination of the three descriptors of E_g, ΔE_{DA}, and ΔE_{ST}.

	V_{OC}	J_{SC}	FF	PCE
Training set (460)	0.731	0.865	0.420	0.804
Testing set (55)	0.731	0.859	0.487	0.794
All data points (515)	0.746	0.866	0.435	0.807

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