Supporting Information for

Analyzing the efficiency, stability and cost potential for fullerene-free organic photovoltaics in one Figure of Merit

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Table S1. Normalized values of number of synthetic steps (NSS), reciprocal yield (RY), number of operation units for the isolation/purification (NUO), number of column chromatographies for the isolation/purification (NCC) and number of hazardous chemicals (NHC) for materials investigated in this work. For this work, all the values are normalized to the maximal values of polymers[S1] (NSSmax = 22; RYmax = 86.9; NUOmax = 39; NCCmax = 13; NHCmax = 44). SC index = 35*N_NSS+25*N_RY+15*N_NUO+15*N_NCC+10*N_NHC

	N_NSS	N_RY	N_NUO	N_NCC	N_NHC	SC index / %	Ref.
P3HT	0.14	0.02	0.1	0	0.09	7.7	[S1]
PCE10	0.73	0.58	0.62	0.54	0.7	64.3	[S1]
PCE11	0.364	0.07	0.333	0.231	0.5	27.9	[S2]
PCBM	0.227	0.266	0.154	0.154	0.136	20.6	[S3]
O-IDTBR	0.5	0.267	0.615	0.461	0.364	43.9	[S4]

Table S2. Photovoltaic parameters of OSCs taken from literature for estimating the i-FoM values.

	V_{OC} / V	J_{SC} / mA cm^{-2}	FF / %	PCE / %	200 hrs Stability	Ref.
P3HT:PCBM	0.56	7.7	65	2.8	0.92	[S5]
PCE10:PCBM	0.82	15.7	68	8.87	0.91	[S6]
PCE11:PCBM	0.73	17.8	70	9.2	0.67	[S7]
P3HT:IDTBR	0.72	12.5	67	6.05	0.98	[S8]
PCE10:IDTBR	1.03	18.5	63	12.0	0.95	-
PCE11:IDTBR	1.08	14.65	62	9.5	1.00	[S9]

Table S3. Parameters used for estimating the SC index of donor:acceptor blends. The SC index (donor) and SC index (acceptor) were calculated according to Po et al.[S1] The D:A ratios of OPV devices are taken from the literature.

	SC index (D) / %	SC index (A) / %	D:A ratio	SC index (M) / %
	Blended with **PCBM**			
P3HT	7.7	20.6	1:1[S10]	14.1
PCE10	64.3	20.6	1:2[S6]	35.2
PCE11	27.9	20.6	1:1.2[S2]	23.9
	Blended with **O-IDTBR**			
P3HT	7.7	43.9	1:1[S4]	25.8
PCE10	64.3	43.9	1:1.5	52.1
PCE11	27.9	43.9	1:1.4[S9]	37.2
	Blended with **i-NFA**			
P3HT	7.7	20.6	1:1	14.1
PCE10	64.3	20.6	1:2	35.2
PCE11	27.9	20.6	1:1.2	23.9

Table S4. Energy levels and bandgaps of the three model polymers used for efficiency prediction using the model described in Figure 2b.

	HOMO / eV	LUMO / eV	Bandgap / eV	Optical / eV	PCE limit / %(1)	PCE limit / %(2)
P3HT	-5.1	-3.2	1.9	1.92	17.6	19.8
PCE10	-5.24	-3.66	1.58	1.58	17.6	19.8
PCE11	-5.34	-3.69	1.65	1.66	17.6	19.8

(1) Calculated under the assumptions of a bandgap-to-V_{OC} loss = 0.5 V, a constant EQE = 0.8 and a FF = 0.75. (2) Calculated under the assumptions of a bandgap-to-V_{OC} loss = 0.45 V, a constant EQE = 0.8 and a FF = 0.8.

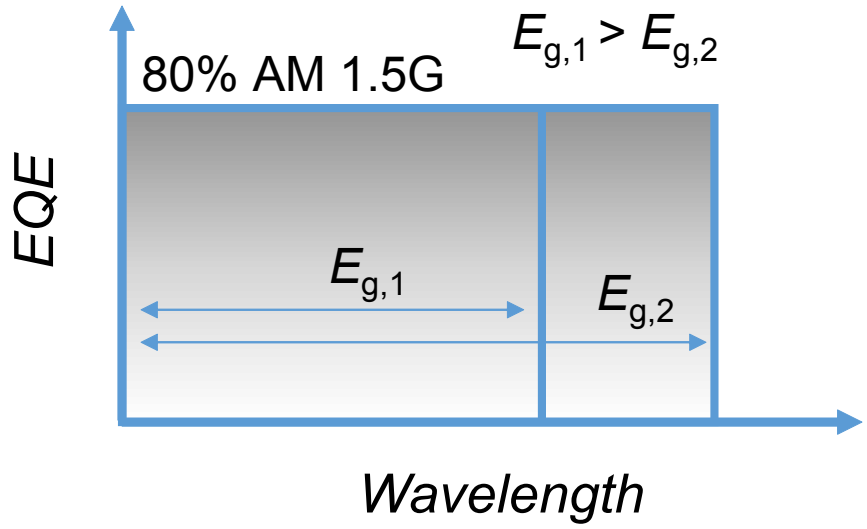

Figure S1. Only the smallest bandgap of donor and acceptor is considered for the J_{SC} calculation under the assumption of rectangular absorption of the AM 1.5G solar spectrum and a constant EQE of 80%.

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