Supporting Materials

Non-Fullerene Acceptor-Based Solar Cells: From structural design to Interface Charge Separation and Charge Transport

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Table S1.Transition energies and oscillators for polymers for n=1.

molecule	state	E (eV)	Absorption peak λ(nm)	Contribution MOs	Strength *f*
P-BZS	S1	3.27	379.02	H → L (0.66639)	1.4863
	S2	3.89	319.15	H-1 → L (0.58321)	0.3679
	S3	3.99	310.98	H-2 → L (0.55825)	0.0352
	S4	4.14	299.37	H → L+1 (0.29482)	0.0379
	S5	4.18	296.12	H → L+1 (0.38820)	0.1495
	S6	4.45	278.19	H → L+2 (0.42496)	0.0399
PDBT-T1	S1	2.87	432.22	H → L (0.64008)	1.5626
	S2	3.36	368.95	H → L+1 (0.40539)	0.1691
	S3	3.54	349.90	H → L+2 (0.31763)	0.1216
	S4	3.67	336.43	H-1 → L (0.27323)	0.0087
	S5	3.76	329.13	H-1 → L (0.28423)	0.1897
	S6	3.87	320.20	H-2 → L (0.35574)	0.1479
QX-M-PO	S1	2.98	416.23	H → L (0.59187)	1.1835
	S2	3.55	349.24	H-2 → L (0.55776)	0.5059
	S3	3.62	342.05	H → L+1 (0.43208)	0.1296
	S4	3.86	320.90	H-1 → L+1 (0.44586)	0.3408
	S5	3.87	320.01	H-8 → L (0.24759)	0.0060
	S6	4.03	307.12	H-3 → L (0.36064)	0.0402
QX-PO	S1	2.95	419.25	H → L (0.57410)	1.1665
	S2	3.55	348.96	H-2 → L (0.50658)	0.5498
	S3	3.60	343.81	H → L+1 (0.36701)	0.0475
	S4	3.84	322.66	H-1 → L+1 (0.44080)	0.3852
	S5	3.87	319.80	H-14 → L (0.24393)	0.0084
	S6	4.01	308.99	H-3 → L (0.36862)	0.0487
QX-PS	S1	2.96	417.79	H → L (0.57592)	1.1747
	S2	3.55	349.23	H-2 → L (0.53626)	0.5458
	S3	3.61	343.45	H → L+1 (0.40308)	0.0877
	S4	3.84	322.16	H-1 → L+1 (0.44722)	0.3727
	S5	3.87	320.11	H-8 → L (0.25663)	0.0075
	S6	4.02	308.23	H → L+2 (0.30622)	0.0255

Table S2. Energy levels of HOMO (H) (eV), LUMO (L) (eV) and energy gap ΔH-L (eV) for ten D/A interfaces.

Interfaces	H	L	Δ_{H-L}
P-BZS/IDIC	-5.09	-3.51	1.58
PDBT-T1/IDIC	-5.08	-3.43	1.65
QX-M-PO/IDIC	-5.05	-3.42	1.63
QX-PO/IDIC	-4.95	-3.46	1.49
QX-PS/IDIC	-5.27	-3.54	1.73
P-BZS/IDTBR	-5.16	-2.72	2.44
PDBT-T1/IDTBR	-5.00	-2.62	2.38
QX-M-PO/IDTBR	-5.07	-2.66	2.41
QX-PO/IDTBR	-4.96	-2.69	2.27
QX-PS/IDTBR	-5.02	-2.66	2.36

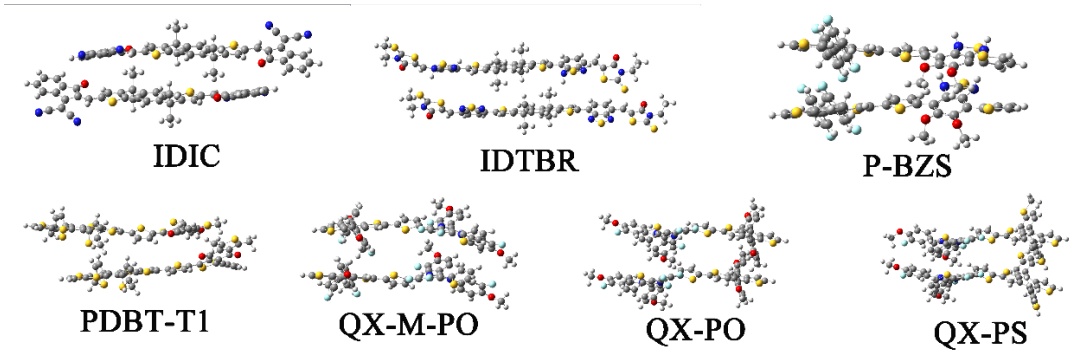

Fig S1. The optimized face-to-face dimer structures of IDIC, IDTBR and five kind ofpolymers.

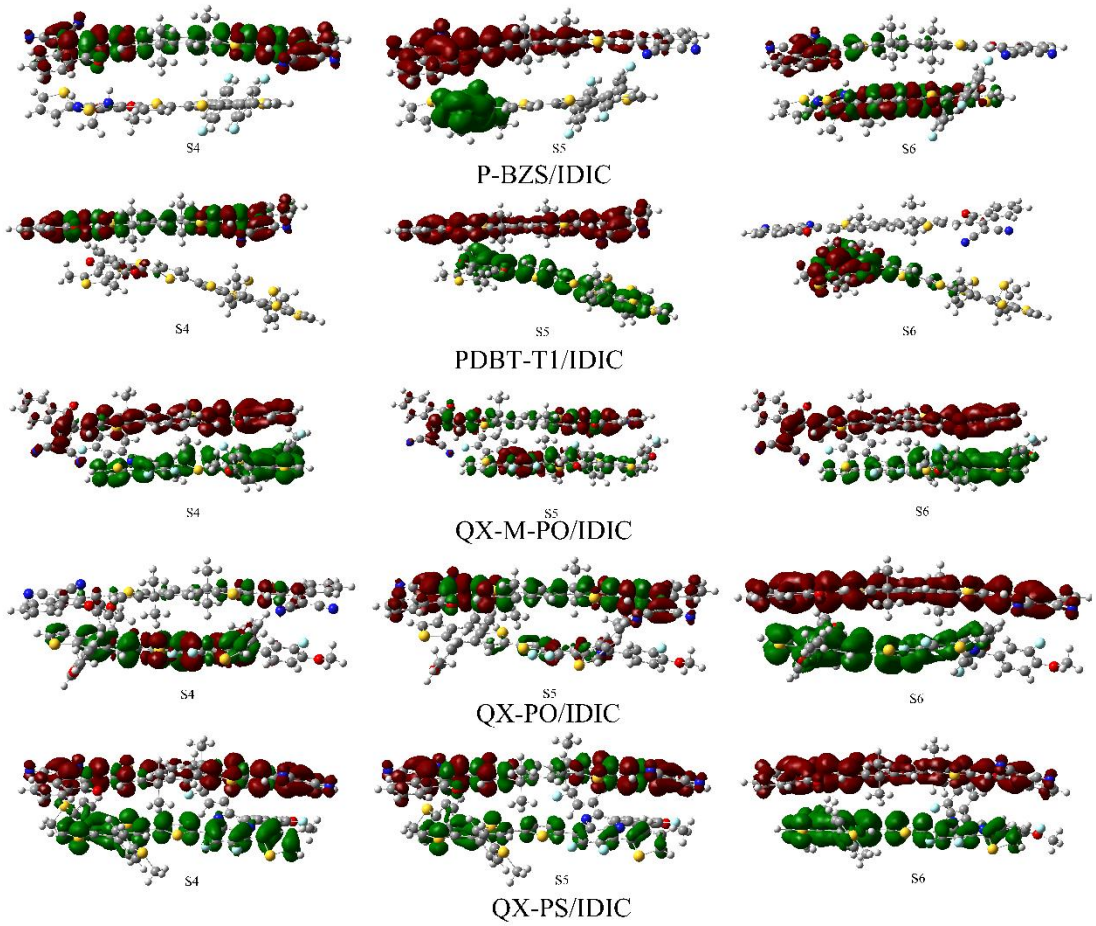

Fig S2. Charge density difference (CDD) plots of polymer/IDIC (S4-S6); where red represents electrons and green represents holes.

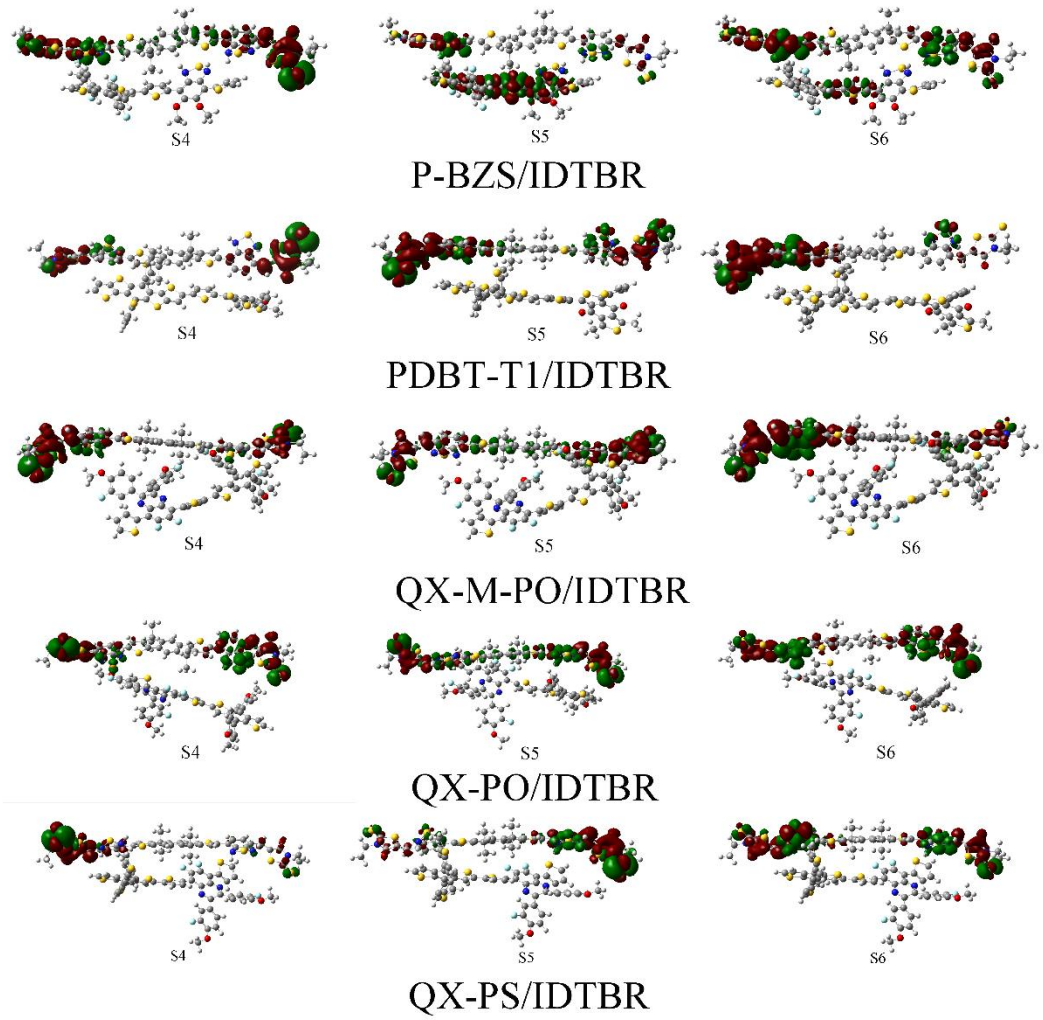

Fig S3. Charge difference densities (CDD) plots of D/A interfaces polymer/IDTBR (S4-S6); where red represents electrons and green represents holes.