Supporting Information

Unraveling Correlations Between Molecular Properties and Device Parameters of Organic Solar Cells Using Machine Learning

Harikrishna Sahu* and Haibo Ma*

Key Laboratory of Mesoscopic Chemistry of MOE, School of Chemistry and Chemical Engineering, Nanjing University, Nanjing 210023, China

E-mail: harikrishnasahu89@gmail.com; haibo@nju.edu.cn

List of Figures

List of Tables

Table S1: Experimental open-circuit voltage (V_{OC}), short circuit current (J_{SC}), fill factor (FF), and power conversion of efficiency (PCE) for 300 SM-OPVs reported in the literature. N^{D}_{atom}, E_H and E_L represent the number of unsaturated atoms in the main conjugation path, energy of the highest occupied molecular orbital (HOMO) and energy of the lowest unoccupied molecular orbital (LUMO) of donor molecules. E_H and E_L of $PC_{71}BM$ ($PC_{61}BM$) are -6.69 (-6.90) and -2.54 (-2.60) eV, respectively.

S No.	Acceptor	V_{OC} (V)	J_{SC} (mA/cm^2)	FF	PCE (%)	N^{D}_{atom}	E_H	E_L	Ref.
1	$PC_{71}BM$	0.89	15.7	0.72	9.84	130	-5.94	-2.39	1
2	$PC_{71}BM$	0.93	14.1	0.75	9.54	68	-6.20	-2.05	2
3	$PC_{71}BM$	0.92	15.5	0.68	9.45	130	-6.02	-2.40	1
4	$PC_{71}BM$	0.89	14.2	0.76	9.36	68	-6.12	-2.01	3
5	$PC_{71}BM$	0.93	14.2	0.70	9.09	54	-6.14	-2.31	4
6	$PC_{71}BM$	0.91	14.9	0.69	9.05	59	-6.26	-2.27	5
7	$PC_{71}BM$	0.97	13.5	0.71	9.01	68	-6.23	-2.07	6
8	$PC_{61}BM$	0.80	16.8	0.68	9.00	86	-5.83	-2.44	7
9	$PC_{71}BM$	0.87	14.3	0.72	8.95	99	-5.83	-2.11	8
10	$PC_{71}BM$	0.89	13.4	0.75	8.91	99	-5.84	-2.10	9
11	$PC_{71}BM$	0.89	13.6	0.74	8.90	68	-6.10	-2.02	10
12	$PC_{71}BM$	0.84	14.6	0.74	8.85	99	-5.77	-2.05	11
13	$PC_{71}BM$	0.89	13.1	0.75	8.54	64	-5.89	-2.07	12
14	$PC_{71}BM$	0.91	12.9	0.71	8.50	74	-6.12	-2.03	13
15	$PC_{61}BM$	0.65	19.0	0.66	8.34	114	-5.69	-2.47	14
16	$PC_{71}BM$	0.98	12.5	0.68	8.34	62	-5.88	-2.06	15
17	$PC_{71}BM$	0.99	14.1	0.61	8.33	68	-6.24	-2.05	16
18	$PC_{71}BM$	0.89	12.3	0.76	8.27	64	-5.89	-2.07	9
19	$PC_{71}BM$	0.94	12.6	0.70	8.26	58	-6.16	-2.02	17
20	$PC_{71}BM$	0.87	13.4	0.72	8.24	64	-5.87	-2.10	12
21	$PC_{71}BM$	0.89	12.6	0.73	8.23	90	-6.02	-1.97	18

22	$PC_{71}BM$	0.82	14.3	0.70	8.13	82	-5.89	-2.46	19
23	$PC_{61}BM$	0.78	16.8	0.62	8.04	78	-5.78	-2.40	20
24	$PC_{71}BM$	0.94	12.2	0.70	8.02	68	-6.12	-2.01	21
25	$PC_{71}BM$	0.90	12.5	0.72	8.02	90	-6.02	-1.97	22
26	$PC_{71}BM$	0.90	13.3	0.67	8.02	60	-6.17	-2.35	23
27	$PC_{71}BM$	0.80	14.5	0.69	8.00	48	-5.88	-2.07	24
28	$PC_{71}BM$	0.82	14.2	0.69	7.95	102	-5.74	-2.27	25
29	$PC_{71}BM$	0.88	14.1	0.66	7.91	62	-6.30	-2.26	26
30	$PC_{71}BM$	0.90	12.2	0.70	7.85	74	-6.21	-2.05	13
31	$PC_{71}BM$	0.98	12.2	0.66	7.83	52	-5.94	-2.10	27
32	$PC_{71}BM$	0.86	12.3	0.74	7.83	58	-6.17	-2.03	28
33	$PC_{71}BM$	0.97	11.5	0.70	7.81	84	-6.12	-2.20	29
34	$PC_{71}BM$	0.92	13.0	0.65	7.80	68	-6.12	-2.01	30
35	$PC_{71}BM$	0.95	11.9	0.70	7.79	64	-6.12	-2.04	31
36	$PC_{71}BM$	0.93	11.4	0.73	7.75	72	-6.14	-1.97	32
37	$PC_{61}BM$	0.78	13.7	0.73	7.74	80	-5.86	-2.19	33
38	$PC_{71}BM$	0.92	11.7	0.71	7.72	78	-6.12	-2.01	30
39	$PC_{71}BM$	0.94	12.4	0.66	7.70	70	-6.14	-2.16	34
40	$PC_{71}BM$	0.90	13.1	0.66	7.61	54	-6.18	-2.30	23
41	$PC_{71}BM$	0.93	13.1	0.65	7.60	74	-6.09	-2.01	35
42	$PC_{71}BM$	0.90	14.5	0.58	7.55	59	-6.26	-2.27	5
43	$PC_{71}BM$	0.79	14.7	0.67	7.54	60	-6.27	-2.17	36
44	$PC_{71}BM$	0.80	14.9	0.64	7.47	74	-5.77	-2.32	19
45	$PC_{71}BM$	0.91	11.9	0.69	7.44	54	-6.44	-2.39	37
46	$PC_{71}BM$	1.07	12.4	0.56	7.36	62	-6.28	-2.07	38
47	$PC_{71}BM$	0.76	14.8	0.65	7.35	62	-6.04	-2.20	39
48	$PC_{61}BM$	0.73	13.6	0.73	7.30	86	-5.87	-2.30	40

49	$PC_{71}BM$	0.99	12.0	0.62	7.24	46	-6.15	-3.10	41
50	$PC_{71}BM$	0.93	11.8	0.68	7.21	68	-6.12	-2.01	42
51	$PC_{71}BM$	0.77	15.3	0.64	7.21	78	-5.98	-2.09	43
52	$PC_{61}BM$	0.84	12.3	0.70	7.20	80	-6.04	-2.26	33
53	$PC_{71}BM$	0.92	12.1	0.64	7.18	58	-6.19	-2.04	30
54	$PC_{71}BM$	0.90	11.2	0.70	7.06	66	-5.93	-1.92	44
55	$PC_{61}BM$	0.86	14.1	0.58	6.98	80	-5.82	-1.99	45
56	$PC_{71}BM$	0.90	12.5	0.62	6.91	56	-6.15	-1.76	46
57	$PC_{71}BM$	0.90	11.0	0.70	6.89	112	-6.02	-1.98	47
58	$PC_{71}BM$	0.88	10.7	0.72	6.86	110	-5.91	-2.32	48
59	$PC_{71}BM$	0.86	11.6	0.69	6.86	48	-6.04	-2.14	49
60	$PC_{71}BM$	0.87	11.8	0.67	6.84	99	-5.84	-2.13	8
61	$PC_{71}BM$	0.93	13.6	0.54	6.83	64	-6.01	-2.37	50
62	$PC_{61}BM$	0.71	16.0	0.64	6.83	80	-5.70	-2.37	51
63	$PC_{71}BM$	0.92	11.1	0.66	6.75	66	-6.13	-2.02	52
64	$PC_{71}BM$	0.89	10.5	0.72	6.73	46	-6.42	-2.26	37
65	$PC_{71}BM$	0.90	12.1	0.63	6.71	52	-6.43	-2.32	53
66	$PC_{71}BM$	0.89	10.9	0.69	6.67	134	-5.83	-2.12	9
67	$PC_{71}BM$	0.90	11.5	0.66	6.67	34	-6.27	-2.23	54
68	$PC_{71}BM$	0.85	13.4	0.59	6.59	76	-5.85	-2.48	55
69	$PC_{71}BM$	0.77	12.7	0.68	6.59	52	-6.01	-1.93	56
70	$PC_{71}BM$	0.78	13.4	0.62	6.59	48	-5.97	-2.10	49
71	$PC_{71}BM$	0.80	14.1	0.61	6.52	50	-5.85	-2.05	57
72	$PC_{71}BM$	0.94	10.7	0.65	6.49	84	-6.05	-1.83	58
73	$PC_{71}BM$	0.84	11.9	0.65	6.47	49	-5.93	-2.01	59
74	$PC_{71}BM$	0.92	11.5	0.61	6.43	62	-5.77	-1.89	15
75	$PC_{71}BM$	0.83	12.1	0.66	6.42	99	-5.82	-2.14	11

76	$PC_{71}BM$	0.91	11.0	0.64	6.40	54	-5.91	-1.99	60
77	$PC_{71}BM$	0.95	12.4	0.55	6.40	70	-5.79	-2.06	61
78	$PC_{61}BM$	0.91	10.8	0.65	6.38	58	-6.19	-2.04	62
79	$PC_{71}BM$	0.86	10.8	0.68	6.37	64	-6.22	-2.26	26
80	$PC_{61}BM$	0.71	15.6	0.58	6.30	86	-5.81	-2.23	40
81	$PC_{71}BM$	0.90	10.5	0.67	6.30	62	-5.87	-1.76	63
82	$PC_{71}BM$	0.88	10.3	0.70	6.30	72	-5.93	-1.74	64
83	$PC_{61}BM$	0.75	12.9	0.65	6.30	67	-5.89	-2.32	65
84	$PC_{71}BM$	0.78	13.2	0.61	6.27	79	-6.05	-2.28	66
85	$PC_{71}BM$	0.90	11.0	0.66	6.26	68	-6.06	-2.01	42
86	$PC_{71}BM$	0.79	14.2	0.56	6.23	74	-6.22	-2.44	67
87	$PC_{71}BM$	0.73	14.9	0.57	6.20	48	-5.88	-2.05	68
88	$PC_{71}BM$	0.92	9.8	0.69	6.20	62	-5.93	-1.71	34
89	$PC_{71}BM$	1.01	14.4	0.43	6.17	49	-6.07	-1.98	69
90	$PC_{71}BM$	0.85	10.8	0.67	6.15	52	-6.13	-2.07	70
91	$PC_{71}BM$	0.77	13.5	0.62	6.15	64	-6.24	-2.26	36
92	$PC_{71}BM$	0.97	10.4	0.65	6.14	67	-6.14	-1.90	71
93	$PC_{71}BM$	0.92	11.5	0.58	6.11	54	-6.34	-2.29	72
94	$PC_{71}BM$	0.99	11.2	0.56	6.11	52	-6.55	-1.96	73
95	$PC_{61}BM$	0.92	14.0	0.47	6.10	51	-6.09	-2.01	74
96	$PC_{61}BM$	0.76	13.5	0.59	6.10	67	-5.96	-2.32	65
97	$PC_{71}BM$	0.94	10.4	0.62	6.07	48	-6.20	-2.13	75
98	$PC_{71}BM$	0.89	10.7	0.65	6.07	26	-6.24	-1.82	76
99	$PC_{71}BM$	0.88	11.4	0.61	6.05	52	-5.74	-1.72	77
100	$PC_{71}BM$	1.03	9.5	0.62	6.04	64	-6.20	-1.85	58
101	$PC_{71}BM$	0.97	12.5	0.51	6.02	44	-6.18	-2.13	78
102	$PC_{71}BM$	0.90	10.0	0.69	6.00	42	-6.39	-2.29	79

103	$PC_{71}BM$	0.78	13.9	0.55	6.00	62	-5.87	-1.91	80
104	$PC_{71}BM$	0.82	11.1	0.66	5.98	55	-5.57	-1.92	81
105	$PC_{71}BM$	1.01	11.7	0.52	5.95	72	-6.37	-2.71	16
106	$PC_{71}BM$	0.92	11.3	0.60	5.94	41	-6.65	-2.90	82
107	$PC_{61}BM$	0.80	12.2	0.62	5.93	72	-5.96	-2.05	83
108	$PC_{71}BM$	0.96	12.0	0.53	5.89	60	-5.78	-2.02	61
109	$PC_{71}BM$	0.66	15.4	0.58	5.88	66	-5.93	-1.94	84
110	$PC_{71}BM$	0.69	13.6	0.64	5.87	74	-6.04	-2.20	85
111	$PC_{61}BM$	0.80	11.5	0.64	5.84	52	-6.08	-2.01	86
112	$PC_{61}BM$	0.71	13.6	0.60	5.80	67	-5.88	-2.27	65
113	$PC_{61}BM$	0.75	12.6	0.62	5.80	86	-5.92	-2.44	65
114	$PC_{61}BM$	0.84	12.0	0.58	5.79	62	-5.96	-2.04	87
115	$PC_{71}BM$	0.85	10.5	0.66	5.76	60	-5.95	-2.09	88
116	$PC_{61}BM$	0.75	12.6	0.61	5.70	67	-5.95	-2.41	65
117	$PC_{71}BM$	0.94	10.4	0.58	5.69	54	-6.07	-2.19	89
118	$PC_{71}BM$	1.03	10.1	0.55	5.67	56	-6.27	-2.06	52
119	$PC_{71}BM$	0.85	11.1	0.60	5.67	56	-6.07	-1.90	84
120	$PC_{71}BM$	0.69	13.5	0.63	5.67	80	-5.93	-2.15	90
121	$PC_{71}BM$	0.89	11.1	0.61	5.66	64	-5.80	-2.00	12
122	$PC_{61}BM$	0.71	14.9	0.55	5.65	80	-5.68	-2.41	91
123	$PC_{71}BM$	0.98	9.6	0.61	5.65	62	-6.11	-2.13	92
124	$PC_{71}BM$	0.86	11.8	0.58	5.62	60	-6.08	-2.30	93
125	$PC_{71}BM$	0.62	15.4	0.58	5.61	74	-5.77	-2.01	94
126	$PC_{71}BM$	0.92	8.8	0.69	5.60	72	-5.93	-1.60	64
127	$PC_{71}BM$	0.92	10.0	0.63	5.58	56	-6.12	-2.02	95
128	$PC_{71}BM$	0.99	11.7	0.50	5.56	56	-5.81	-2.00	61
129	$PC_{61}BM$	0.82	13.1	0.52	5.51	74	-5.83	-1.98	45

130	$PC_{61}BM$	0.96	10.3	0.59	5.50	58	-6.19	-2.07	96
131	$PC_{61}BM$	0.80	11.4	0.60	5.50	64	-5.94	-2.05	97
132	$PC_{71}BM$	0.86	10.4	0.62	5.50	62	-6.06	-2.15	98
133	$PC_{61}BM$	0.72	12.7	0.60	5.50	67	-5.95	-2.32	65
134	$PC_{71}BM$	0.84	10.9	0.60	5.47	32	-5.72	-1.59	99
135	$PC_{71}BM$	0.91	10.8	0.56	5.45	42	-6.03	-2.16	100
136	$PC_{61}BM$	0.93	9.8	0.60	5.44	54	-6.18	-1.97	101
137	$PC_{71}BM$	0.82	11.9	0.55	5.44	54	-6.01	-1.96	102
138	$PC_{61}BM$	0.90	9.1	0.66	5.42	64	-6.13	-2.06	103
139	$PC_{71}BM$	0.74	10.5	0.69	5.40	90	-5.75	-2.08	104
140	$PC_{71}BM$	0.89	11.4	0.53	5.37	34	-6.17	-2.17	105
141	$PC_{71}BM$	0.91	10.5	0.57	5.37	52	-5.83	-1.90	27
142	$PC_{71}BM$	0.97	8.8	0.64	5.30	66	-6.15	-1.97	106
143	$PC_{71}BM$	0.63	14.6	0.58	5.30	74	-5.75	-1.69	107
144	$PC_{71}BM$	0.94	9.8	0.58	5.28	35	-6.67	-2.92	82
145	$PC_{71}BM$	0.94	8.0	0.70	5.26	64	-6.14	-2.05	108
146	$PC_{71}BM$	0.86	10.5	0.58	5.25	68	-6.08	-1.79	109
147	$PC_{71}BM$	0.85	11.2	0.56	5.24	36	-5.82	-1.93	110
148	$PC_{71}BM$	0.68	14.5	0.56	5.23	78	-5.79	-1.95	43
149	$PC_{71}BM$	0.87	10.5	0.57	5.22	74	-6.12	-1.85	58
150	$PC_{71}BM$	0.79	11.5	0.58	5.21	42	-5.93	-2.15	100
151	$PC_{71}BM$	0.76	9.9	0.69	5.21	90	-5.75	-2.08	48
152	$PC_{71}BM$	0.86	10.9	0.56	5.19	64	-5.83	-1.84	111
153	$PC_{71}BM$	0.91	9.7	0.60	5.16	66	-6.06	-1.95	106
154	$PC_{71}BM$	0.72	11.9	0.62	5.15	62	-5.96	-2.03	112
155	$PC_{71}BM$	0.92	8.6	0.65	5.11	56	-6.22	-2.04	52
156	$PC_{71}BM$	0.95	9.0	0.64	5.10	44	-6.07	-1.89	113

157	$PC_{71}BM$	0.90	11.6	0.49	5.09	62	-6.01	-2.04	114
158	$PC_{61}BM$	0.97	8.9	0.62	5.07	62	-6.10	-1.79	96
159	$PC_{61}BM$	0.87	9.2	0.63	5.07	82	-5.97	-2.18	115
160	$PC_{71}BM$	0.86	9.9	0.59	5.05	57	-6.19	-2.08	116
161	$PC_{71}BM$	0.98	10.1	0.51	5.05	58	-6.15	-2.09	117
162	$PC_{71}BM$	0.90	10.2	0.55	5.05	26	-6.78	-2.42	118
163	$PC_{71}BM$	0.79	13.0	0.49	5.04	57	-6.17	-2.04	119
164	$PC_{71}BM$	0.69	13.4	0.56	5.03	82	-5.88	-2.11	120
165	$PC_{61}BM$	0.70	11.5	0.63	5.03	64	-6.10	-2.29	121
166	$PC_{71}BM$	0.90	8.3	0.69	4.99	64	-6.04	-1.95	122
167	$PC_{71}BM$	0.82	10.9	0.57	4.97	60	-5.94	-2.14	123
168	$PC_{71}BM$	0.84	9.9	0.61	4.97	55	-5.48	-1.82	81
169	$PC_{71}BM$	0.82	10.8	0.56	4.96	38	-5.70	-1.56	124
170	$PC_{61}BM$	0.80	8.6	0.72	4.93	59	-6.01	-1.95	125
171	$PC_{61}BM$	0.82	10.8	0.56	4.92	64	-5.96	-2.01	126
172	$PC_{71}BM$	0.98	9.5	0.53	4.91	54	-6.32	-1.87	58
173	$PC_{71}BM$	0.86	9.4	0.62	4.90	56	-6.08	-1.98	95
174	$PC_{71}BM$	0.88	9.9	0.56	4.88	32	-5.92	-1.74	99
175	$PC_{61}BM$	1.01	14.0	0.34	4.86	61	-6.01	-2.00	127
176	$PC_{61}BM$	1.08	14.0	0.32	4.84	51	-6.11	-1.82	128
177	$PC_{71}BM$	0.76	10.5	0.61	4.83	110	-5.80	-2.04	48
178	$PC_{71}BM$	0.96	9.6	0.52	4.80	26	-6.88	-2.28	118
179	$PC_{61}BM$	0.89	9.7	0.56	4.80	62	-6.02	-2.12	129
180	$PC_{61}BM$	0.80	11.9	0.50	4.78	80	-5.67	-2.31	130
181	$PC_{71}BM$	0.98	8.7	0.56	4.76	22	-6.44	-2.21	131
182	$PC_{71}BM$	0.91	10.5	0.50	4.75	58	-6.01	-1.99	114
183	$PC_{71}BM$	0.72	13.6	0.48	4.73	62	-6.01	-2.21	132

184	$PC_{71}BM$	0.95	8.7	0.58	4.72	40	-6.12	-2.36	41
185	$PC_{61}BM$	0.97	8.7	0.60	4.70	62	-6.16	-1.96	96
186	$PC_{71}BM$	0.91	7.4	0.69	4.68	68	-6.23	-1.94	133
187	$PC_{71}BM$	0.77	9.9	0.63	4.67	28	-6.14	-1.63	76
188	$PC_{71}BM$	0.92	11.2	0.44	4.66	34	-6.14	-2.14	134
189	$PC_{71}BM$	0.97	10.3	0.46	4.65	56	-5.65	-2.02	135
190	$PC_{71}BM$	0.72	10.6	0.60	4.65	32	-5.57	-1.48	136
191	$PC_{71}BM$	0.92	12.1	0.42	4.65	34	-6.13	-2.12	134
192	$PC_{71}BM$	0.69	12.5	0.58	4.64	74	-5.94	-2.09	85
193	$PC_{61}BM$	1.02	9.3	0.49	4.63	41	-6.27	-2.09	137
194	$PC_{61}BM$	0.97	9.1	0.52	4.62	62	-6.17	-1.78	138
195	$PC_{71}BM$	0.90	9.5	0.54	4.61	43	-6.53	-2.87	139
196	$PC_{71}BM$	0.69	11.9	0.57	4.60	63	-5.95	-2.19	140
197	$PC_{71}BM$	0.80	10.3	0.59	4.60	68	-5.98	-1.95	141
198	$PC_{71}BM$	0.98	8.2	0.58	4.58	41	-6.13	-1.96	92
199	$PC_{71}BM$	0.83	12.6	0.44	4.57	48	-6.05	-2.20	142
200	$PC_{61}BM$	0.95	8.0	0.60	4.56	54	-6.20	-1.99	62
201	$PC_{61}BM$	0.90	7.4	0.71	4.56	64	-6.04	-1.95	122
202	$PC_{71}BM$	0.88	9.4	0.56	4.56	42	-5.77	-1.73	77
203	$PC_{61}BM$	0.79	8.9	0.65	4.54	62	-6.03	-2.10	126
204	$PC_{71}BM$	0.85	7.4	0.72	4.52	52	-6.13	-2.01	70
205	$PC_{71}BM$	1.00	10.2	0.44	4.50	22	-6.53	-1.99	143
206	$PC_{61}BM$	0.88	9.9	0.51	4.46	47	-6.20	-2.01	144
207	$PC_{61}BM$	0.89	9.0	0.55	4.45	50	-6.04	-1.93	145
208	$PC_{61}BM$	0.90	7.9	0.64	4.43	66	-6.05	-1.98	146
209	$PC_{71}BM$	0.92	10.0	0.48	4.40	38	-6.04	-2.06	147
210	$PC_{71}BM$	0.87	9.5	0.53	4.40	50	-6.03	-1.95	148

211	$PC_{71}BM$	0.65	13.1	0.52	4.40	74	-5.72	-1.77	107
212	$PC_{61}BM$	0.76	11.7	0.50	4.40	56	-5.89	-1.93	149
213	$PC_{71}BM$	0.98	10.2	0.46	4.40	54	-5.98	-2.02	150
214	$PC_{71}BM$	1.01	9.0	0.48	4.36	28	-6.41	-2.20	151
215	$PC_{71}BM$	0.77	9.6	0.59	4.34	56	-6.18	-2.19	152
216	$PC_{71}BM$	0.88	10.1	0.49	4.33	64	-6.06	-2.29	153
217	$PC_{61}BM$	0.83	8.8	0.66	4.32	43	-6.26	-2.35	154
218	$PC_{71}BM$	0.69	11.2	0.56	4.32	40	-5.98	-2.07	155
219	$PC_{71}BM$	0.84	9.3	0.55	4.25	70	-5.94	-1.92	156
220	$PC_{61}BM$	0.77	10.8	0.51	4.25	114	-6.00	-2.10	157
221	$PC_{71}BM$	0.93	9.4	0.49	4.25	54	-5.82	-1.92	158
222	$PC_{71}BM$	0.88	10.8	0.44	4.24	35	-5.90	-1.97	159
223	$PC_{61}BM$	0.94	7.8	0.58	4.21	64	-6.05	-2.10	160
224	$PC_{61}BM$	0.95	7.8	0.57	4.20	64	-5.89	-2.07	161
225	$PC_{71}BM$	0.87	8.7	0.56	4.20	48	-6.06	-1.97	162
226	$PC_{71}BM$	0.93	10.0	0.46	4.19	60	-5.91	-2.06	61
227	$PC_{71}BM$	0.92	9.0	0.53	4.18	22	-6.28	-2.16	163
228	$PC_{71}BM$	0.93	10.1	0.45	4.18	52	-6.10	-2.05	114
229	$PC_{71}BM$	0.87	11.7	0.41	4.18	34	-6.06	-2.07	134
230	$PC_{61}BM$	0.88	6.3	0.75	4.16	64	-6.28	-2.17	164
231	$PC_{71}BM$	0.91	9.5	0.48	4.15	46	-6.42	-2.08	52
232	$PC_{61}BM$	1.11	11.2	0.33	4.14	51	-6.16	-1.96	127
233	$PC_{61}BM$	0.96	13.6	0.32	4.12	61	-5.99	-1.92	127
234	$PC_{71}BM$	0.99	8.3	0.50	4.09	52	-6.47	-2.14	165
235	$PC_{71}BM$	0.74	10.2	0.54	4.08	50	-5.98	-2.12	89
236	$PC_{71}BM$	0.87	7.1	0.68	4.07	48	-6.25	-2.02	56
237	$PC_{71}BM$	0.94	10.0	0.43	4.06	54	-5.80	-1.90	166

238	$PC_{61}BM$	0.90	7.5	0.60	4.05	55	-6.12	-2.04	167
239	$PC_{61}BM$	0.83	8.4	0.60	4.04	64	-5.94	-2.01	160
240	$PC_{71}BM$	0.82	9.7	0.52	4.04	64	-5.85	-1.77	111
241	$PC_{71}BM$	0.85	9.5	0.50	4.02	68	-5.69	-2.23	168
242	$PC_{71}BM$	0.92	6.9	0.63	4.00	68	-6.10	-1.96	169
243	$PC_{61}BM$	0.78	8.1	0.63	4.00	49	-6.18	-2.02	167
244	$PC_{61}BM$	0.73	9.1	0.63	3.97	70	-6.05	-2.11	170
245	$PC_{71}BM$	0.88	8.9	0.52	3.97	28	-5.93	-1.84	110
246	$PC_{71}BM$	0.93	8.5	0.50	3.96	27	-6.25	-2.20	171
247	$PC_{61}BM$	1.03	7.3	0.52	3.95	63	-6.47	-2.47	172
248	$PC_{71}BM$	0.94	8.0	0.54	3.94	59	-6.19	-1.91	71
249	$PC_{71}BM$	0.90	10.1	0.43	3.91	52	-5.84	-1.81	173
250	$PC_{61}BM$	0.72	9.2	0.58	3.83	62	-5.93	-2.02	126
251	$PC_{71}BM$	0.88	10.6	0.41	3.76	69	-5.90	-1.95	69
252	$PC_{61}BM$	0.76	11.0	0.46	3.75	63	-5.93	-2.08	45
253	$PC_{61}BM$	0.87	7.1	0.61	3.73	64	-6.02	-2.07	126
254	$PC_{71}BM$	0.85	10.6	0.44	3.73	35	-5.85	-1.96	159
255	$PC_{71}BM$	0.76	8.3	0.58	3.70	52	-5.99	-1.87	174
256	$PC_{71}BM$	1.01	9.8	0.38	3.70	32	-6.73	-2.55	175
257	$PC_{61}BM$	0.79	8.8	0.53	3.66	64	-5.92	-1.98	126
258	$PC_{71}BM$	0.94	6.0	0.67	3.64	42	-6.73	-2.47	53
259	$PC_{71}BM$	0.84	9.9	0.44	3.59	48	-5.87	-2.08	123
260	$PC_{71}BM$	0.82	10.5	0.42	3.54	35	-5.84	-1.86	159
261	$PC_{61}BM$	1.05	10.5	0.32	3.53	51	-6.14	-1.86	127
262	$PC_{71}BM$	0.93	8.2	0.46	3.51	52	-5.85	-1.76	173
263	$PC_{71}BM$	0.86	11.9	0.34	3.47	37	-6.07	-2.42	176
264	$PC_{71}BM$	0.90	7.9	0.49	3.45	32	-6.13	-1.72	177

265	$PC_{71}BM$	0.99	9.0	0.38	3.40	54	-5.96	-2.08	161
266	$PC_{61}BM$	0.98	10.1	0.49	3.40	37	-6.87	-2.36	178
267	$PC_{61}BM$	0.92	8.8	0.42	3.40	47	-5.90	-1.73	128
268	$PC_{71}BM$	0.91	7.0	0.57	3.34	54	-6.15	-1.97	122
269	$PC_{61}BM$	0.88	7.0	0.53	3.27	37	-6.34	-2.06	167
270	$PC_{71}BM$	0.78	10.2	0.49	3.26	61	-6.15	-1.83	179
271	$PC_{61}BM$	0.83	7.3	0.57	3.26	76	-5.95	-2.09	180
272	$PC_{71}BM$	0.83	8.1	0.48	3.24	58	-6.12	-1.98	181
273	$PC_{61}BM$	0.83	8.2	0.65	3.23	43	-6.24	-2.32	154
274	$PC_{71}BM$	0.74	7.9	0.55	3.21	69	-5.86	-2.07	182
275	$PC_{71}BM$	0.80	8.4	0.51	3.20	68	-5.85	-1.86	141
276	$PC_{61}BM$	0.91	6.8	0.52	3.14	54	-6.15	-1.97	122
277	$PC_{71}BM$	0.82	8.9	0.43	3.10	62	-5.83	-1.76	173
278	$PC_{71}BM$	0.66	8.2	0.56	3.09	74	-5.86	-2.03	94
279	$PC_{61}BM$	0.78	7.1	0.55	3.07	71	-5.96	-2.06	167
280	$PC_{71}BM$	0.92	7.9	0.42	3.07	28	-6.13	-2.29	183
281	$PC_{71}BM$	0.90	7.3	0.46	3.04	32	-6.06	-1.69	184
282	$PC_{71}BM$	0.70	8.2	0.53	3.02	48	-5.91	-2.06	49
283	$PC_{71}BM$	0.99	7.7	0.38	2.89	80	-6.03	-1.73	185
284	$PC_{61}BM$	0.36	15.0	0.50	2.70	22	-5.70	-1.73	186
285	$PC_{61}BM$	0.94	8.2	0.34	2.59	25	-6.45	-1.87	187
286	$PC_{71}BM$	0.84	8.0	0.38	2.56	66	-5.94	-2.23	188
287	$PC_{61}BM$	0.79	6.1	0.49	2.50	42	-5.70	-1.89	189
288	$PC_{71}BM$	0.76	9.5	0.33	2.38	43	-6.06	-2.47	176
289	$PC_{61}BM$	0.67	8.4	0.45	2.33	40	-6.00	-2.13	190
290	$PC_{61}BM$	0.58	7.0	0.57	2.30	18	-6.01	-1.36	191
291	$PC_{71}BM$	0.81	5.7	0.49	2.30	52	-5.99	-1.78	192

292	$PC_{61}BM$	0.97	3.4	0.57	2.10	30	-6.20	-1.93	193
293	$PC_{61}BM$	0.76	6.3	0.38	1.76	40	-6.24	-2.05	194
294	$PC_{61}BM$	0.76	6.3	0.36	1.74	20	-6.36	-2.04	195
295	$PC_{61}BM$	0.90	5.3	0.32	1.54	25	-6.55	-1.94	195
296	$PC_{61}BM$	0.75	4.1	0.44	1.34	33	-5.77	-1.79	196
297	$PC_{61}BM$	0.80	4.4	0.34	1.17	25	-5.90	-1.67	196
298	$PC_{61}BM$	0.84	3.0	0.40	1.00	24	-5.76	-1.68	197
299	$PC_{61}BM$	0.47	1.9	0.52	0.52	26	-5.66	-2.11	198
300	$PC_{61}BM$	1.06	1.5	0.34	0.50	22	-5.94	-1.82	199

Table S2: Statistical analysis of device characteristics.

Device parameters	minimum	maximum	average	median	standard deviation	variance
PCE (%)	0.50	9.84	5.36	5.21	1.756	3.08
V_{OC}(V)	0.36	1.11	0.864	0.88	0.099	0.0098
J_{SC}(mA/cm^2)	1.48	19.01	10.79	10.77	2.581	6.66
FF	0.32	0.763	0.579	0.586	0.100	0.01

1 Descriptors for ML models

In our recent studies,[200,201] we introduced 28 descriptors to capture the energy conversion process. These descriptors and their possible impact on the device performance are briefly described below:

(1) *Number of unsaturated atoms in the main conjugation path of donor molecules*, $N^{\mathrm{D}}_{\mathrm{atom}}$. This descriptor represents the conjugation length of a molecule, and it is widely considered to be associated with photon absorption, exciton diffusion length, stability of charge carriers, etc.[202,203]

(2) *Vertical ionization potential of donor molecules*, $\mathrm{IP}(v)$. The IP is associated with the energy of HOMO (E_{H}) which in turn correlates with the donor valence band edge energies and the V_{OC}.[204]

(3) *Polarizability of donor molecules.* Large polarizability of organic molecules may reduce the exciton binding energy by stabilizing the charge-separated states.

(4) *Energy of the electronic transition to a singlet excited state with the largest oscillator strength*, E_{g}. This parameter is related to photon absorption by donor molecules; therefore it is expected to correlate with the J_{SC}.

(5) *Reorganization energy for holes in donor molecules*, λ_h. This quantity is expected to correlate with the barrier for charge transport, and therefore should be smaller for higher mobility materials.[205]

(6) *Hole-electron binding energy in donor molecules*, E_{bind}. It is a measure of the strength of hole-electron interaction and can be estimated as the difference between the fundamental gap and optical gap.[206] It strongly affects the yield of hole-electron recombination, and a small E_{bind} is always desired to increase the chance of migration of excitons to the D/A interface.

(7) *The energetic difference of HOMO of donor and LUMO of acceptor*, $E^{\mathrm{DA}}_{\mathrm{HL}}$. This descriptor is an approximation to the energy of the charge-transfer state (E_{CT}) for the D/A interface, which is known to have good correlation with V_{OC} of an OPV.[207,208] Thus, this

descriptor can roughly estimate the driving force to dissociate excitons in the D/A interface.

(8) *Energy of the electronic transition to the lowest-lying triplet state*, E_{T}. The charge-transfer state at the D/A heterojunction can relax to the lowest-lying triplet exciton state of individual molecules if the process is energetically favorable, which may leads to recombination of holes and electrons to the ground state.[207,209] To take account the possible triplet loss channel, in addition to $E_{\mathrm{HL}}^{\mathrm{DA}}$, E_{T} is also considered as a descriptor.

(9) *The energetic difference of LUMO of donor and LUMO of acceptor*, $E_{\mathrm{LL}}^{\mathrm{DA}}$. This descriptor quantifies the degree of alignment of LUMOs of donor and acceptor molecules. If $E_{\mathrm{LL}}^{\mathrm{DA}}$ is too large there is a substantial energy loss at the D/A interface; if it is not large enough the driving force for the charge separation can be insufficient.

(10) *Change in dipole moment in going from the ground state to the first excited state for donor molecules*, Δ_{ge}. It is associated with the degree of photoinduced charge transfer within a molecule, and a large value of this parameter is expected to promote the formation of a polarized exciton and reduce the geminate recombination of the hole and electron.[210]

(11,12) *The energetic differences of HOMO and HOMO-1*, $\Delta_{\mathrm{H}} = E_{\mathrm{HOMO}} - E_{\mathrm{HOMO-1}}$ and *LUMO and LUMO+1*, $\Delta_{\mathrm{L}} = E_{\mathrm{LUMO+1}} - E_{\mathrm{LUMO}}$ *of donor molecules.* In the case of small Δ_{H} and Δ_{L}, orbitals other than HOMO/LUMO may also significantly contribute to the exciton formation, exciton dissociation, and hole/electron transport influencing the device parameters of an OPV.[201]

(13) *The energetic difference of LUMO and LUMO+1 of acceptors*, $\Delta_{\mathrm{L}}^{\mathrm{A}} = E_{\mathrm{LUMO+1}} - E_{\mathrm{LUMO}}$. Small $\Delta_{\mathrm{L}}^{\mathrm{A}}$ values of acceptors known to accelerate exciton dissociation at the D/A interface, as there is a possibility of having more than one electron accepting states in the anionic form as proposed in refs 211–213.

(14) *The largest oscillator strength for the electronic transition*, f_{osc}. It determines the probability of interaction of a molecule with light over a certain range of energy. This parameter is directly related to the photon absorption.

(15,16) *Energy of the first electronic transition*, E_{S_1} and the associated oscillator strength,

$f_{\mathrm{osc}}^{\mathrm{S}_1}$. E_{S_1} is the minimum energy of a photon required for absorption by a molecule. Also, in order to examine the energetic condition for the singlet fission process, it is important to consider both E_{S_1} and E_{T} as descriptors. Further, it is worth to include $f_{\mathrm{osc}}^{\mathrm{S}_1}$ as a descriptor, as it describes the importance of the first electronic transition.

(17) *Maximal photogenerated current*, J_{ph}. The maximum obtainable current density can be evaluated by assuming that photon absorption occurs at energies $\geq E_{\mathrm{S}_1}$, and it is calculated by numerically integrating with the energy range from E_{S_1} to the superior limit of the sunlight wavelength (AM1.5 condition) using the following equation,

$$J_{\mathrm{ph}} = e \int_{E_{\mathrm{S}_1}}^{\infty} \phi_{\mathrm{ph}}(\lambda) d\lambda. \tag{1}$$

Here, ϕ_{ph} and e are solar photon flux density and elementary charge, respectively. The reference density was obtained from the American Society for Testing and Materials (ASTM G173-03, AM1.5g). This parameter is known to be directly correlated with the J_{SC}.

(18) *Area of absorption spectra for donors*, Δ_{area}. The absorption spectrum was calculated using the following equation with an half-width half-maximum of 3500 cm^{-1} for the first 20 electronic excitations,

$$\varepsilon(\widetilde{\nu}) = \sum_{i=1}^{20} \varepsilon_i(\widetilde{\nu}) = \sum_{i=1}^{20} \frac{\sqrt{\pi} \cdot e^2 \cdot N}{1000 \cdot \ln(10) \cdot c^2 \cdot m_e} \cdot \frac{f_i}{\sigma} exp[-(\frac{\widetilde{\nu} - \widetilde{\nu}_i}{\sigma})^2]. \tag{2}$$

Area of each spectrum was calculated using the composite trapezoidal rule. This descriptor is expected to correlate with the J_{SC}.

(19) *The most favourable excited state for electronic transition in donor molecules*, S_{N}. For many molecules, excitation other the first electronic transition has the largest oscillator strength, and in these cases, there is a high probability of hole-electron recombination. To account this effect, S_{N} is considered as a descriptor.

(20,21) *Contribution of HOMO/HOMO-1 for the* $S_0 \rightarrow S_{\mathrm{N}}$ *transition*, $C_{\mathrm{H}}/C_{\mathrm{H-1}}$. In our previous study,[201] it is noticed that orbitals other than HOMO also contribute to the

$S_0 \rightarrow S_\mathrm{N}$ transition; thus these two descriptors may be related to the photon absorption.

(22,23) *Contribution of LUMO/LUMO+1 for the* $S_0 \rightarrow S_\mathrm{N}$ *transition*, $C_\mathrm{L}/C_\mathrm{L+1}$. Orbitals energetically close to LUMO also participate in photon absorption, and therefore, these parameters may influence the J_SC.

(24) *HOMO-LUMO gap for donors*, Δ_HL. It is calculated as the difference of HOMO and LUMO energies of donor molecules, generally used as an optical gap instead of the E_g for its low computational cost.

(25) *Fundamental gap for donors*, E_fund. It is calculated as the difference between ionization potential and electron affinity, which is related to the energy required for the electron-hole separation.

(26) *Number of* π*-electrons in donors*, N_elec. In OPVs, excitons are formed by excitations of π-electrons from occupied to unoccupied orbitals; thus N_elec may be closely related to the energy conversion process.

(27) *Number of heteroatoms present in the main conjugation path for donors*, $N_\mathrm{het}^\mathrm{D}$. The presence of heteroatoms such as nitrogen, sulfur, and oxygen, in a conjugated molecule, may regulate the geometry through non-covalent interactions and influence its photophysical properties.

(28) *Name of acceptors*, *Acceptor*. This is a categorical descriptor to distinguish two acceptors: $\mathrm{PC_{61}BM}$ and $\mathrm{PC_{71}BM}$.

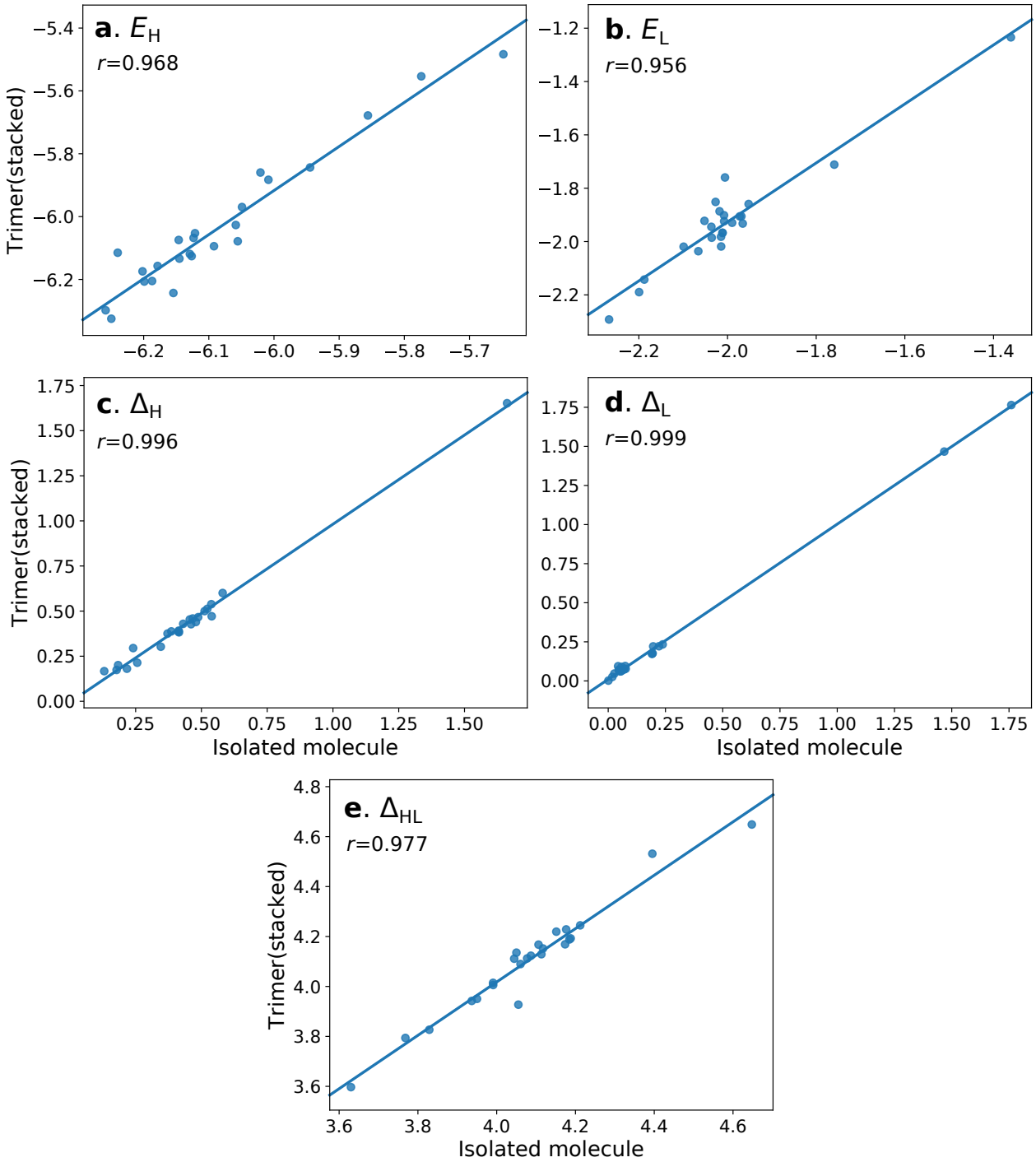

Figure S1: Comparison between properties of isolated molecules and π-stacked trimers for 24 systems: (a) E_{H}, (b) E_{L}, (c) Δ_{H}, (d) Δ_{L}, and (e) Δ_{HL}. In the case of π-stacked trimers, single-point QM/MM calculations were carried out by considering the middle one as a high layer (M06-2X/6-31G(d)) and the other two as low layers (UFF), where ground-state geometry of individual molecules were optimised at the M06-2X/6-31G(d) level.

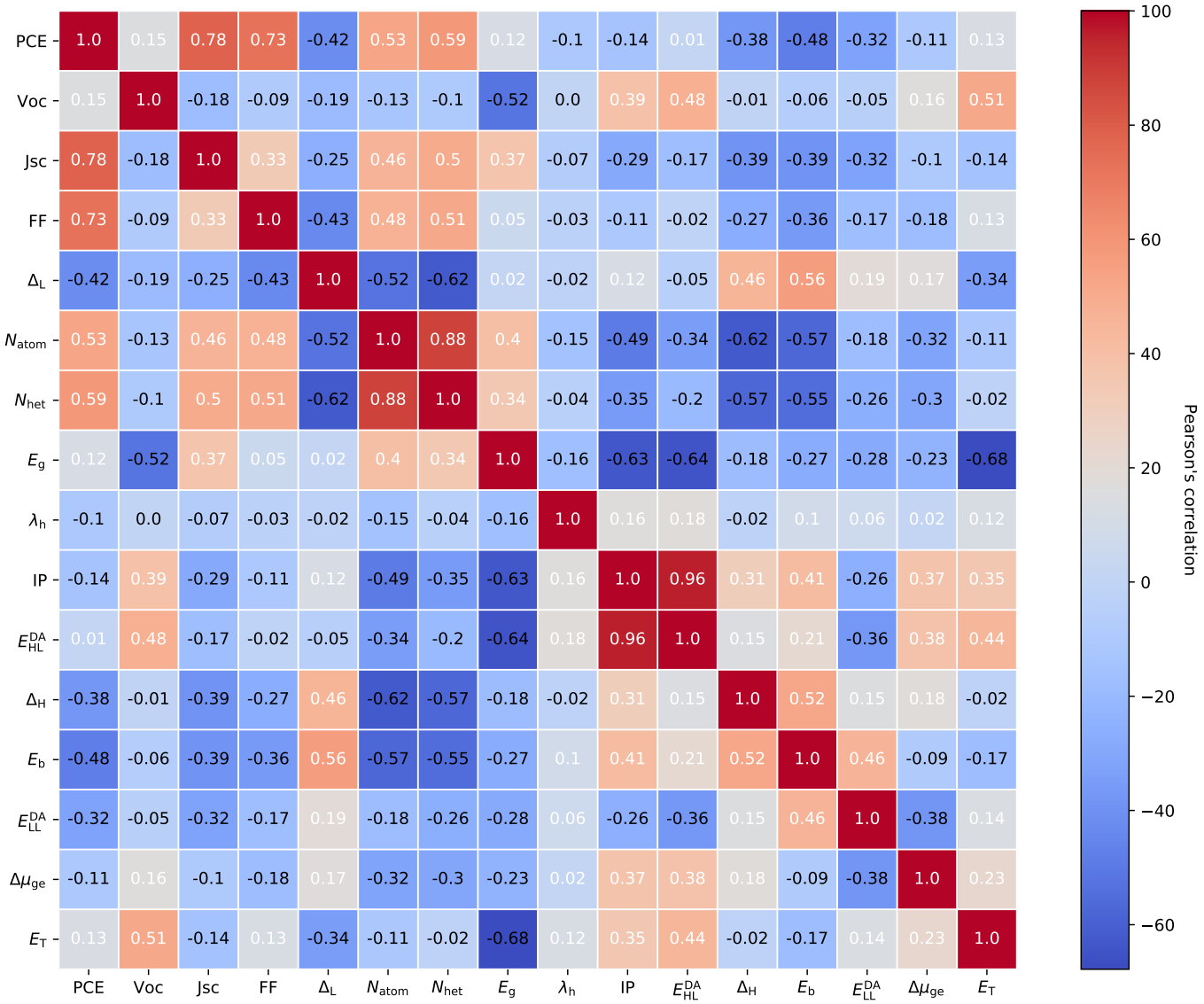

Figure S2: Pearson's correlation coefficients for all possible combinations of 12 important descriptor(s) and/or device parameter(s).

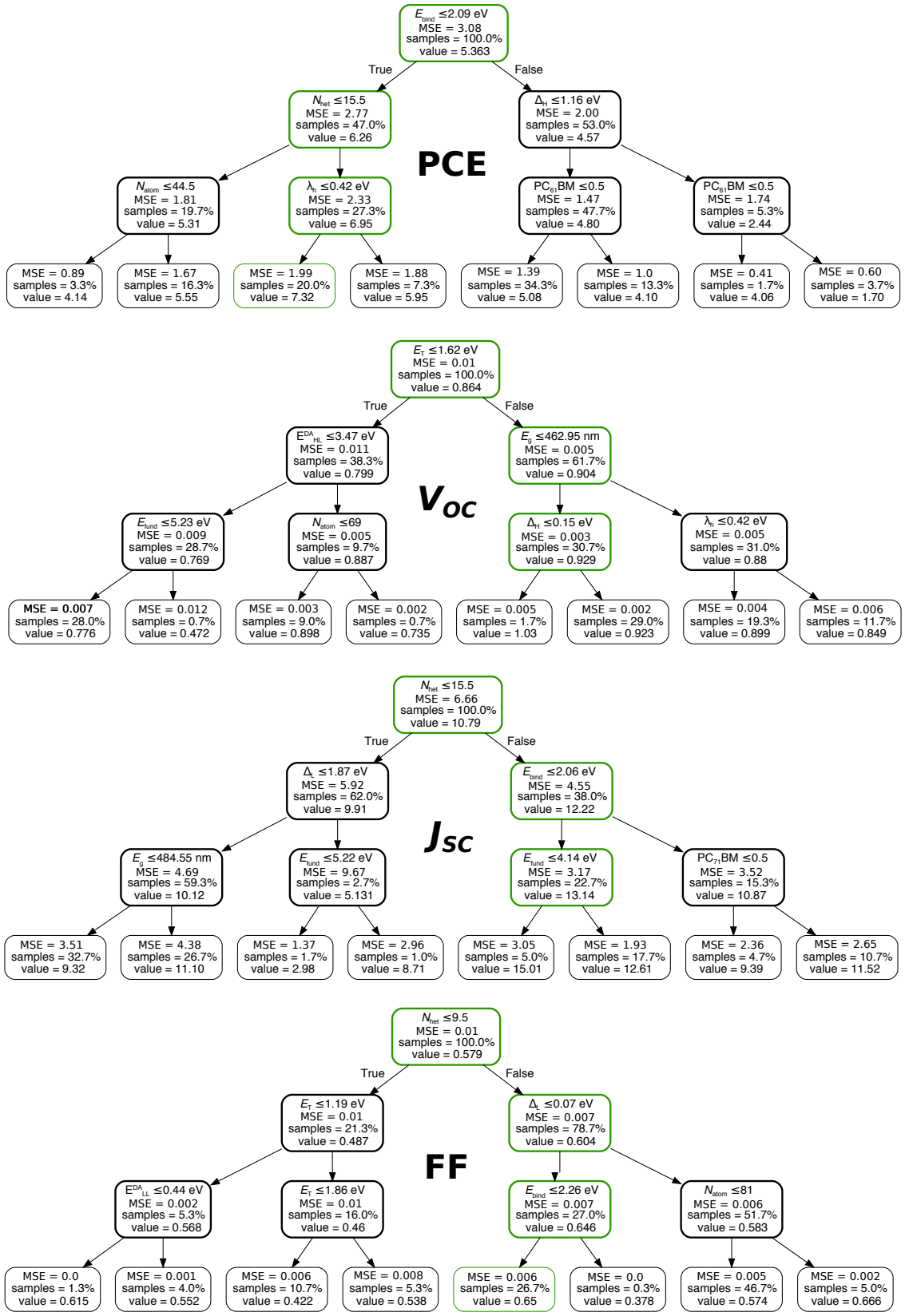

Figure S3: Regression trees for PCE, V_{OC}, J_{SC} and FF constructed using 300 data points with a maximum depth of 3. In a decision tree, conditions are depicted as nodes with reported mean squared error (MSE), percentage of samples, and the average value of the respective device characteristics.

2 ML models

Table S3: Prediction of the device characteristics (PCE, J_{SC}, V_{OC} and FF) by the GBRT algorithm. MAPE, RMSE, and r represent mean absolute percentage error, root mean square error, and Pearson's correlation coefficient, respectively. Results for the testing set (50 points) and 10-fold cross-validation on 250 data points are shown outside and inside the parenthesis, respectively.

Device characteristics	r	RMSE	MAPE (%)
PCE	0.78 (0.81)	0.998 (1.090)	16.6 (20.8)
V_{OC}	0.71 (0.70)	0.076 (0.071)	7.3 (6.7)
J_{SC}	0.70 (0.70)	1.813 (1.871)	15.1 (16.4)
FF	0.76(0.71)	0.066 (0.071)	10.0 (10.4)

Table S4: Prediction of the device characteristics (PCE, J_{SC}, V_{OC} and FF) by the RF algorithm. MAPE, RMSE, and r represent mean absolute percentage error, root mean square error, and Pearson's correlation coefficient, respectively. Results for the testing set (50 points) and 10-fold cross-validation on 250 data points are shown outside and inside the parenthesis, respectively.

Device characteristics	r	RMSE	MAPE (%)
PCE	0.76(0.78)	1.034 (1.166)	17.5 (22.9)
V_{OC}	0.70(0.68)	0.076 (0.073)	7.2 (6.7)
J_{SC}	0.70(0.71)	1.794 (1.881)	15.2 (16.8)
FF	0.76(0.71)	0.067 (0.072)	10.4 (10.9)

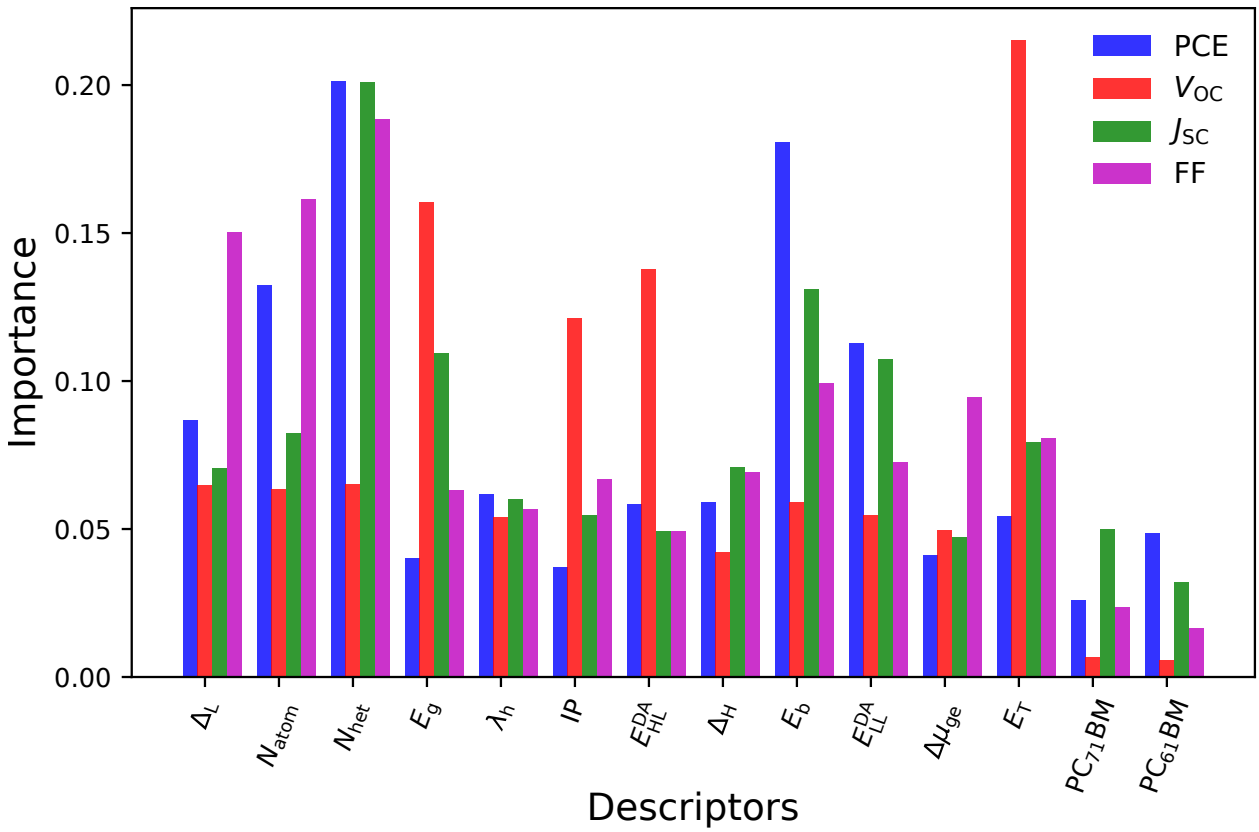

Figure S4: Permutation importance of descriptors for the RF model.

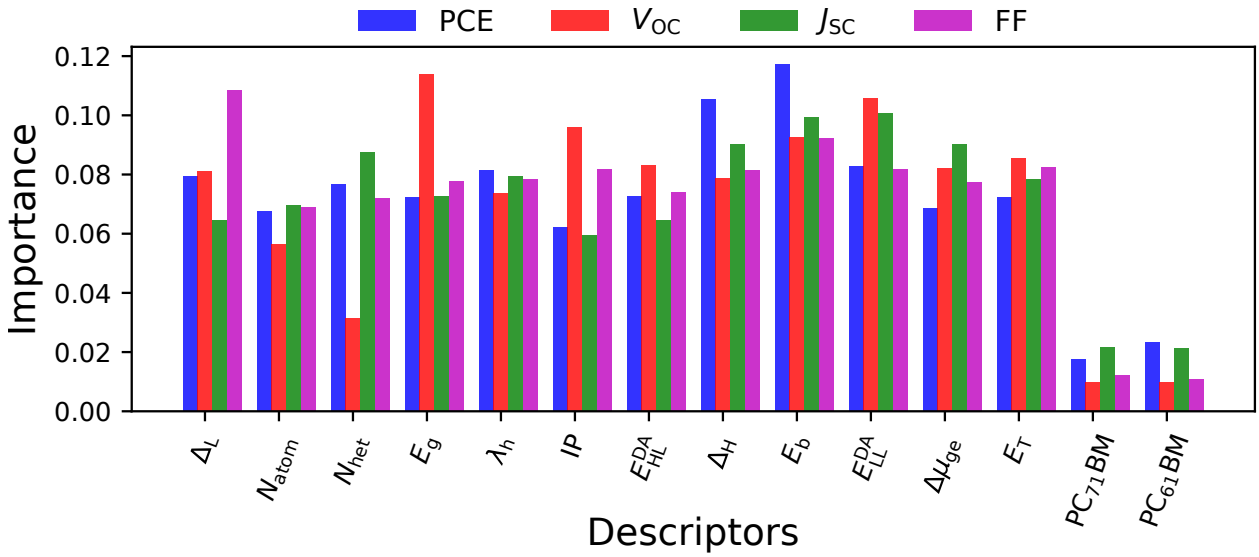

Figure S5: Gini importance of descriptors for the GBRT model.

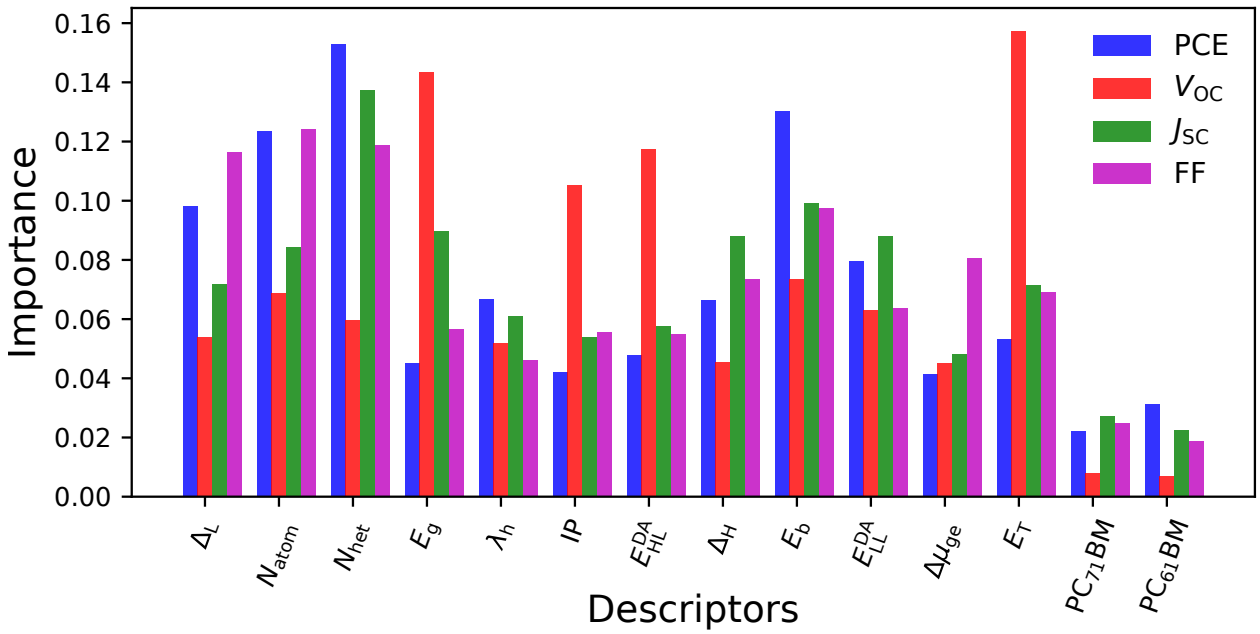

Figure S6: Gini importance of descriptors for the RF model.

References

(1) Wan, J.; Xu, X.; Zhang, G.; Li, Y.; Feng, K.; Peng, Q. Highly Efficient Halogen-Free Solvent Processed Small-Molecule Organic Solar Cells Enabled by Material Design and Device Engineering. *Energy Environ. Sci.* **2017**, *10*, 1739–1745.

(2) Wang, Z.; Xu, X.; Li, Z.; Feng, K.; Li, K.; Li, Y.; Peng, Q. Solution-Processed Organic Solar Cells with 9.8% Efficiency Based on a New Small Molecule Containing a 2D Fluorinated Benzodithiophene Central Unit. *Adv. Electron. Mater.* **2016**, *2*, 1600061.

(3) Li, M.; Liu, F.; Wan, X.; Ni, W.; Kan, B.; Feng, H.; Zhang, Q.; Yang, X.; Wang, Y.; Zhang, Y. et al. Subtle Balance Between Length Scale of Phase Separation and Domain Purification in Small-Molecule Bulk-Heterojunction Blends Under Solvent Vapor Treatment. *Adv. Mater.* **2015**, *27*, 6296–6302.

(4) Xu, S.; Zhou, Z.; Fan, H.; Ren, L.; Liu, F.; Zhu, X.; Russell, T. P. An Electron-Rich 2-Alkylthieno[3,4-*b*]thiophene Building Block with Excellent Electronic and Morphological Tunability for High-Performance Small-Molecule Solar Cells. *J. Mater. Chem. A* **2016**, *4*, 17354–17362.

(5) Zhang, Q.; Kan, B.; Liu, F.; Long, G.; Wan, X.; Chen, X.; Zuo, Y.; Ni, W.; Zhang, H.; Li, M. et al. Small-Molecule Solar Cells with Efficiency Over 9%. *Nat. Photonics* **2015**, *9*, 35.

(6) Cui, C.; Guo, X.; Min, J.; Guo, B.; Cheng, X.; Zhang, M.; Brabec, C. J.; Li, Y. High-Performance Organic Solar Cells Based on a Small Molecule with Alkylthio-Thienyl-Conjugated Side Chains without Extra Treatments. *Adv. Mater.* **2015**, *27*, 7469–7475.

(7) Liang, T.; Xiao, L.; Gao, K.; Xu, W.; Peng, X.; Cao, Y. Modifying the Chemical Structure of a Porphyrin Small Molecule with Benzothiophene Groups for the Re-

producible Fabrication of High Performance Solar Cells. *ACS Appl. Mater. Interfaces* **2017**, *9*, 7131–7138.

(8) Wang, J.-L.; Liu, K.-K.; Liu, S.; Xiao, F.; Chang, Z.-F.; Zheng, Y.-Q.; Dou, J.-H.; Zhang, R.-B.; Wu, H.-B.; Pei, J. et al. Donor End-Capped Hexafluorinated Oligomers for Organic Solar Cells with 9.3% Efficiency by Engineering the Position of π-Bridge and Sequence of Two-Step Annealing. *Chem. Mater.* **2017**, *29*, 1036–1046.

(9) Wang, J.-L.; Liu, K.-K.; Yan, J.; Wu, Z.; Liu, F.; Xiao, F.; Chang, Z.-F.; Wu, H.-B.; Cao, Y.; Russell, T. P. Series of Multifluorine Substituted Oligomers for Organic Solar Cells with Efficiency Over 9% and Fill Factor of 0.77 by Combination Thermal and Solvent Vapor Annealing. *J. Am. Chem. Soc.* **2016**, *138*, 7687–7697.

(10) Sun, K.; Xiao, Z.; Lu, S.; Zajaczkowski, W.; Pisula, W.; Hanssen, E.; White, J. M.; Williamson, R. M.; Subbiah, J.; Ouyang, J. et al. A Molecular Nematic Liquid Crystalline Material for High-Performance Organic Photovoltaics. *Nat. Commun.* **2015**, *6*, 6013.

(11) Jin-Liang, W.; Kai-Kai, L.; Sha, L.; Fei, X.; Feng, L.; Hong-Bin, W.; Yong, C. Developing High-Performance Electron-Rich Unit End-Capped Wide Bandgap Oligomeric Donor by Weak Electron-Deficient Central Core Strategy. *Sol. RRL* **2018**, *2*, 1700212.

(12) Wang, J.-L.; Xiao, F.; Yan, J.; Wu, Z.; Liu, K.-K.; Chang, Z.-F.; Zhang, R.-B.; Chen, H.; Wu, H.-B.; Cao, Y. Difluorobenzothiadiazole-Based Small-Molecule Organic Solar Cells with 8.7% Efficiency by Tuning of π-Conjugated Spacers and Solvent Vapor Annealing. *Adv. Funct. Mater.* **2016**, *26*, 1803–1812.

(13) Kan, B.; Zhang, Q.; Liu, F.; Wan, X.; Wang, Y.; Ni, W.; Yang, X.; Zhang, M.; Zhang, H.; Russell, T. P. et al. Small Molecules Based on Alkyl/Alkylthio-thieno[3,2-*b*]thiophene-Substituted Benzo[1,2-*b*:4,5-*b*']dithiophene for Solution-Processed Solar Cells with High Performance. *Chem. Mater.* **2015**, *27*, 8414–8423.

(14) Lai, T.; Xiao, L.; Deng, K.; Liang, T.; Chen, X.; Peng, X.; Cao, Y. Dimeric Porphyrin Small Molecules for Efficient Organic Solar Cells with High Photoelectron Response in the Near-Infrared Region. *ACS Appl. Mater. Interfaces* **2018**, *10*, 668–675.

(15) Busireddy, M. R.; Madhu, C.; Chereddy, N. R.; Appalanaidu, E.; Sharma, G. D.; Vaidya, J. R. Optimization of the Donor Material Structure and Processing Conditions to Obtain Efficient Small-Molecule Donors for Bulk Heterojunction Solar Cells. *ChemPhotoChem* **2018**, *2*, 81–88.

(16) Deng, D.; Yang, Y.; Zou, W.; Zhang, Y.; Wang, Z.; Wang, Z.; Zhang, J.; Lu, K.; Ma, W.; Wei, Z. Aromatic End-Capped Acceptor Effects on Molecular Stacking and the Photovoltaic Performance of Solution-Processable Small Molecules. *J. Mater. Chem. A* **2018**, DOI:10.1039/C8TA04102D.

(17) Ni, W.; Li, M.; Wan, X.; Feng, H.; Kan, B.; Zuo, Y.; Chen, Y. A high-Performance Photovoltaic Small Molecule Developed by Modifying the Chemical Structure and Optimizing the Morphology of the Active Layer. *RSC Adv.* **2014**, *4*, 31977–31980.

(18) Badgujar, S.; Lee, G.-Y.; Park, T.; Song, C. E.; Park, S.; Oh, S.; Shin, W. S.; Moon, S.-J.; Lee, J.-C.; Lee, S. K. High-Performance Small Molecule *via* Tailoring Intermolecular Interactions and its Application in Large-Area Organic Photovoltaic Modules. *Adv. Energy Mater.* **2016**, *6*, 1600228.

(19) Xiao, L.; Chen, S.; Gao, K.; Peng, X.; Liu, F.; Cao, Y.; Wong, W.-Y.; Wong, W.-K.; Zhu, X. New Terthiophene-Conjugated Porphyrin Donors for Highly Efficient Organic Solar Cells. *ACS Appl. Mater. Interfaces* **2016**, *8*, 30176–30183.

(20) Gao, K.; Li, L.; Lai, T.; Xiao, L.; Huang, Y.; Huang, F.; Peng, J.; Cao, Y.; Liu, F.; Russell, T. P. et al. Deep Absorbing Porphyrin Small Molecule for High-Performance Organic Solar Cells with Very Low Energy Losses. *J. Am. Chem. Soc.* **2015**, *137*, 7282–7285.

(21) Liu, Y.; Chen, C.-C.; Hong, Z.; Gao, J.; (Michael) Yang, Y.; Zhou, H.; Dou, L.; Li, G.; Yang, Y. Solution-Processed Small-Molecule Solar Cells: Breaking the 10% Power Conversion Efficiency. *Sci. Rep.* **2013**, *3*, 3356.

(22) Oh, S.; Badgujar, S.; Kim, D. H.; Lee, W.-E.; Khan, N.; Jahandar, M.; Rasool, S.; Song, C. E.; Lee, H. K.; Shin, W. S. et al. A Thermally and Mechanically Stable Solar Cell Made of a Small-Molecule Donor and a Polymer Acceptor. *J. Mater. Chem. A* **2017**, *5*, 15923–15931.

(23) Liu, W.; Zhou, Z.; Vergote, T.; Xu, S.; Zhu, X. A Thieno[3,4-*b*]thiophene-Based Small-Molecule Donor with a π-Extended Dithienobenzodithiophene Core for Efficient Solution-Processed Organic Solar Cells. *Mater. Chem. Front.* **2017**, *1*, 2349–2355.

(24) Huang, Y.; Wen, W.; Mukherjee, S.; Ade, H.; Kramer, E. J.; Bazan, G. C. High-Molecular-Weight Insulating Polymers Can Improve the Performance of Molecular Solar Cells. *Adv. Mater.* **2014**, *26*, 4168–4172.

(25) Cuesta, V.; Vartanian, M.; de la Cruz, P.; Singhal, R.; Sharma, G. D.; Langa, F. Comparative Study on the Photovoltaic Characteristics of A-D-A and D-A-D Molecules Based on Zn-porphyrin; a D-A-D Molecule with Over 8.0% Efficiency. *J. Mater. Chem. A* **2017**, *5*, 1057–1065.

(26) Zhang, Q.; Wang, Y.; Kan, B.; Wan, X.; Liu, F.; Ni, W.; Feng, H.; Russell, T. P.; Chen, Y. A Solution-Processed High Performance Organic Solar Cell Using a Small Molecule with the Thieno[3,2-*b*]thiophene Central Unit. *Chem. Commun.* **2015**, *51*, 15268–15271.

(27) Busireddy, M. R.; Chereddy, N. R.; Shanigaram, B.; Kotamarthi, B.; Biswas, S.; Sharma, G. D.; Vaidya, J. R. Dithieno[3,2-*b*:2',3'-*d*]pyrrole-benzo[*c*][1,2,5]thiadiazole Conjugate Small Molecule Donors: Effect of Fluorine Content on Their Photovoltaic Properties. *Phys. Chem. Chem. Phys.* **2017**, *19*, 20513–20522.

(28) Guo, Y.-Q.; Wang, Y.; Song, L.-C.; Liu, F.; Wan, X.; Zhang, H.; Chen, Y. Small Molecules with Asymmetric 4-Alkyl-8-alkoxybenzo[1,2-*b*:4,5-*b*']dithiophene as the Central Unit for High-Performance Solar Cells with High Fill Factors. *Chem. Mater.* **2017**, *29*, 3694–3703.

(29) Yuan, L.; Zhao, Y.; Zhang, J.; Zhang, Y.; Zhu, L.; Lu, K.; Yan, W.; Wei, Z. Oligomeric Donor Material for High-Efficiency Organic Solar Cells: Breaking Down a Polymer. *Adv. Mater.* **2015**, *27*, 4229–4233.

(30) Zhou, J.; Zuo, Y.; Wan, X.; Long, G.; Zhang, Q.; Ni, W.; Liu, Y.; Li, Z.; He, G.; Li, C. et al. Solution-Processed and High-Performance Organic Solar Cells Using Small Molecules with a Benzodithiophene Unit. *J. Am. Chem. Soc.* **2013**, *135*, 8484–8487.

(31) Du, Z.; Chen, W.; Chen, Y.; Qiao, S.; Bao, X.; Wen, S.; Sun, M.; Han, L.; Yang, R. High Efficiency Solution-Processed Two-Dimensional Small Molecule Organic Solar Cells Obtained *via* Low-Temperature Thermal Annealing. *J. Mater. Chem. A* **2014**, *2*, 15904–15911.

(32) Li, H.; Fang, J.; Zhang, J.; Zhou, R.; Wu, Q.; Deng, D.; Abdullah Adil, M.; Lu, K.; Guo, X.; Wei, Z. A Novel Small Molecule Based on Naphtho[1,2-*b*:5,6-*b*']dithiophene Benefits Both Fullerene and Non-Fullerene Solar Cells. *Mater. Chem. Front.* **2018**, *2*, 143–148.

(33) Zhang, S.; Zhang, J.; Abdelsamie, M.; Shi, Q.; Zhang, Y.; Parker, T. C.; Jucov, E. V.; Timofeeva, T. V.; Amassian, A.; Bazan, G. C. et al. Intermediate-Sized Conjugated Donor Molecules for Organic Solar Cells: Comparison of Benzodithiophene and Benzobisthiazole-Based Cores. *Chem. Mater.* **2017**, *29*, 7880–7887.

(34) Liang, R.-Z.; Wang, K.; Wolf, J.; Babics, M.; Wucher, P.; Thehaiban, M. K. A.; Beaujuge, P. M. Benzo[1,2-*b*:4,5-*b*']Dithiophene-6,7-Difluoroquinoxaline Small Molecule Donors with >8% BHJ Solar Cell Efficiency. *Adv. Energy Mater.* **2017**, *7*, 1602804.

(35) Ye, C.; Wang, Y.; Bi, Z.; Guo, X.; Fan, Q.; Chen, J.; Ou, X.; Ma, W.; Zhang, M. High-Performance Organic Solar Cells Based on a Small Molecule with Thieno[3,2-*b*]thiophene as π-Bridge. *Org. Electron.* **2018**, *53*, 273–279.

(36) Li, M.; Qiu, Z.; Zhang, G.; Liu, Y.; Xiong, L.; Bai, D.; Zhu, M.; Peng, Q.; Zhu, W. Efficient Chemical Structure and Device Engineering for Achieving Difluorinated 2,2'-bithiophene-Based Small Molecular Organic Solar Cells with 9.0% Efficiency. *J. Mater. Chem. A* **2018**, *6*, 12493–12505.

(37) Cheng, M.; Chen, C.; Yang, X.; Huang, J.; Zhang, F.; Xu, B.; Sun, L. Novel Small Molecular Materials Based on Phenoxazine Core Unit for Efficient Bulk Heterojunction Organic Solar Cells and Perovskite Solar Cells. *Chem. Mater.* **2015**, *27*, 1808–1814.

(38) Deng, D.; Zhang, Y.; Wang, Z.; Wu, Q.; Ma, W.; Lu, K.; Wei, Z. A Simple but Efficient Small Molecule with a High Open Circuit Voltage of 1.07 V in Solution-Processable Organic Solar Cells. *Asian J. Org. Chem.* **2018**, *7*, 558–562.

(39) Zhang, Z.; Zhou, Z.; Hu, Q.; Liu, F.; Russell, T. P.; Zhu, X. 1,3-Bis(thieno[3,4-*b*]thiophen-6-yl)-4*H*-thieno[3,4-*c*]pyrrole-4,6(5*H*)-dione-Based Small-Molecule Donor for Efficient Solution-Processed Solar Cells. *ACS Appl. Mater. Interfaces* **2017**, *9*, 6213–6219.

(40) Cheacharoen, R.; Mateker, W. R.; Zhang, Q.; Kan, B.; Sarkisian, D.; Liu, X.; Love, J. A.; Wan, X.; Chen, Y.; Nguyen, T.-Q. et al. Assessing the Stability of High Performance Solution Processed Small Molecule Solar Cells. *Sol. Energy Mater. Sol. Cells* **2017**, *161*, 368–376.

(41) Rout, Y.; Misra, R.; Singhal, R.; Biswas, S.; Sharma, G. D. Phenothiazine-Based Small-Molecule Organic Solar Cells with Power Conversion Efficiency Over 7% and Open Circuit Voltage of About 1.0 V Using Solvent Vapor Annealing. *Phys. Chem. Chem. Phys.* **2018**, *20*, 6321–6329.

(42) Min, J.; Cui, C.; Heumueller, T.; Fladischer, S.; Cheng, X.; Spiecker, E.; Li, Y.; Brabec, C. J. Side-Chain Engineering for Enhancing the Properties of Small Molecule Solar Cells: A Trade-off Beyond Efficiency. *Adv. Energy Mater.* **2016**, *6*, 1600515.

(43) Qiu, Z.; Xu, X.; Yang, L.; Pei, Y.; Zhu, M.; Peng, Q.; Liu, Y. Tuning the Central Donor Core *via* Intramolecular Noncovalent Interactions Based on D(A-Ar)$_2$ Type Small Molecules for High Performance Organic Solar Cells. *Sol. Energy* **2018**, *161*, 138–147.

(44) Yuan, L.; Lu, K.; Xia, B.; Zhang, J.; Wang, Z.; Wang, Z.; Deng, D.; Fang, J.; Zhu, L.; Wei, Z. Acceptor End-Capped Oligomeric Conjugated Molecules with Broadened Absorption and Enhanced Extinction Coefficients for High-Efficiency Organic Solar Cells. *Adv. Mater.* **2016**, *28*, 5980–5985.

(45) Zhao, Y.; Wang, H.; Zeng, W.; Xia, S.; Zhou, F.; Chen, H.; He, F.; Yang, C. Regulating the Optoelectronic Properties of Small Molecule Donors with Multiple Alternative Electron-Donor and Acceptor Units for Organic Solar Cells. *J. Mater. Chem. A* **2018**, *6*, 8101–8108.

(46) Cheng, M.; Xu, B.; Chen, C.; Yang, X.; Zhang, F.; Tan, Q.; Hua, Y.; Kloo, L.; Sun, L. Phenoxazine-Based Small Molecule Material for Efficient Perovskite Solar Cells and Bulk Heterojunction Organic Solar Cells. *Adv. Energy Mater.* **2015**, *5*, 1401720.

(47) Badgujar, S.; Song, C. E.; Oh, S.; Shin, W. S.; Moon, S.-J.; Lee, J.-C.; Jung, I. H.; Lee, S. K. Highly Efficient and Thermally Stable Fullerene-Free Organic Solar Cells Based on a Small Molecule Donor and Acceptor. *J. Mater. Chem. A* **2016**, *4*, 16335–16340.

(48) Wang, J.-L.; Wu, Z.; Miao, J.-S.; Liu, K.-K.; Chang, Z.-F.; Zhang, R.-B.; Wu, H.-B.; Cao, Y. Solution-Processed Diketopyrrolopyrrole-Containing Small-Molecule Organic

Solar Cells with 7.0% Efficiency: In-Depth Investigation on the Effects of Structure Modification and Solvent Vapor Annealing. *Chem. Mater.* **2015**, *27*, 4338–4348.

(49) Yun, J. H.; Park, S.; Heo, J. H.; Lee, H.-S.; Yoon, S.; Kang, J.; Im, S. H.; Kim, H.; Lee, W.; Kim, B. et al. Enhancement of Charge Transport Properties of Small Molecule Semiconductors by Controlling Fluorine Substitution and Effects on Photovoltaic Properties of Organic Solar Cells and Perovskite Solar Cells. *Chem. Sci.* **2016**, *7*, 6649–6661.

(50) Yang, D.; Sasabe, H.; Sano, T.; Kido, J. Low-Band-Gap Small Molecule for Efficient Organic Solar Cells with a Low Energy Loss below 0.6 eV and a High Open-Circuit Voltage of Over 0.9 V. *ACS Energy Lett.* **2017**, *2*, 2021–2025.

(51) Qin, H.; Li, L.; Guo, F.; Su, S.; Peng, J.; Cao, Y.; Peng, X. Solution-Processed Bulk Heterojunction Solar Cells Based on a Porphyrin Small Molecule with 7% Power Conversion Efficiency. *Energy Environ. Sci.* **2014**, *7*, 1397–1401.

(52) Shen, S.; Jiang, P.; He, C.; Zhang, J.; Shen, P.; Zhang, Y.; Yi, Y.; Zhang, Z.; Li, Z.; Li, Y. Solution-Processable Organic Molecule Photovoltaic Materials with Bithienyl-benzodithiophene Central Unit and Indenedione End Groups. *Chem. Mater.* **2013**, *25*, 2274–2281.

(53) Yunchuang, W.; Bin, K.; Xin, K.; Feng, L.; Xiangjian, W.; Hongtao, Z.; Chenxi, L.; Yongsheng, C. Two Thieno[3,2-*b*]thiophene-Based Small Molecules as Bifunctional Photoactive Materials for Organic Solar Cells. *Sol. RRL* **2018**, *2*, 1700179.

(54) Gautam, P.; Misra, R.; Biswas, S.; Sharma, G. D. A D-π-A1-π-A2 Push-Pull Small Molecule Donor for Solution Processed Bulk Heterojunction Organic Solar Cells. *Phys. Chem. Chem. Phys.* **2016**, *18*, 13918–13926.

(55) Arrechea, S.; Aljarilla, A.; de la Cruz, P.; Singh, M. K.; Sharma, G. D.; Langa, F. New Cyclopentadithiophene (CDT) Linked Porphyrin Donors with Different End-Capping

Acceptors for Efficient Small Molecule Organic Solar Cells. *J. Mater. Chem. C* **2017**, *5*, 4742–4751.

(56) Zhao, J.; Xia, B.; Lu, K.; Deng, D.; Yuan, L.; Zhang, J.; Zhu, L.; Zhu, X.; Li, H.; Wei, Z. Dialkoxyphenyldithiophene-Based Small Molecules with Enhanced Absorption for Solution Processed Organic Solar Cells. *RSC Adv.* **2016**, *6*, 60595–60601.

(57) Jung, J. W.; Russell, T. P.; Jo, W. H. A Small Molecule Composed of Dithienopyran and Diketopyrrolopyrrole as Versatile Electron Donor Compatible with Both Fullerene and Nonfullerene Electron Acceptors for High Performance Organic Solar Cells. *Chem. Mater.* **2015**, *27*, 4865–4870.

(58) Wang, C.; Li, C.; Wen, S.; Ma, P.; Wang, G.; Wang, C.; Li, H.; Shen, L.; Guo, W.; Ruan, S. Enhanced Photovoltaic Performance of Tetrazine-Based Small Molecules with Conjugated Side Chains. *ACS Sustainable Chem. Eng.* **2017**, *5*, 8684–8692.

(59) Busireddy, M. R.; Raju Mantena, V. N.; Chereddy, N. R.; Shanigaram, B.; Kotamarthi, B.; Biswas, S.; Sharma, G. D.; Vaidya, J. R. A Dithieno[3,2-*b*:2',3'-*d*]pyrrole Based, NIR Absorbing, Solution Processable, Small Molecule Donor for Efficient Bulk Heterojunction Solar Cells. *Phys. Chem. Chem. Phys.* **2016**, *18*, 32096–32106.

(60) Love, J. A.; Nagao, I.; Huang, Y.; Kuik, M.; Gupta, V.; Takacs, C. J.; Coughlin, J. E.; Qi, L.; van der Poll, T. S.; Kramer, E. J. et al. Silaindacenodithiophene-Based Molecular Donor: Morphological Features and Use in the Fabrication of Compositionally Tolerant, High-Efficiency Bulk Heterojunction Solar Cells. *J. Am. Chem. Soc.* **2014**, *136*, 3597–3606.

(61) Intemann, J. J.; Yao, K.; Ding, F.; Xu, Y.; Xin, X.; Li, X.; Jen, A. K.-Y. Enhanced Performance of Organic Solar Cells with Increased End Group Dipole Moment in Indacenodithieno[3,2-*b*]thiophene-Based Molecules. *Adv. Funct. Mater.* **2015**, *25*, 4889–4897.

(62) Zhou, J.; Wan, X.; Liu, Y.; Zuo, Y.; Li, Z.; He, G.; Long, G.; Ni, W.; Li, C.; Su, X. et al. Small Molecules Based on Benzo[1,2-*b*:4,5-*b*']dithiophene Unit for High-Performance Solution-Processed Organic Solar Cells. *J. Am. Chem. Soc.* **2012**, *134*, 16345–16351.

(63) Wolf, J.; Babics, M.; Wang, K.; Saleem, Q.; Liang, R.-Z.; Hansen, M. R.; Beaujuge, P. M. Benzo[1,2-*b*:4,5-*b*']dithiophene-Pyrido[3,4-*b*]pyrazine Small-Molecule Donors for Bulk Heterojunction Solar Cells. *Chem. Mater.* **2016**, *28*, 2058–2066.

(64) Wang, K.; Liang, R.-Z.; Wolf, J.; Saleem, Q.; Babics, M.; Wucher, P.; Abdelsamie, M.; Amassian, A.; Hansen, M. R.; Beaujuge, P. M. Donor and Acceptor Unit Sequences Influence Material Performance in Benzo[1,2-*b*:4,5-*b*']dithiophene–6,7-Difluoroquinoxaline Small Molecule Donors for BHJ Solar Cells. *Adv. Funct. Mater.* **2016**, *26*, 7103–7114.

(65) Liu, X.; Sun, Y.; Hsu, B. B. Y.; Lorbach, A.; Qi, L.; Heeger, A. J.; Bazan, G. C. Design and Properties of Intermediate-Sized Narrow Band-Gap Conjugated Molecules Relevant to Solution-Processed Organic Solar Cells. *J. Am. Chem. Soc.* **2014**, *136*, 5697–5708.

(66) Nho, S.; Kim, D. H.; Park, S.; Tran, H. N.; Lim, B.; Cho, S. Carbazole and Rhodanine Based Donor Molecule with Improved Processability for High Performance Organic Photovoltaics. *Dyes Pigm.* **2018**, *151*, 272–278.

(67) Tang, A.; Zhan, C.; Yao, J. Series of Quinoidal Methyl-Dioxocyano-Pyridine Based π-Extended Narrow-Bandgap Oligomers for Solution-Processed Small-Molecule Organic Solar Cells. *Chem. Mater.* **2015**, *27*, 4719–4730.

(68) Moon, M.; Walker, B.; Lee, J.; Park, S. Y.; Ahn, H.; Kim, T.; Lee, T. H.; Heo, J.; Seo, J. H.; Shin, T. J. et al. Dithienogermole-Containing Small-Molecule Solar Cells with 7.3% Efficiency: In-Depth Study on the Effects of Heteroatom Substitution of Si with Ge. *Adv. Energy Mater.* **2015**, *5*, 1402044.

(69) Tu, Q.; Yin, Z.; Ma, Y.; Chen, S.-C.; Zheng, Q. Ladder-Type Heteroheptacene-Cored Semiconductors for Small-Molecule Solar Cells. *Dyes Pigm.* **2018**, *149*, 747–754.

(70) Liu, Y.; Yang, Y. M.; Chen, C.-C.; Chen, Q.; Dou, L.; Hong, Z.; Li, G.; Yang, Y. Solution-Processed Small Molecules Using Different Electron Linkers for High-Performance Solar Cells. *Adv. Mater.* **2013**, *25*, 4657–4662.

(71) Liu, Y.; Sun, Y.; Li, M.; Feng, H.; Ni, W.; Zhang, H.; Wan, X.; Chen, Y. Efficient Carbazole-Based Small-Molecule Organic Solar Cells with an Improved Fill Factor. *RSC Adv.* **2018**, *8*, 4867–4871.

(72) Kan, B.; Li, M.; Zhang, Q.; Liu, F.; Wan, X.; Wang, Y.; Ni, W.; Long, G.; Yang, X.; Feng, H. et al. A Series of Simple Oligomer-like Small Molecules Based on Oligothiophenes for Solution-Processed Solar Cells with High Efficiency. *J. Am. Chem. Soc.* **2015**, *137*, 3886–3893.

(73) Revoju, S.; Biswas, S.; Eliasson, B.; Sharma, G. D. Effect of Acceptor Strength on Optical, Electrochemical and Photovoltaic Properties of Phenothiazine-Based Small Molecule for Bulk Heterojunction Organic Solar Cells. *Dyes Pigm.* **2018**, *149*, 830–842.

(74) Li, Z.; He, G.; Wan, X.; Liu, Y.; Zhou, J.; Long, G.; Zuo, Y.; Zhang, M.; Chen, Y. Solution Processable Rhodanine-Based Small Molecule Organic Photovoltaic Cells with a Power Conversion Efficiency of 6.1%. *Adv. Energy Mater.* **2012**, *2*, 74–77.

(75) Kumar, C. V.; Cabau, L.; Koukaras, E. N.; Viterisi, A.; Sharma, G. D.; Palomares, E. Solution Processed Organic Solar Cells Based on A-D-D'-D-A Small Molecule with Benzo[1,2-*b*:4,5-*b*']dithiophene Donor (D') Unit, Cyclopentadithiophene Donor (D) and Ethylrhodanine Acceptor Unit having 6% Light to Energy Conversion Efficiency. *J. Mater. Chem. A* **2015**, *3*, 4892–4902.

(76) Revoju, S.; Biswas, S.; Eliasson, B.; Sharma, G. D. Asymmetric Triphenylamine-Phenothiazine Based Small Molecules with Varying Terminal Acceptors for Solution

Processed Bulk-Heterojunction Organic Solar Cells. *Phys. Chem. Chem. Phys.* **2018**, *20*, 6390–6400.

(77) Kumar, C. V.; Cabau, L.; Koukaras, E. N.; Sharma, G. D.; Palomares, E. Efficient Solution Processed D1-A-D2-A-D1 Small Molecules Bulk Heterojunction Solar Cells Based on Alkoxy Triphenylamine and Benzo[1,2-*b*:4,5-*b*']thiophene Units. *Org. Electron.* **2015**, *26*, 36–47.

(78) Wang, J.; Wang, W.; Dong, X.; Wang, G.; Zhang, Z.-G.; Li, Y.; Shen, P. STFTYT: A Simple and Broadly Absorbing Small Molecule for Efficient Organic Solar Cells with a Very Low Energy Loss. *Org. Electron.* **2018**, *57*, 45–52.

(79) Min, J.; Luponosov, Y. N.; Gasparini, N.; Xue, L.; Drozdov, F. V.; Peregudova, S. M.; Dmitryakov, P. V.; Gerasimov, K. L.; Anokhin, D. V.; Zhang, Z.-G. et al. Integrated Molecular, Morphological and Interfacial Engineering Towards Highly Efficient and Stable Solution-Processed Small Molecule Solar Cells. *J. Mater. Chem. A* **2015**, *3*, 22695–22707.

(80) Duan, R.; Cui, Y.; Zhao, Y.; Li, C.; Chen, L.; Hou, J.; Wagner, M.; Baumgarten, M.; He, C.; Müllen, K. The Importance of End Groups for Solution-Processed Small-Molecule Bulk-Heterojunction Photovoltaic Cells. *ChemSusChem* **2016**, *9*, 973–980.

(81) Jo, H.; Park, S.; Choi, H.; Lee, S.; Song, K.; Biswas, S.; Sharma, A.; Sharma, G. D.; Ko, J. S,N-Heteropentacene Based Small Molecules with A-D-A Structure for Solution Processed Organic Bulk Heterojunction Solar Cells. *RSC Adv.* **2015**, *5*, 102115–102125.

(82) Gautam, P.; Misra, R.; Sharma, G. D. Dicyanoquinodimethane-Substituted Benzothiadiazole For Efficient Small-Molecule Solar Cells. *Phys. Chem. Chem. Phys.* **2016**, *18*, 7235–7241.

(83) Zhang, X.; Yao, J.; Zhan, C. Boosting Organic Solar Cell Electrical Performance by Introducing Large Aromatics onto Small-Molecule Peripheral Side-Chains. *Adv. Mater. Interfaces* **2016**, *3*, 1600323.

(84) Chen, J.; Duan, L.; Xiao, M.; Wang, Q.; Liu, B.; Xia, H.; Yang, R.; Zhu, W. Tuning the Central Fused Ring and Terminal Units to Improve the Photovoltaic Performance of Ar(A-D)$_2$ Type Small Molecules in Solution-Processed Organic Solar Cells. *J. Mater. Chem. A* **2016**, *4*, 4952–4961.

(85) Kim, J.-H.; Park, J. B.; Yang, H.; Jung, I. H.; Yoon, S. C.; Kim, D.; Hwang, D.-H. Controlling the Morphology of BDTT-DPP-Based Small Molecules *via* End-Group Functionalization for Highly Efficient Single and Tandem Organic Photovoltaic Cells. *ACS Appl. Mater. Interfaces* **2015**, *7*, 23866–23875.

(86) Ni, W.; Wan, X.; Li, M.; Wang, Y.; Chen, Y. A-D-A Small Molecules for Solution-Processed Organic Photovoltaic Cells. *Chem. Commun.* **2015**, *51*, 4936–4950.

(87) Lin, Y.; Ma, L.; Li, Y.; Liu, Y.; Zhu, D.; Zhan, X. A Solution-Processable Small Molecule Based on Benzodithiophene and Diketopyrrolopyrrole for High-Performance Organic Solar Cells. *Adv. Energy Mater.* **2013**, *3*, 1166–1170.

(88) Wang, K.; Guo, B.; Xu, Z.; Guo, X.; Zhang, M.; Li, Y. Solution-Processable Organic Molecule for High-Performance Organic Solar Cells with Low Acceptor Content. *ACS Appl. Mater. Interfaces* **2015**, *7*, 24686–24693.

(89) Do, K.; Cho, N.; Siddiqui, S.; Singh, S. P.; Sharma, G. D.; Ko, J. New D-A-D-A-D Push-Pull Organic Semiconductors with Different Benzo[1,2-*b*:4, 5-*b*'] Dithiophene Cores for Solution Processed Bulk Heterojunction Solar Cells. *Dyes Pigm.* **2015**, *120*, 126–135.

(90) Hoang, Q. V.; Rasool, S.; Oh, S.; Van Vu, D.; Kim, D. H.; Lee, H. K.; Song, C. E.; Lee, S. K.; Lee, J.-C.; Moon, S.-J. et al. Effects of Morphology Evolution on Solution-

Processed Small Molecule Photovoltaics *via* a Solvent Additive. *J. Mater. Chem. C* **2017**, *5*, 7837–7844.

(91) Liang, T.; Xiao, L.; Liu, C.; Gao, K.; Qin, H.; Cao, Y.; Peng, X. Porphyrin Small Molecules Containing Furan- and Selenophene-Substituted Diketopyrrolopyrrole for Bulk Heterojunction Organic Solar Cells. *Org. Electron.* **2016**, *29*, 127–134.

(92) Patil, Y.; Misra, R.; Chen, F. C.; Sharma, G. D. Small Molecule Based N-Phenyl Carbazole Substituted Diketopyrrolopyrroles as Donors for Solution-Processed Bulk Heterojunction Organic Solar Cells. *Phys. Chem. Chem. Phys.* **2016**, *18*, 22999–23005.

(93) Jung, J. W. A Low Band Gap Conjugated Small Molecule Based on Isoindigo Flanked with Diketopyrrolopyrrole for Efficient Organic Solar Cells. *Dyes Pigm.* **2017**, *137*, 512–517.

(94) Tang, A.; Zhan, C.; Yao, J. Comparative Study of Effects of Terminal Non-Alkyl Aromatic and Alkyl Groups on Small-Molecule Solar Cell Performance. *Adv. Energy Mater.* **2015**, *5*, 1500059.

(95) Wang, Z.; Li, Z.; Liu, J.; Mei, J.; Li, K.; Li, Y.; Peng, Q. Solution-Processable Small Molecules for High-Performance Organic Solar Cells with Rigidly Fluorinated 2,2'-Bithiophene Central Cores. *ACS Appl. Mater. Interfaces* **2016**, *8*, 11639–11648.

(96) Lim, N.; Cho, N.; Paek, S.; Kim, C.; Lee, J. K.; Ko, J. High-Performance Organic Solar Cells with Efficient Semiconducting Small Molecules Containing an Electron-Rich Benzodithiophene Derivative. *Chem. Mater.* **2014**, *26*, 2283–2288.

(97) Qian, D.; Liu, B.; Wang, S.; Himmelberger, S.; Linares, M.; Vagin, M.; Müller, C.; Ma, Z.; Fabiano, S.; Berggren, M. et al. Modulating Molecular Aggregation by Facile Heteroatom Substitution of Diketopyrrolopyrrole Based Small Molecules for Efficient Organic Solar Cells. *J. Mater. Chem. A* **2015**, *3*, 24349–24357.

(98) Liu, J.; Sun, Y.; Moonsin, P.; Kuik, M.; Proctor, C. M.; Lin, J.; Hsu, B. B.; Promarak, V.; Heeger, A. J.; Nguyen, T.-Q. Tri-Diketopyrrolopyrrole Molecular Donor Materials for High-Performance Solution-Processed Bulk Heterojunction Solar Cells. *Adv. Mater.* **2013**, *25*, 5898–5903.

(99) Kumar, C. H. P.; Ganesh, K.; Suresh, T.; Sharma, A.; Bhanuprakash, K.; Sharma, G. D.; Chandrasekharam, M. Influence of Thermal and Solvent Annealing on the Morphology and Photovoltaic Performance of Solution Processed, D-A-D Type Small Molecule-Based Bulk Heterojunction Solar Cells. *RSC Adv.* **2015**, *5*, 93579–93590.

(100) Patil, Y.; Misra, R.; Sharma, A.; Sharma, G. D. D-A-D-π-D-A-D Type Diketopyrrolopyrrole Based Small Molecule Electron Donors for Bulk Heterojunction Organic Solar Cells. *Phys. Chem. Chem. Phys.* **2016**, *18*, 16950–16957.

(101) Liu, Y.; Wan, X.; Wang, F.; Zhou, J.; Long, G.; Tian, J.; Chen, Y. High-Performance Solar Cells using a Solution-Processed Small Molecule Containing Benzodithiophene Unit. *Adv. Mater.* **2011**, *23*, 5387–5391.

(102) Duan, X.; Xiao, M.; Chen, J.; Wang, X.; Peng, W.; Duan, L.; Tan, H.; Lei, G.; Yang, R.; Zhu, W. Improving Photovoltaic Performance of the Linear A-Ar-A-Type Small Molecules with Diketopyrropyrrole Arms by Tuning the Linkage Position of the Anthracene Core. *ACS Appl. Mater. Interfaces* **2015**, *7*, 18292–18299.

(103) Patra, D.; Huang, T.-Y.; Chiang, C.-C.; Maturana, R. O. V.; Pao, C.-W.; Ho, K.-C.; Wei, K.-H.; Chu, C.-W. 2-Alkyl-5-thienyl-Substituted Benzo[1,2-*b*:4,5-*b*']dithiophene-Based Donor Molecules for Solution-Processed Organic Solar Cells. *ACS Appl. Mater. Interfaces* **2013**, *5*, 9494–9500.

(104) Yin, Q.-R.; Miao, J.-S.; Wu, Z.; Chang, Z.-F.; Wang, J.-L.; Wu, H.-B.; Cao, Y. Rational Design of Diketopyrrolopyrrole-Based Oligomers for High Performance Small

Molecular Photovoltaic Materials *via* an Extended Framework and Multiple Fluorine Substitution. *J. Mater. Chem. A* **2015**, *3*, 11575–11586.

(105) Fu, L.; Fu, W.; Cheng, P.; Xie, Z.; Fan, C.; Shi, M.; Ling, J.; Hou, J.; Zhan, X.; Chen, H. A Diketopyrrolopyrrole Molecule End-Capped with a Furan-2-carboxylate Moiety: The Planarity of Molecular Geometry and Photovoltaic Properties. *J. Mater. Chem. A* **2014**, *2*, 6589–6597.

(106) Qiu, B.; Yuan, J.; Xiao, X.; He, D.; Qiu, L.; Zou, Y.; Zhang, Z.-g.; Li, Y. Effect of Fluorine Substitution on Photovoltaic Properties of Alkoxyphenyl Substituted Benzo[1,2-*b*:4,5-*b*']dithiophene-Based Small Molecules. *ACS Appl. Mater. Interfaces* **2015**, *7*, 25237–25246.

(107) Bura, T.; Leclerc, N.; Bechara, R.; Lévêque, P.; Heiser, T.; Ziessel, R. Triazatruxene-Diketopyrrolopyrrole Dumbbell-Shaped Molecules as Photoactive Electron Donor for High-Efficiency Solution Processed Organic Solar Cells. *Adv. Energy Mater.* **2013**, *3*, 1118–1124.

(108) Deng, D.; Zhang, Y.; Yuan, L.; He, C.; Lu, K.; Wei, Z. Effects of Shortened Alkyl Chains on Solution-Processable Small Molecules with Oxo-Alkylated Nitrile End-Capped Acceptors for High-Performance Organic Solar Cells. *Adv. Energy Mater.* **2014**, *4*, 1400538.

(109) Vijay Kumar, C.; Cabau, L.; Koukaras, E. N.; Siddiqui, S. A.; Sharma, G. D.; Palomares, E. Efficient Bulk Heterojunction Solar Cells Based on Solution Processed Small Molecules Based on the Same Benzo[1,2-*b*:4, 5-*b*']thiophene Unit as Core Donor and Different Terminal Units. *Nanoscale* **2015**, *7*, 7692–7703.

(110) Patil, Y.; Misra, R.; Chen, F. C.; Keshtov, M. L.; Sharma, G. D. Symmetrical and Unsymmetrical Triphenylamine Based Diketopyrrolopyrroles and Their Use as Donors

for Solution Processed Bulk Heterojunction Organic Solar Cells. *RSC Adv.* **2016**, *6*, 99685–99694.

(111) Sim, J.; Do, K.; Song, K.; Sharma, A.; Biswas, S.; Sharma, G. D.; Ko, J. D-A-D-A-D Push Pull Organic Small Molecules Based on 5,10-Dihydroindolo[3,2-*b*]indole (DINI) Central Core Donor for Solution Processed Bulk Heterojunction Solar Cells. *Org. Electron.* **2016**, *30*, 122–130.

(112) Huang, J.; Zhan, C.; Zhang, X.; Zhao, Y.; Lu, Z.; Jia, H.; Jiang, B.; Ye, J.; Zhang, S.; Tang, A. et al. Solution-Processed DPP-Based Small Molecule that Gives High Photovoltaic Efficiency with Judicious Device Optimization. *ACS Appl. Mater. Interfaces* **2013**, *5*, 2033–2039.

(113) Li, Y.; Lee, D. H.; Lee, J.; Nguyen, T. L.; Hwang, S.; Park, M. J.; Choi, D. H.; Woo, H. Y. Two Regioisomeric π-Conjugated Small Molecules: Synthesis, Photophysical, Packing, and Optoelectronic Properties. *Adv. Funct. Mater.* **2017**, *27*, 1701942.

(114) Bai, H.; Wang, Y.; Cheng, P.; Li, Y.; Zhu, D.; Zhan, X. Acceptor-Donor-Acceptor Small Molecules Based on Indacenodithiophene for Efficient Organic Solar Cells. *ACS Appl. Mater. Interfaces* **2014**, *6*, 8426–8433.

(115) Zhang, C.-H.; Wang, L.-P.; Tan, W.-Y.; Wu, S.-P.; Liu, X.-P.; Yu, P.-P.; Huang, J.; Zhu, X.-H.; Wu, H.-B.; Zhao, C.-Y. et al. Effective Modulation of an Aryl Acetylenic Molecular System Based on Dithienyldiketopyrrolopyrrole for Organic Solar Cells. *J. Mater. Chem. C* **2016**, *4*, 3757–3764.

(116) Patra, D.; Chiang, C.-C.; Chen, W.-A.; Wei, K.-H.; Wu, M.-C.; Chu, C.-W. Solution-Processed Benzotrithiophene-Based Donor Molecules for Efficient Bulk Heterojunction Solar Cells. *J. Mater. Chem. A* **2013**, *1*, 7767–7774.

(117) Yi, Z.; Ni, W.; Zhang, Q.; Li, M.; Kan, B.; Wan, X.; Chen, Y. Effect of Thermal

Annealing on Active Layer Morphology and Performance for Small Molecule Bulk Heterojunction Organic Solar Cells. *J. Mater. Chem. C* **2014**, *2*, 7247–7255.

(118) Jadhav, T.; Misra, R.; Biswas, S.; Sharma, G. D. Bulk Heterojunction Organic Solar Cells Based on Carbazole-BODIPY Conjugate Small Molecules as Donors with High Open Circuit Voltage. *Phys. Chem. Chem. Phys.* **2015**, *17*, 26580–26588.

(119) Hong, J.; Choi, J. Y.; An, T. K.; Sung, M. J.; Kim, Y.; Kim, Y.-H.; Kwon, S.-K.; Park, C. E. A Novel Small Molecule Based on Dithienophosphole Oxide for Bulk Heterojunction Solar Cells Without Pre- or Post-Treatments. *Dyes Pigm.* **2017**, *142*, 516–523.

(120) Hoang, Q. V.; Song, C. E.; Kang, I.-N.; Moon, S.-J.; Lee, S. K.; Lee, J.-C.; Shin, W. S. Low Band Gap Diketopyrrolopyrrole-Based Small Molecule Bulk Heterojunction Solar Cells: Influence of Terminal Side Chain on Morphology and Photovoltaic Performance. *RSC Adv.* **2016**, *6*, 28658–28665.

(121) Ata, I.; Popovic, D.; Lindén, M.; Mishra, A.; Bäuerle, P. The Influence of the Central Acceptor Unit on the Optoelectronic Properties and Photovoltaic Performance of A-D-A-D-A-Type Co-Oligomers. *Org. Chem. Front.* **2017**, *4*, 755–766.

(122) Wang, L.; Zhang, Y.; Yin, N.; Lin, Y.; Gao, W.; Luo, Q.; Tan, H.; Yang, H.-B.; Ma, C.-Q. Correlation of the π-Conjugation Chain Length and the Property and Photovoltaic Performance of Benzo[1,2-*b*:4,5-*b*']dithiophene-Cored A-π-D-π-A Type Molecules. *Sol. Energy Mater. Sol. Cells* **2016**, *157*, 831–843.

(123) Wu, Y.; Cheng, X.; Xu, G.; Li, Y.; Cui, C.; Li, Y. Manipulating the Photovoltaic Properties of Small-Molecule Donor Materials by Tailoring End-Capped Alkylthio Substitution. *RSC Adv.* **2016**, *6*, 108908–108916.

(124) Tang, A.; Zhan, C.; Yao, J.; Zhou, E. Design of Diketopyrrolopyrrole (DPP)-Based Small Molecules for Organic-Solar-Cell Applications. *Adv. Mater.* **2017**, *29*, 1600013.

(125) He, G.; Li, Z.; Wan, X.; Zhou, J.; Long, G.; Zhang, S.; Zhang, M.; Chen, Y. Efficient Small Molecule Bulk Heterojunction Solar Cells With High Fill Factors *via* Introduction of π-Stacking Moieties as End Group. *J. Mater. Chem. A* **2013**, *1*, 1801–1809.

(126) Aldrich, T. J.; Leonardi, M. J.; Dudnik, A. S.; Eastham, N. D.; Harutyunyan, B.; Fauvell, T. J.; Manley, E. F.; Zhou, N.; Butler, M. R.; Harschneck, T. et al. Enhanced Fill Factor Through Chalcogen Side-Chain Manipulation in Small-Molecule Photovoltaics. *ACS Energy Lett.* **2017**, *2*, 2415–2421.

(127) Wang, L.; Yin, L.; Ji, C.; Li, Y. Tuning the Photovoltaic Performance of BT-TPA Chromophore Based Solution-Processed Solar Cells Through Molecular Design Incorporating of Bithiophene Unit and Fluorine-Substitution. *Dyes Pigm.* **2015**, *118*, 37–44.

(128) Wang, L.; Yin, L.; Ji, C.; Zhang, Y.; Gao, H.; Li, Y. High Open-Circuit Voltage of the Solution-Processed Organic Solar Cells Based on Benzothiadiazole–triphenylamine Small Molecules Incorporating π-Linkage. *Org. Electron.* **2014**, *15*, 1138–1148.

(129) Feng, G.; Xu, Y.; Zhang, J.; Wang, Z.; Zhou, Y.; Li, Y.; Wei, Z.; Li, C.; Li, W. All-Small-Molecule Organic Solar Cells Based on an Electron Donor Incorporating Binary Electron-Deficient Units. *J. Mater. Chem. A* **2016**, *4*, 6056–6063.

(130) Li, L.; Huang, Y.; Peng, J.; Cao, Y.; Peng, X. Enhanced Performance of Solution-Processed Solar Cells Based on Porphyrin Small Molecules with a Diketopyrrolopyrrole Acceptor Unit and a Pyridine Additive. *J. Mater. Chem. A* **2013**, *1*, 2144–2150.

(131) Min, J.; Luponosov, Y. N.; Gerl, A.; Polinskaya, M. S.; Peregudova, S. M.; Dmitryakov, P. V.; Bakirov, A. V.; Shcherbina, M. A.; Chvalun, S. N.; Grigorian, S. et al. Alkyl Chain Engineering of Solution-Processable Star-Shaped Molecules for High-Performance Organic Solar Cells. *Adv. Energy Mater.* **2014**, *4*, 1301234.

(132) Wang, H.; Liu, F.; Bu, L.; Gao, J.; Wang, C.; Wei, W.; Russell, T. P. The Role of Additive in Diketopyrrolopyrrole-Based Small Molecular Bulk Heterojunction Solar Cells. *Adv. Mater.* **2013**, *25*, 6519–6525.

(133) Zhu, X.; Xia, B.; Lu, K.; Li, H.; Zhou, R.; Zhang, J.; Zhang, Y.; Shuai, Z.; Wei, Z. Naphtho[1,2-*b*:5,6-*b*']dithiophene-Based Small Molecules for Thick-Film Organic Solar Cells with High Fill Factors. *Chem. Mater.* **2016**, *28*, 943–950.

(134) Chen, Y.; Wang, G.; Yang, L.; Wu, J.; Melkonyan, F. S.; Huang, Y.; Lu, Z.; Marks, T. J.; Facchetti, A. Novel Unsymmetrical Squaraine-Based Small Molecules for Organic Solar Cells. *J. Mater. Chem. C* **2018**, *6*, 847–854.

(135) Xiao, L.; Wang, H.; Gao, K.; Li, L.; Liu, C.; Peng, X.; Wong, W.-Y.; Wong, W.-K.; Zhu, X. A-D-A Type Small Molecules Based on Boron Dipyrromethene for Solution-Processed Organic Solar Cells. *Chem. Asian J.* **2015**, *10*, 1513–1518.

(136) Chandrasekharam, M.; Reddy, M. A.; Ganesh, K.; Sharma, G.; Singh, S. P.; Rao, J. L. Synthesis and Photovoltaic Properties of D-A-D Type Small Molecules Containing Diketopyrrolopyrrole (DPP) Acceptor Central Unit with Different Donor Terminal Units. *Org. Electron.* **2014**, *15*, 2116–2125.

(137) Long, G.; Wan, X.; Kan, B.; Liu, Y.; He, G.; Li, Z.; Zhang, Y.; Zhang, Y.; Zhang, Q.; Zhang, M. et al. Investigation of Quinquethiophene Derivatives with Different End Groups for High Open Circuit Voltage Solar Cells. *Adv. Energy Mater.* **2013**, *3*, 639–646.

(138) Ha, J.-j.; Kim, Y. J.; Park, J.-g.; An, T. K.; Kwon, S.-K.; Park, C. E.; Kim, Y.-H. Thieno[3,4-*c*]pyrrole-4,6-dione-Based Small Molecules for Highly Efficient Solution-Processed Organic Solar Cells. *Chem. Asian J.* **2014**, *9*, 1045–1053.

(139) Gautam, P.; Misra, R.; Siddiqui, S. A.; Sharma, G. D. Unsymmetrical Donor-Acceptor-Acceptor-π-Donor Type Benzothiadiazole-Based Small Molecule for a Solution Pro-

cessed Bulk Heterojunction Organic Solar Cell. *ACS Appl. Mater. Interfaces* **2015**, *7*, 10283–10292.

(140) Li, W.; Kelchtermans, M.; Wienk, M. M.; Janssen, R. A. J. Effect of Structure on the Solubility and Photovoltaic Properties of Bis-Diketopyrrolopyrrole Molecules. *J. Mater. Chem. A* **2013**, *1*, 15150–15157.

(141) Narayanaswamy, K.; Yadagiri, B.; Bagui, A.; Gupta, V.; Singh, S. P. Multichromophore Donor Materials Derived from Diketopyrrolopyrrole and Phenoxazine: Design, Synthesis, and Photovoltaic Performance. *Eur. J. Org. Chem.* **2017**, 4896–4904.

(142) Aytun, T.; Barreda, L.; Ruiz-Carretero, A.; Lehrman, J. A.; Stupp, S. I. Improving Solar Cell Efficiency Through Hydrogen Bonding: A Method for Tuning Active Layer Morphology. *Chem. Mater.* **2015**, *27*, 1201–1209.

(143) Bürckstümmer, H.; Tulyakova, E. V.; Deppisch, M.; Lenze, M. R.; Kronenberg, N. M.; Gsänger, M.; Stolte, M.; Meerholz, K.; Würthner, F. Efficient Solution-Processed Bulk Heterojunction Solar Cells by Antiparallel Supramolecular Arrangement of Dipolar Donor-Acceptor Dyes. *Angew. Chem., Int. Ed.* **2011**, *50*, 11628–11632.

(144) Liu, Y.; Wan, X.; Wang, F.; Zhou, J.; Long, G.; Tian, J.; You, J.; Yang, Y.; Chen, Y. Spin-Coated Small Molecules for High Performance Solar Cells. *Adv. Energy Mater.* **2011**, *1*, 771–775.

(145) Liang, L.; Wang, J.-T.; Xiang, X.; Ling, J.; Zhao, F.-G.; Li, W.-S. Influence of Moiety Sequence on the Performance of Small Molecular Photovoltaic Materials. *J. Mater. Chem. A* **2014**, *2*, 15396–15405.

(146) Du, Z.; Chen, W.; Qiu, M.; Chen, Y.; Wang, N.; Wang, T.; Sun, M.; Yu, D.; Yang, R. Utilizing Alkoxyphenyl Substituents for Side-Chain Engineering of Efficient Benzo[1,2-*b*:4,5-*b*']dithiophene-Based Small Molecule Organic Solar Cells. *Phys. Chem. Chem. Phys.* **2015**, *17*, 17391–17398.

(147) Walker, B.; Tamayo, A. B.; Dang, X.-D.; Zalar, P.; Seo, J. H.; Garcia, A.; Tantiwiwat, M.; Nguyen, T.-Q. Nanoscale Phase Separation and High Photovoltaic Efficiency in Solution-Processed, Small-Molecule Bulk Heterojunction Solar Cells. *Adv. Funct. Mater.* **2009**, *19*, 3063–3069.

(148) Choi, Y. S.; Jo, W. H. A Strategy to Enhance Both V_{OC} and J_{SC} of A-D-A Type Small Molecules Based on Diketopyrrolopyrrole for High Efficient Organic Solar Cells. *Org. Electron.* **2013**, *14*, 1621–1628.

(149) Loser, S.; Miyauchi, H.; Hennek, J. W.; Smith, J.; Huang, C.; Facchetti, A.; Marks, T. J. A "zig-zag" Naphthodithiophene Core for Increased Efficiency in Solution-Processed Small Molecule Solar Cells. *Chem. Commun.* **2012**, *48*, 8511–8513.

(150) Shang, Q.; Wang, M.; Wei, J.; Zheng, Q. Indenothiophene-Based Asymmetric Small Molecules for Organic Solar Cells. *RSC Adv.* **2017**, *7*, 18144–18150.

(151) Luponosov, Y. N.; Solodukhin, A. N.; Mannanov, A. L.; Trukhanov, V. A.; Peregudova, S. M.; Pisarev, S. A.; Bakirov, A. V.; Shcherbina, M. A.; Chvalun, S. N.; Paraschuk, D. Y. et al. Highly Soluble and Thermally Stable Alkyl-Free Star-Shaped D-π-A Oligomer with Electron-Withdrawing Phenyldicyanovinyl Groups for Organic Photovoltaics. *Org. Electron.* **2017**, *51*, 180–189.

(152) Liu, F.; Fan, H.; Zhang, Z.; Zhu, X. Low-Bandgap Small-Molecule Donor Material Containing Thieno[3,4-*b*]thiophene Moiety for High-Performance Solar Cells. *ACS Appl. Mater. Interfaces* **2016**, *8*, 3661–3668.

(153) Wang, W.; Shen, P.; Dong, X.; Weng, C.; Wang, G.; Bin, H.; Zhang, J.; Zhang, Z.-G.; Li, Y. Development of Spiro[cyclopenta[1,2-*b*:5,4-*b*']dithiophene-4,9'-fluorene]-Based A-π-D-π-A Small Molecules with Different Acceptor Units for Efficient Organic Solar Cells. *ACS Appl. Mater. Interfaces* **2017**, *9*, 4614–4625.

(154) Wessendorf, C. D.; Schulz, G. L.; Mishra, A.; Kar, P.; Ata, I.; Weidelener, M.; Urdanpilleta, M.; Hanisch, J.; Mena-Osteritz, E.; Lindén, M. et al. Efficiency Improvement of Solution-Processed Dithienopyrrole-Based A-D-A Oligothiophene Bulk-Heterojunction Solar Cells by Solvent Vapor Annealing. *Adv. Energy Mater.* **2014**, *4*, 1400266.

(155) Sun, S.-X.; Huo, Y.; Li, M.-M.; Hu, X.; Zhang, H.-J.; Zhang, Y.-W.; Zhang, Y.-D.; Chen, X.-L.; Shi, Z.-F.; Gong, X. et al. Understanding the Halogenation Effects in Diketopyrrolopyrrole-Based Small Molecule Photovoltaics. *ACS Appl. Mater. Interfaces* **2015**, *7*, 19914–19922.

(156) Gedefaw, D.; Prosa, M.; Bolognesi, M.; Seri, M.; Andersson, M. R. Recent Development of Quinoxaline Based Polymers/Small Molecules for Organic Photovoltaics. *Adv. Energy Mater.* **2017**, *7*, 1700575.

(157) Tao, Q.; Duan, L.; Xiong, W.; Huang, G.; Wang, P.; Tan, H.; Wang, Y.; Yang, R.; Zhu, W. D(A-A')$_2$ Architecture: An Efficient Strategy to Improve Photovoltaic Performance of Small Molecules for Solution-Processed Organic Solar Cells. *Dyes Pigm.* **2016**, *133*, 153–160.

(158) Yong, W.; Zhang, M.; Xin, X.; Li, Z.; Wu, Y.; Guo, X.; Yang, Z.; Hou, J. Solution-Processed Indacenodithiophene-Based Small Molecule for Bulk Heterojunction Solar Cells. *J. Mater. Chem. A* **2013**, *1*, 14214–14220.

(159) Paek, S.; Cho, N.; Song, K.; Jun, M.-J.; Lee, J. K.; Ko, J. Efficient Organic Semiconductors Containing Fluorine-Substituted Benzothiadiazole for Solution-Processed Small Molecule Organic Solar Cells. *J. Phys. Chem. C* **2012**, *116*, 23205–23213.

(160) Eastham, N. D.; Dudnik, A. S.; Harutyunyan, B.; Aldrich, T. J.; Leonardi, M. J.; Manley, E. F.; Butler, M. R.; Harschneck, T.; Ratner, M. A.; Chen, L. X. et al. En-

hanced Light Absorption in Fluorinated Ternary Small-Molecule Photovoltaics. *ACS Energy Lett.* **2017**, *2*, 1690–1697.

(161) Wang, J.-L.; Yin, Q.-R.; Miao, J.-S.; Wu, Z.; Chang, Z.-F.; Cao, Y.; Zhang, R.-B.; Wang, J.-Y.; Wu, H.-B.; Cao, Y. Rational Design of Small Molecular Donor for Solution-Processed Organic Photovoltaics with 8.1% Efficiency and High Fill Factor *via* Multiple Fluorine Substituents and Thiophene Bridge. *Adv. Funct. Mater.* **2015**, *25*, 3514–3523.

(162) Chandrasekharan, A.; Hambsch, M.; Jin, H.; Maasoumi, F.; Shaw, P. E.; Raynor, A.; Burn, P. L.; Lo, S.-C.; Meredith, P.; Namdas, E. B. Effect of Capping Group on the Properties of Non-Polymeric Diketopyrrolopyrroles for Solution-Processed Bulk Heterojunction Solar Cells. *Org. Electron.* **2017**, *50*, 339–346.

(163) Luponosov, Y. N.; Min, J.; Solodukhin, A. N.; Bakirov, A. V.; Dmitryakov, P. V.; Shcherbina, M. A.; Peregudova, S. M.; Cherkaev, G. V.; Chvalun, S. N.; Brabec, C. J. et al. Star-Shaped D-π-A Oligothiophenes with a Tris(2-methoxyphenyl)amine Core and Alkyldicyanovinyl Groups: Synthesis and Physical and Photovoltaic Properties. *J. Mater. Chem. C* **2016**, *4*, 7061–7076.

(164) Lin, Y.; Ma, L.; Li, Y.; Liu, Y.; Zhu, D.; Zhan, X. Small-Molecule Solar Cells with Fill Factors up to 0.75 *via* a Layer-by-Layer Solution Process. *Adv. Energy Mater.* **2014**, *4*, 1300626.

(165) Li, M.; Ni, W.; Wan, X.; Zhang, Q.; Kan, B.; Chen, Y. Benzo[1,2-*b*:4,5-*b*']dithiophene (BDT)-Based Small Molecules for Solution Processed Organic Solar Cells. *J. Mater. Chem. A* **2015**, *3*, 4765–4776.

(166) Liu, D.; Xiao, M.; Du, Z.; Yan, Y.; Han, L.; Roy, V. A. L.; Sun, M.; Zhu, W.; Lee, C. S.; Yang, R. Solution-Processed, Indacenodithiophene-Based, Small-Molecule

Organic Field-Effect Transistors and Solar Cells. *J. Mater. Chem. C* **2014**, *2*, 7523–7530.

(167) Chen, Y.; Wan, X.; Long, G. High Performance Photovoltaic Applications Using Solution-Processed Small Molecules. *Acc. Chem. Res.* **2013**, *46*, 2645–2655.

(168) Huang, Y.; Li, L.; Peng, X.; Peng, J.; Cao, Y. Solution Processed Small Molecule Bulk Heterojunction Organic Photovoltaics Based on a Conjugated Donor-Acceptor Porphyrin. *J. Mater. Chem.* **2012**, *22*, 21841–21844.

(169) Cui, C.; Min, J.; Ho, C.-L.; Ameri, T.; Yang, P.; Zhao, J.; Brabec, C. J.; Wong, W.-Y. A New Two-Dimensional Oligothiophene End-Capped with Alkyl Cyanoacetate Groups for Highly Efficient Solution-Processed Organic Solar Cells. *Chem. Commun.* **2013**, *49*, 4409–4411.

(170) Liao, X.; Wu, F.; Zhang, L.; Chen, L.; Chen, Y. Solution-Processed Small Molecules Based on Benzodithiophene and Difluorobenzothiadiazole for Inverted Organic Solar Cells. *Polym. Chem.* **2015**, *6*, 7726–7736.

(171) Min, J.; Luponosov, Y. N.; Baran, D.; Chvalun, S. N.; Shcherbina, M. A.; Bakirov, A. V.; Dmitryakov, P. V.; Peregudova, S. M.; Kausch-Busies, N.; Ponomarenko, S. A. et al. Effects of Oligothiophene π-Bridge Length on Physical and Photovoltaic Properties of Star-Shaped Molecules for Bulk Heterojunction Solar Cells. *J. Mater. Chem. A* **2014**, *2*, 16135–16147.

(172) Li, P.; Tong, H.; Liu, J.; Ding, J.; Xie, Z.; Wang, L. An A'-A-D-A-A' Type Small Molecule Based on 2,7-Carbazole for Solution-Processed Organic Solar Cells with High Open-Circuit Voltage. *RSC Adv.* **2013**, *3*, 23098–23104.

(173) Liu, X.; Li, S.; Li, J.; Wang, J.; Tan, Z.; Yan, F.; Li, H.; Lo, Y. H.; Chui, C.-H.; Wong, W.-Y. Synthesis, Characterization and Photovoltaic Properties of Benzo[1,2-*b*:4,5-*b*']dithiophene-Bridged Molecules. *RSC Adv.* **2014**, *4*, 63260–63267.

(174) Lee, O. P.; Yiu, A. T.; Beaujuge, P. M.; Woo, C. H.; Holcombe, T. W.; Millstone, J. E.; Douglas, J. D.; Chen, M. S.; Fréchet, J. M. J. Efficient Small Molecule Bulk Heterojunction Solar Cells with High Fill Factors *via* Pyrene-Directed Molecular Self-Assembly. *Adv. Mater.* **2011**, *23*, 5359–5363.

(175) Lin, L.-Y.; Lu, C.-W.; Huang, W.-C.; Chen, Y.-H.; Lin, H.-W.; Wong, K.-T. New A-A-D-A-A-Type Electron Donors for Small Molecule Organic Solar Cells. *Org. Lett.* **2011**, *13*, 4962–4965.

(176) Lim, H. C.; Kim, J.-J.; Jang, J.; Hong, J.-I. Effect of the π-Linker on the Performance of Organic Photovoltaic Devices Based on Push-Pull D-π-π-A Molecules. *New J. Chem.* **2018**, *42*, 11458–11464.

(177) Lin, J. D. A.; Liu, J.; Kim, C.; Tamayo, A. B.; Proctor, C. M.; Nguyen, T.-Q. Effect of Structural Variation on Photovoltaic Characteristics of Phenyl Substituted Diketopyrrolopyrroles. *RSC Adv.* **2014**, *4*, 14101–14108.

(178) Schulze, K.; Uhrich, C.; Schüppel, R.; Leo, K.; Pfeiffer, M.; Brier, E.; Reinold, E.; Bäuerle, P. Efficient Vacuum-Deposited Organic Solar Cells Based on a New Low-Bandgap Oligothiophene and Fullerene C_{60}. *Adv. Mater.* **2006**, *18*, 2872–2875.

(179) Castro, E.; Cabrera-Espinoza, A.; Deemer, E.; Echegoyen, L. Low-Energy-Gap Organic Based Acceptor-Donor-Acceptor π-Conjugated Small Molecules for Bulk-Heterojunction Organic Solar Cells. *Eur. J. Org. Chem.* **2015**, *2015*, 4629–4634.

(180) Huo, Y.; Zhu, J.; Wang, X.-Z.; Yan, C.; Chai, Y.-F.; Chen, Z.-Z.; Zhan, X.; Zhang, H.-L. Small Molecule Donors Based on Benzodithiophene and Diketopyrrolopyrrole Compatible with Both Fullerene and Non-Fullerene Acceptors. *J. Mater. Chem. C* **2018**, *6*, 5843–5848.

(181) Shaker, M.; Lee, J.-H.; Trinh, C. K.; Kim, W.; Lee, K.; Lee, J.-S. A Facile Method to

Synthesize [A'(D'AD)$_2$]-Based Push-Pull small Molecules for Organic Photovoltaics. *RSC Adv.* **2015**, *5*, 66005–66012.

(182) Yuan, L.; Zhao, Y.; Lu, K.; Deng, D.; Yan, W.; Wei, Z. Small Molecules Incorporating Regioregular Oligothiophenes and Fluorinated Benzothiadiazole Groups for Solution-Processed Organic Solar Cells. *J. Mater. Chem. C* **2014**, *2*, 5842–5849.

(183) Zhang, J.; Xu, L.; Chen, J.; Shen, P.; Ye, M.; Yuan, N.-Y.; Ding, J.-N. A Star-Shaped Photovoltaic Organic Molecule Based on 1,3-Diethyl-2-thiobarbituric Acid Reaches a Power Conversion Efficiency of 3.07%. *Thin Solid Films* **2018**, *645*, 129–133.

(184) Sharma, G. D.; Reddy, M. A.; Ganesh, K.; Singh, S. P.; Chandrasekharam, M. Indole and Triisopropyl Phenyl as Capping Units for a Diketopyrrolopyrrole (DPP) Acceptor Central Unit: An Efficient D-A-D Type Small Molecule for Organic Solar Cells. *RSC Adv.* **2014**, *4*, 732–742.

(185) Deng, J.; Chen, J.; Tao, Q.; Yan, D.; Fu, Y.; Tan, H. Improved Photovoltaic Performance of 2,7-Pyrene Based Small Molecules *via* the Use of 3-Carbazole as Terminal Unit. *Tetrahedron* **2018**, *74*, 3989–3995.

(186) Yoo, S.; Domercq, B.; Kippelen, B. Efficient Thin-Film Organic Solar Cells Based on Pentacene/C_{60} Heterojunctions. *Appl. Phys. Lett.* **2004**, *85*, 5427–5429.

(187) Bürckstümmer, H.; Kronenberg, N. M.; Gsänger, M.; Stolte, M.; Meerholz, K.; Würthner, F. Tailored Merocyanine Dyes for Solution-Processed BHJ Solar Cells. *J. Mater. Chem.* **2010**, *20*, 240–243.

(188) Ryu, K. Y.; Sung, D.-B.; Won, S.-Y.; Jo, A.; Ahn, K.; Kim, H. Y.; ArulKashmir, A.; Kwak, K.; Lee, C.; Kim, W.-S. et al. Synthesis of Organic Semiconductor Bearing B←N Bridged Thienylthiazole and Diketopyrrolopyrrole for the Applicaton of High Open-Circuit Voltage Organic Photovoltaics. *Dyes Pigm.* **2018**, *149*, 858–866.

(189) Verreet, B.; Schols, S.; Cheyns, D.; Rand, B. P.; Gommans, H.; Aernouts, T.; Heremans, P.; Genoe, J. The Characterization of Chloroboron (III) Subnaphthalocyanine Thin Films and Their Application as a Donor Material for Organic Solar Cells. *J. Mater. Chem.* **2009**, *19*, 5295–5297.

(190) Tamayo, A. B.; Walker, B.; Nguyen, T.-Q. A Low Band Gap, Solution Processable Oligothiophene with a Diketopyrrolopyrrole Core for Use in Organic Solar Cells. *J. Phys. Chem. C* **2008**, *112*, 11545–11551.

(191) Chu, C.-W.; Shao, Y.; Shrotriya, V.; Yang, Y. Efficient Photovoltaic Energy Conversion in Tetracene-C_{60} Based Heterojunctions. *Appl. Phys. Lett.* **2005**, *86*, 243506.

(192) Alqahtani, O.; Babics, M.; Gorenflot, J.; Savikhin, V.; Ferron, T.; Balawi, A. H.; Paulke, A.; Kan, Z.; Pope, M.; Clulow, A. J. et al. Mixed Domains Enhance Charge Generation and Extraction in Bulk-Heterojunction Solar Cells with Small-Molecule Donors. *Adv. Energy Mater.* **2018**, *8*, 1702941.

(193) Mutolo, K. L.; Mayo, E. I.; Rand, B. P.; Forrest, S. R.; Thompson, M. E. Enhanced Open-Circuit Voltage in Subphthalocyanine/C_{60} Organic Photovoltaic Cells. *J. Am. Chem. Soc.* **2006**, *128*, 8108–8109.

(194) Mei, J.; Graham, K. R.; Stalder, R.; Reynolds, J. R. Synthesis of Isoindigo-Based Oligothiophenes for Molecular Bulk Heterojunction Solar Cells. *Org. Lett.* **2010**, *12*, 660–663.

(195) Kronenberg, N. M.; Deppisch, M.; Wurthner, F.; Lademann, H. W. A.; Deing, K.; Meerholz, K. Bulk Heterojunction Organic Solar Cells Based on Merocyanine Colorants. *Chem. Commun.* **2008**, 6489–6491.

(196) Rousseau, T.; Cravino, A.; Bura, T.; Ulrich, G.; Ziessel, R.; Roncali, J. BODIPY Derivatives as Donor Materials for Bulk Heterojunction Solar Cells. *Chem. Commun.* **2009**, 1673–1675.

(197) Lloyd, M. T.; Mayer, A. C.; Subramanian, S.; Mourey, D. A.; Herman, D. J.; Bapat, A. V.; Anthony, J. E.; Malliaras, G. G. Efficient Solution-Processed Photovoltaic Cells Based on an Anthradithiophene/Fullerene Blend. *J. Am. Chem. Soc.* **2007**, *129*, 9144–9149.

(198) Lloyd, M.; Mayer, A.; Tayi, A.; Bowen, A.; Kasen, T.; Herman, D.; Mourey, D.; Anthony, J.; Malliaras, G. Photovoltaic Cells From a Soluble Pentacene Derivative. *Org. Electron.* **2006**, *7*, 243–248.

(199) Barlier, V. S.; Schlenker, C. W.; Chin, S. W.; Thompson, M. E. Acetylide-Bridged Tetracene Dimers. *Chem. Commun.* **2011**, *47*, 3754–3756.

(200) Sahu, H.; Yang, F.; Ye, X.; Ma, J.; Fang, W.; Ma, H. Designing Promising Molecules for Organic Solar Cells *via* Machine Learning Assisted Virtual Screening. *J. Mater. Chem. A* **2019**, *7*, 17480–17488.

(201) Sahu, H.; Rao, W.; Troisi, A.; Ma, H. Toward Predicting Efficiency of Organic Solar Cells *via* Machine Learning and Improved Descriptors. *Adv. Energy Mater.* **2018**, *8*, 1801032.

(202) Liu, C.; Wang, K.; Gong, X.; Heeger, A. J. Low Bandgap Semiconducting Polymers for Polymeric Photovoltaics. *Chem. Soc. Rev.* **2016**, *45*, 4825–4846.

(203) Ostroverkhova, O. Organic Optoelectronic Materials: Mechanisms and Applications. *Chem. Rev.* **2016**, *116*, 13279–13412.

(204) Thompson, B.; Fréchet, J. Polymer-Fullerene Composite Solar Cells. *Angew. Chem. Int. Ed.* **2008**, *47*, 58–77.

(205) Oberhofer, H.; Reuter, K.; Blumberger, J. Charge Transport in Molecular Materials: An Assessment of Computational Methods. *Chem. Rev.* **2017**, *117*, 10319–10357.

(206) Brédas, J.-L. Mind the Gap! *Mater. Horiz.* **2014**, *1*, 17–19.

(207) Zhang, J.; Zhu, L.; Wei, Z. Toward Over 15% Power Conversion Efficiency for Organic Solar Cells: Current Status and Perspectives. *Small Methods* **2017**, *1*, 1700258.

(208) Burke, T. M.; Sweetnam, S.; Vandewal, K.; McGehee, M. D. Beyond Langevin Recombination: How Equilibrium Between Free Carriers and Charge Transfer States Determines the Open-Circuit Voltage of Organic Solar Cells. *Adv. Energy Mater.* **2015**, *5*, 1500123.

(209) Schwarz, K. N.; Geraghty, P. B.; Jones, D. J.; Smith, T. A.; Ghiggino, K. P. Suppressing Subnanosecond Bimolecular Charge Recombination in a High-Performance Organic Photovoltaic Material. *J. Phys. Chem. C* **2016**, *120*, 24002–24010.

(210) Rolczynski, B. S.; Szarko, J. M.; Son, H. J.; Liang, Y.; Yu, L.; Chen, L. X. Ultrafast Intramolecular Exciton Splitting Dynamics in Isolated Low-Band-Gap Polymers and Their Implications in Photovoltaic Materials Design. *J. Am. Chem. Soc.* **2012**, *134*, 4142–4152.

(211) Kuzmich, A.; Padula, D.; Ma, H.; Troisi, A. Trends in the Electronic and Geometric Structure of Non-Fullerene Based Acceptors for Organic Solar Cells. *Energy Environ. Sci.* **2017**, *10*, 395–401.

(212) Ma, H.; Troisi, A. Modulating the Exciton Dissociation Rate by up to More than Two Orders of Magnitude by Controlling the Alignment of LUMO+1 in Organic Photovoltaics. *J. Phys. Chem. C* **2014**, *118*, 27272–27280.

(213) Liu, T.; Troisi, A. What Makes Fullerene Acceptors Special as Electron Acceptors in Organic Solar Cells and How to Replace Them. *Adv. Mater.* **2013**, *25*, 1038–1041.