Supporting Information for: Boron-based non-fullerene small molecule acceptors via nitrogen substitutions: a theoretical study

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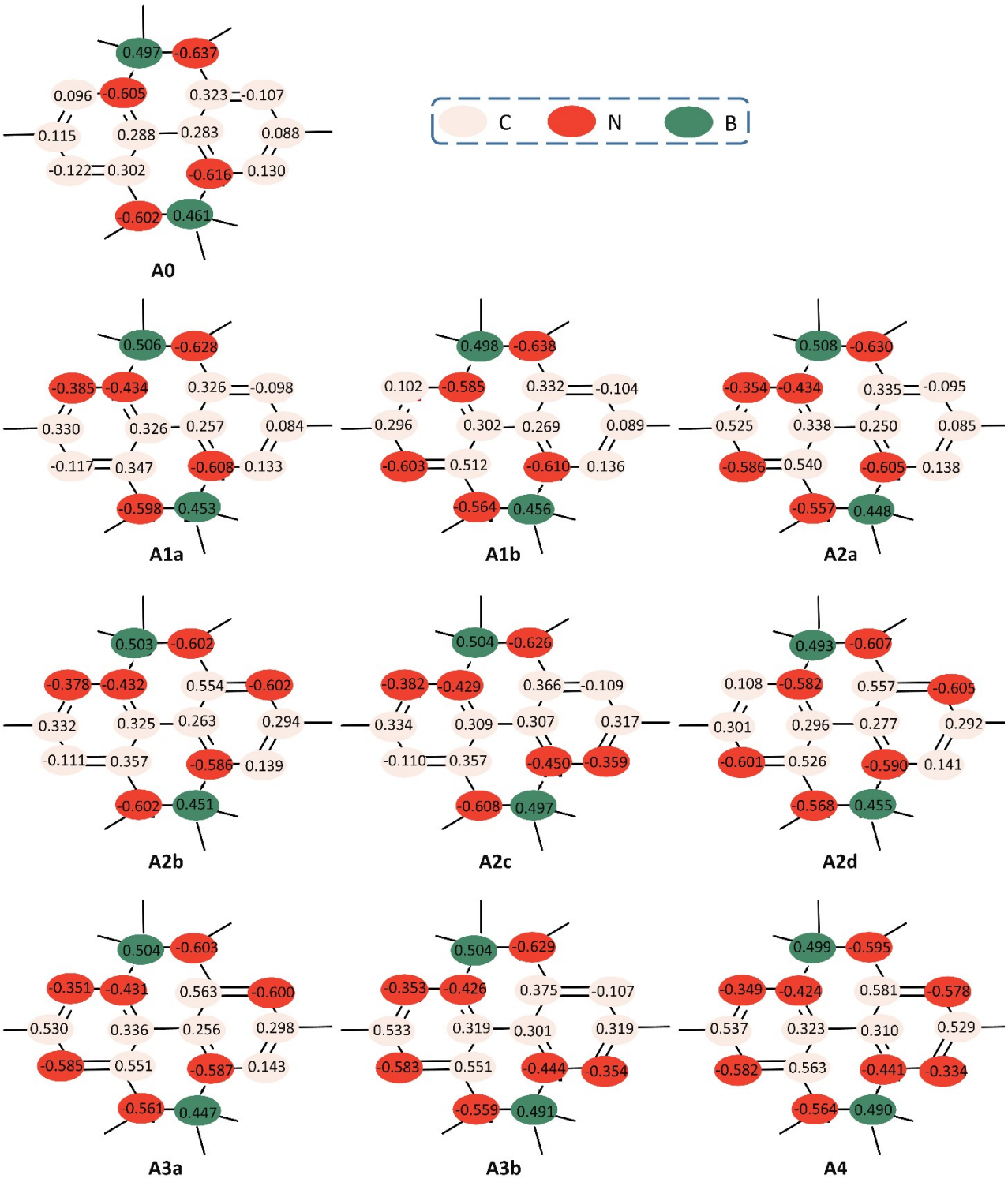


Fig. S1 The Mulliken atom charge of core in studied acceptors.

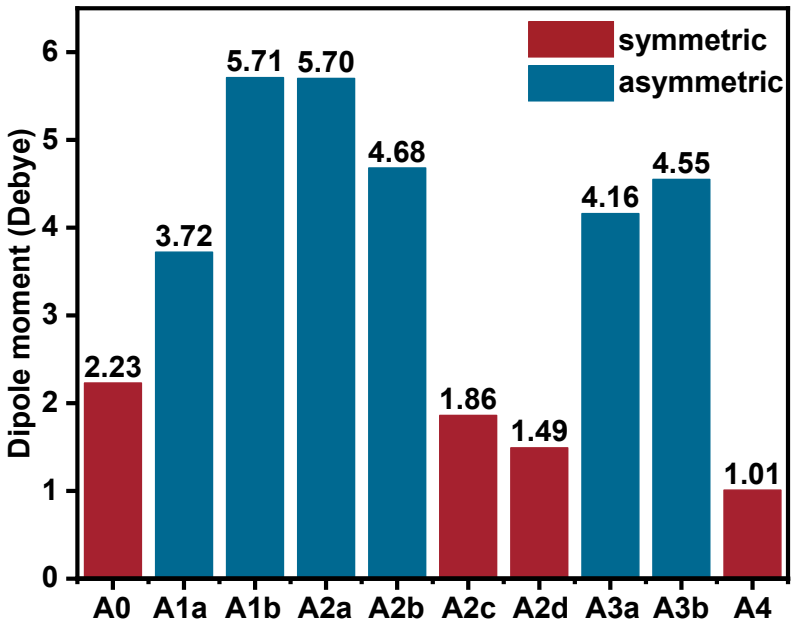


Fig. S2 The dipole moments of studied molecules (the red bars stand for the symmetric molecules and the blue ones mean the asymmetric molecules).

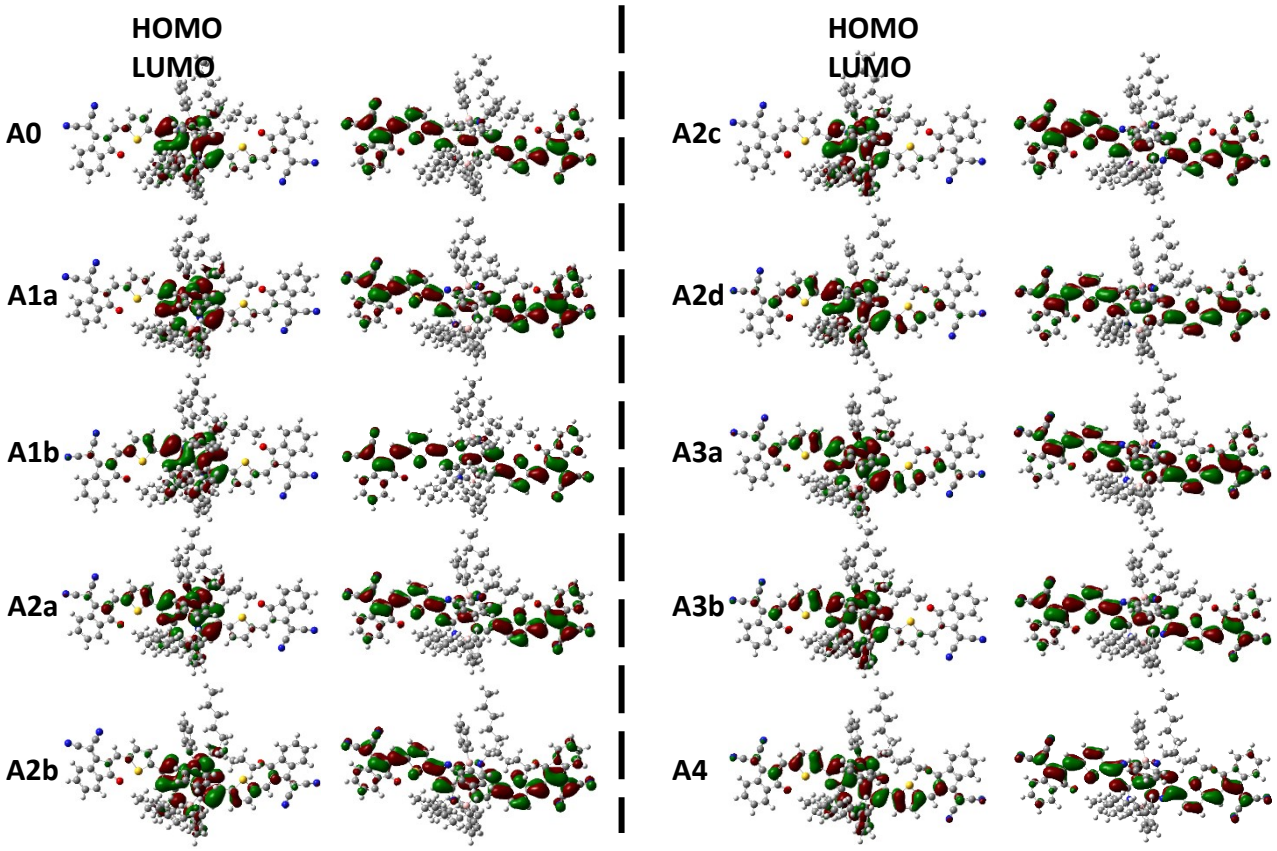


Fig. S3 The contour plots of the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) for studied acceptors.

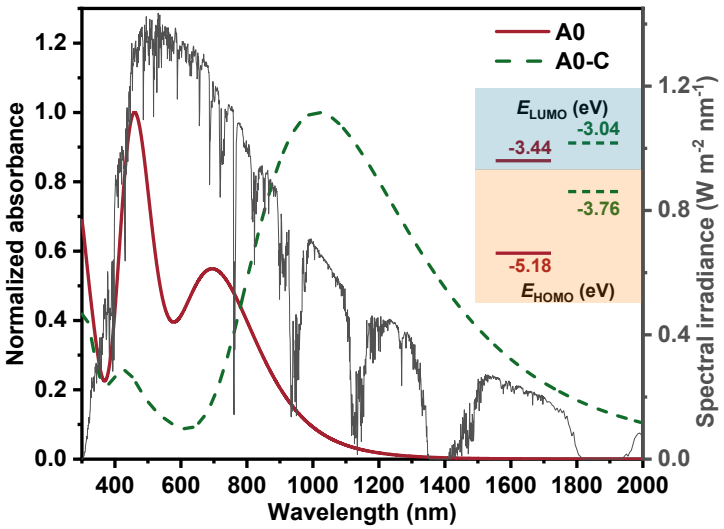


Fig. S4 The absorption spectra and frontier molecular orbitals of A0 (in red solid line) and its carbon counterpart A0-C (in green dash line) together with the sunlight irradiation spectrum (in grey solid line).

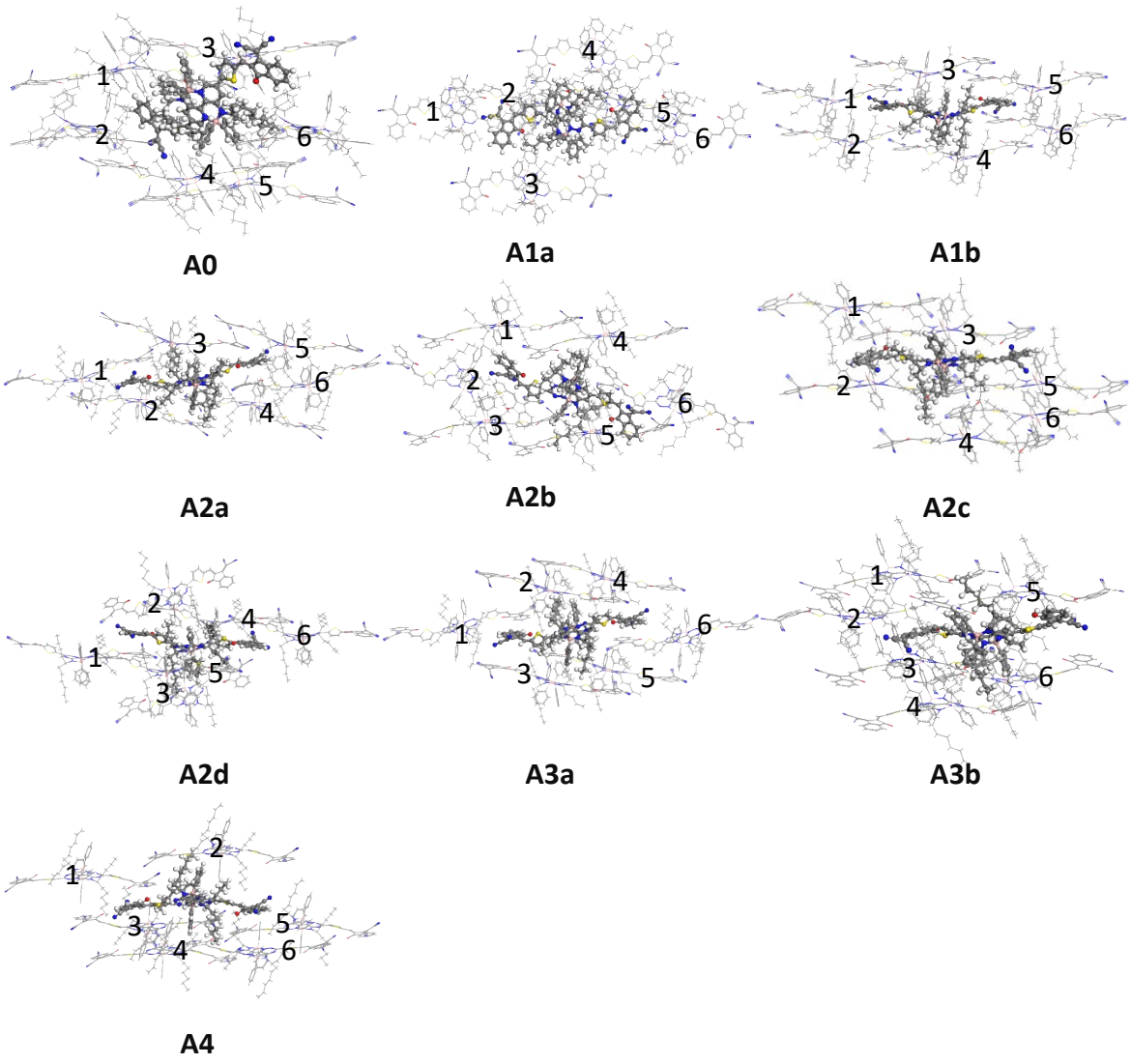


Fig. S5 The detailed information for the primary transfer pathways (marked by numbers) in the predicted crystal structures of the studied molecules.

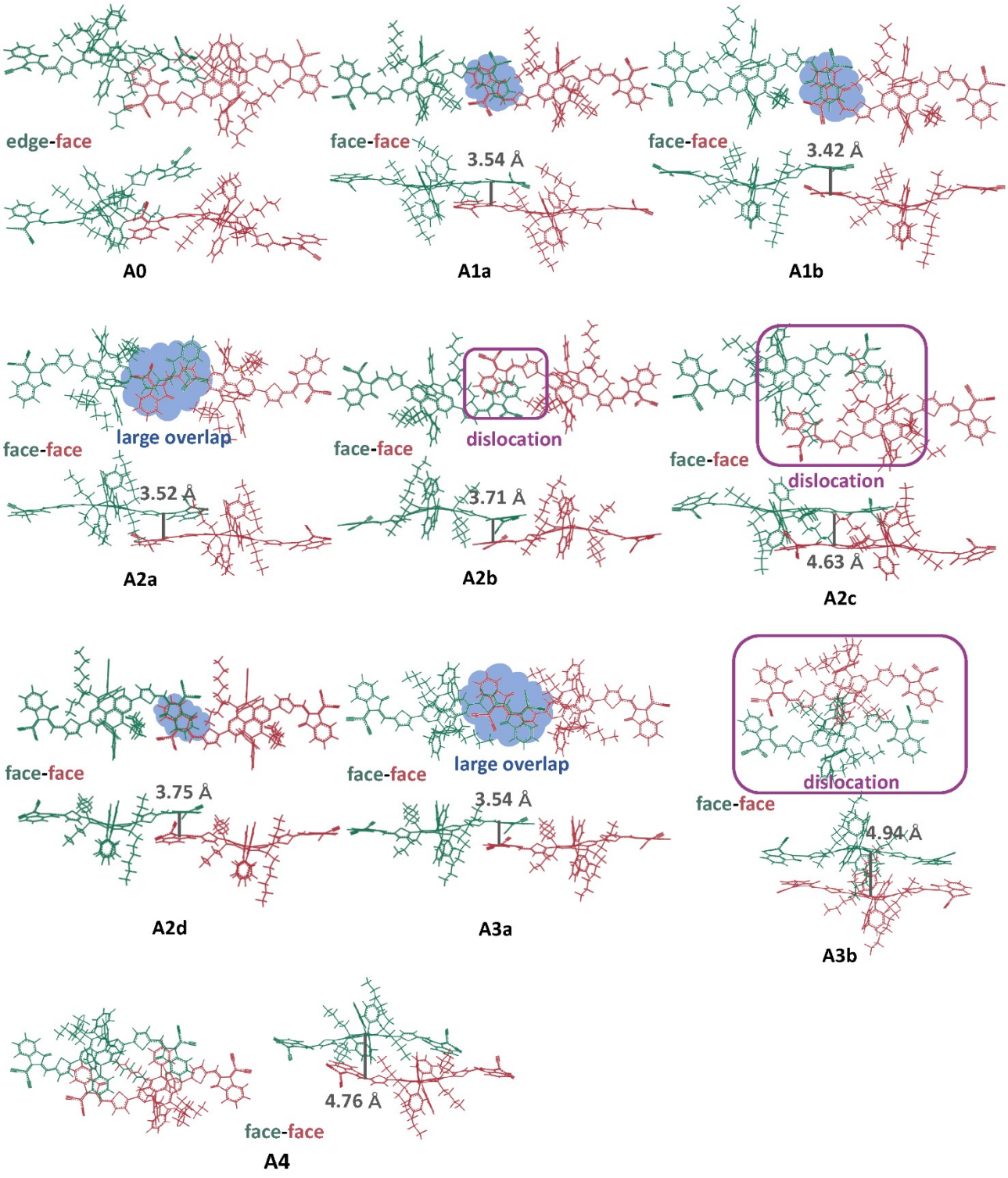


Fig. S6 The detailed packing information for the most favoured hopping pathway of acceptors.

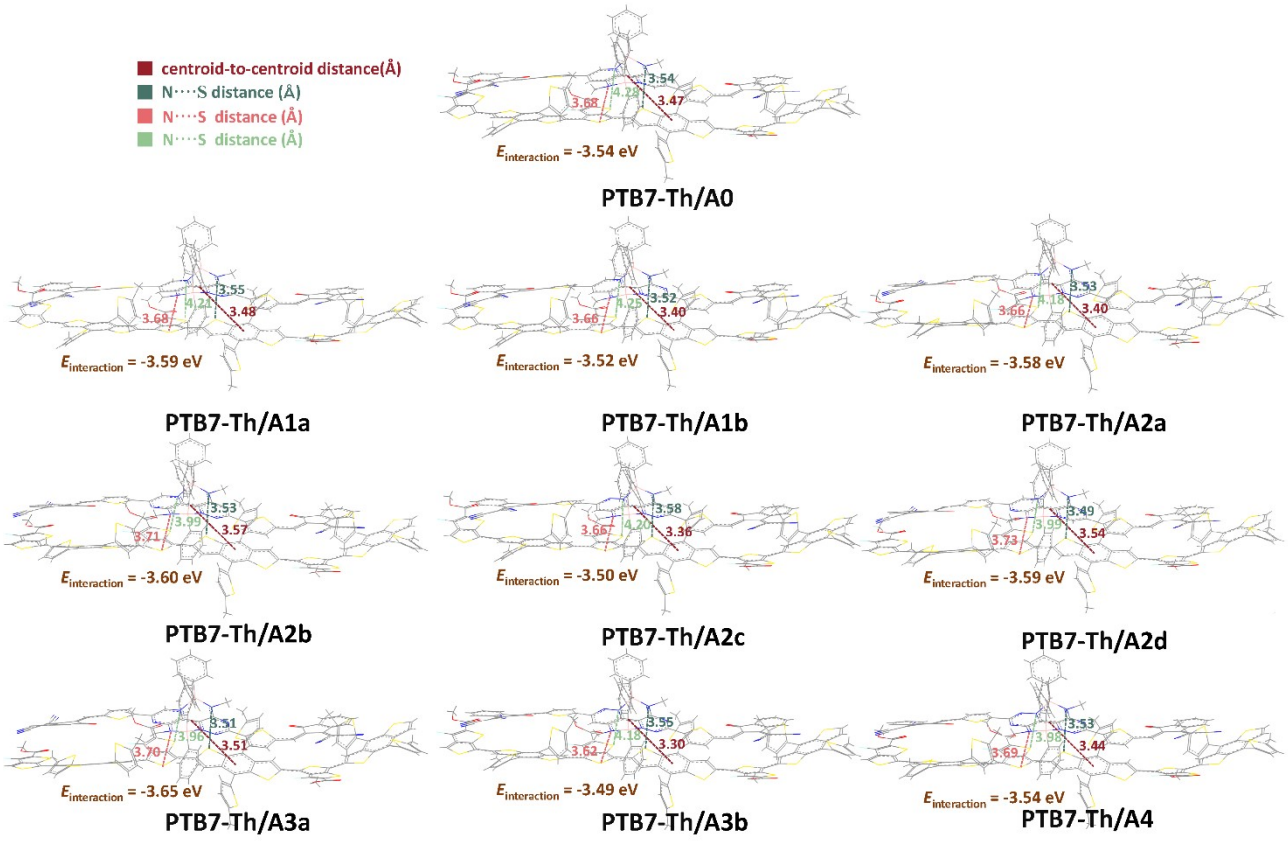


Fig. S7 The optimized structures of the PTB7-Th/acceptors with the centroid-to-centroid distances, N···S distances, and the weak interaction energy ($E_{interaction}$).

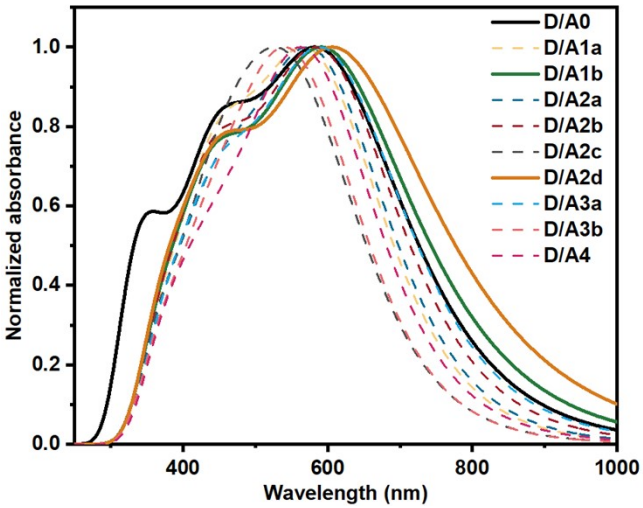


Fig. S8 The calculated absorption spectra of the studied donor/acceptor (D/A) interfaces, composed by the donor PTB7-Th and the studied acceptors.

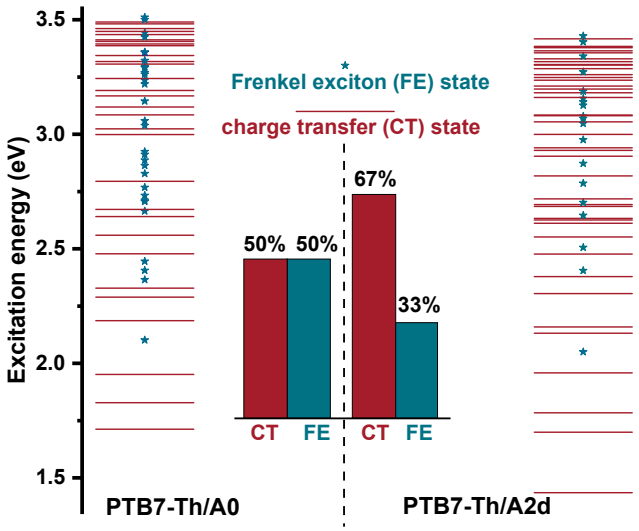


Fig. S9 The types (charge transfer state: CT, Frenkerl exciton state: FE) of the lowest sixty excited states and the corresponding percentage in the PTB7-Th/A0 and PTB7-Th/A2d.

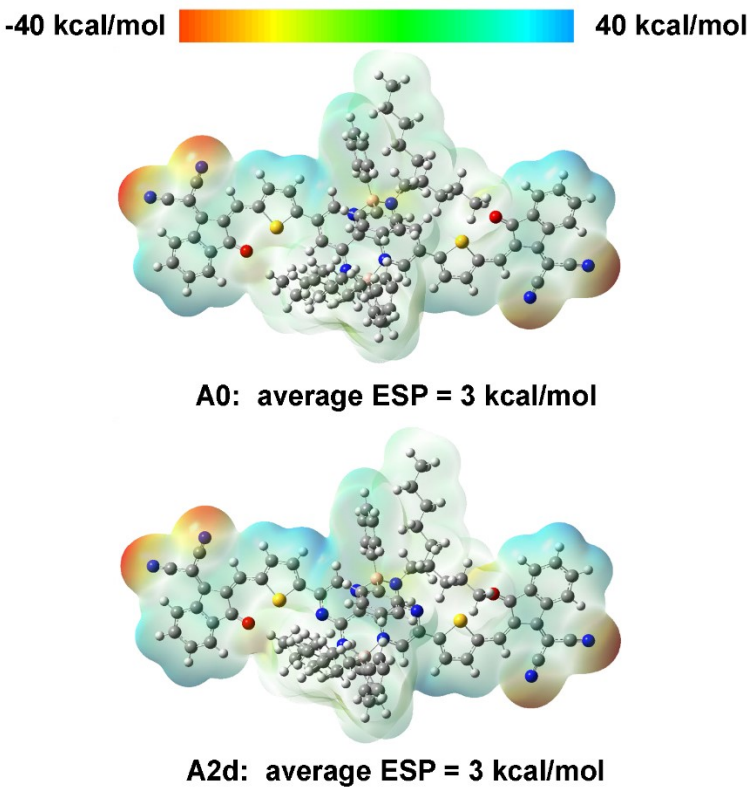
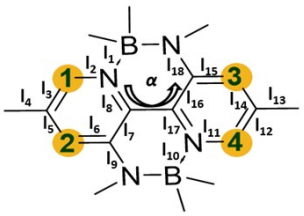


Fig. S10 The electrostatic potential (ESP) maps and average ESP of the A0 and A2d.

Table S1 The calculated bond length l_n (Å) and dihedral angle α (°) in molecules.



acceptor	A0	A1a	A1b	A2a	A2b	A2c	A2d	A3a	A3b	A4
l_1	1.63	1.62	1.63	1.62	1.63	1.63	1.64	1.63	1.63	1.63
l_2	1.34	1.32	1.34	1.33	1.32	1.32	1.34	1.33	1.33	1.33
l_3	1.40	1.35	1.40	1.34	1.35	1.35	1.40	1.34	1.34	1.35
l_4	1.46	1.46	1.45	1.46	1.46	1.46	1.45	1.46	1.46	1.45
l_5	1.39	1.39	1.34	1.35	1.39	1.38	1.34	1.33	1.33	1.33
l_6	1.41	1.41	1.35	1.35	1.41	1.41	1.35	1.35	1.35	1.35
l_7	1.44	1.44	1.45	1.45	1.44	1.44	1.45	1.45	1.45	1.45
l_8	1.36	1.35	1.35	1.34	1.35	1.35	1.35	1.34	1.33	1.33
l_9	1.35	1.34	1.33	1.32	1.33	1.33	1.33	1.32	1.32	1.32
l_{10}	1.63	1.64	1.64	1.64	1.63	1.63	1.64	1.64	1.63	1.62
l_{11}	1.34	1.33	1.33	1.33	1.34	1.32	1.34	1.34	1.31	1.33
l_{12}	1.40	1.40	1.40	1.40	1.40	1.34	1.40	1.40	1.35	1.34
l_{13}	1.46	1.46	1.46	1.46	1.45	1.46	1.45	1.45	1.46	1.46
l_{14}	1.39	1.39	1.39	1.39	1.34	1.39	1.34	1.33	1.39	1.33
l_{15}	1.39	1.41	1.41	1.41	1.35	1.41	1.34	1.35	1.41	1.35
l_{16}	1.45	1.44	1.44	1.44	1.45	1.45	1.45	1.45	1.45	1.45
l_{17}	1.36	1.36	1.36	1.36	1.35	1.34	1.35	1.35	1.34	1.33
l_{18}	1.35	1.35	1.35	1.35	1.34	1.34	1.34	1.33	1.34	1.32
|α|	10.82	12.71	13.07	14.24	11.86	12.10	12.49	12.92	13.81	11.87

Table S2 The calculated vertical ionization potential energy (VIP), vertical electron affinity energy (VEA), first vertical excitation energy (E_1), and exciton binding energy (E_b).

acceptor	VIP (eV)	VEA (eV)	E_1 (eV)	E_b (eV)
A0	5.21	3.42	1.41	0.38
A1a	5.53	3.43	1.68	0.42
A1b	5.36	3.50	1.47	0.40
A2a	5.69	3.51	1.74	0.44
A2b	5.66	3.54	1.66	0.45
A2c	5.83	3.46	1.90	0.47
A2d	5.47	3.62	1.45	0.40
A3a	5.79	3.65	1.68	0.46
A3b	6.00	3.56	1.93	0.51
A4	6.11	3.72	1.88	0.51

Table S3 The calculated the type of exciton, excited energy (*E*), oscillator strength *f*, transferred charge $|\Delta q|$, and D index of the PTB7-Th/A0 and PTB7-Th/A2d interfaces.

PTB7-Th/A0						PTB7-Th/A2d					
S_n	nature	*E* (eV)	*f*	$\|\Delta q\|$ (e)	D (Å)	S_n	nature	*E* (eV)	*f*	$\|\Delta q\|$ (e)	D (Å)
S_1	CT_1	1.71	0.04	0.78	2.37	S_1	CT_1	1.44	0.05	0.89	2.88
S_2	CT_2	1.83	0.74	0.31	0.75	S_2	CT_2	1.70	0.82	0.40	1.18
S_3	CT_3	1.95	0.06	0.81	2.58	S_3	CT_3	1.78	0.17	0.65	1.85
S_4	FE_1	2.10	2.45	0.01	0.58	S_4	CT_4	1.96	0.05	0.91	3.41
S_5	CT_4	2.19	0.01	0.93	3.07	S_5	FE_1	2.05	2.10	0.19	1.25
S_6	CT_5	2.29	0.02	0.48	2.39	S_6	CT_5	2.13	0.09	0.91	2.92
S_7	CT_6	2.33	0.06	0.46	2.95	S_7	CT_6	2.16	0.24	0.84	2.38
S_8	FE_2	2.37	0.02	0.35	1.70	S_8	CT_7	2.30	0.06	0.59	2.10
S_9	FE_3	2.41	0.06	0.48	3.16	S_9	FE_2	2.38	0.06	0.35	1.05
S_{10}	FE_4	2.45	0.17	0.09	0.69	S_{10}	CT_8	2.40	0.02	0.86	4.12
S_{11}	CT_7	2.48	0.05	0.87	2.83	S_{11}	FE_3	2.48	0.02	0.09	0.51
S_{12}	CT_8	2.56	0.05	0.73	2.32	S_{12}	CT_9	2.51	0.02	0.87	3.64
S_{13}	CT_9	2.64	0.04	0.74	5.48	S_{13}	CT_{10}	2.55	0.02	0.80	3.70
S_{14}	FE_5	2.66	0.16	0.21	1.98	S_{14}	CT_{11}	2.61	0.34	0.24	1.11
S_{15}	CT_{10}	2.67	0.02	0.78	2.02	S_{15}	CT_{12}	2.63	0.06	0.81	2.40
S_{16}	FE_6	2.71	0.62	0.06	1.14	S_{16}	FE_4	2.63	0.18	0.26	0.59
S_{17}	FE_7	2.71	0.59	0.33	1.03	S_{17}	CT_{13}	2.65	0.15	0.56	2.06
S_{18}	FE_8	2.73	0.26	0.11	0.67	S_{18}	CT_{14}	2.69	0.36	0.38	1.81
S_{19}	FE_9	2.77	0.08	0.09	0.33	S_{19}	CT_{15}	2.69	0.30	0.64	1.83
S_{20}	CT_{11}	2.79	0.05	0.76	5.04	S_{20}	FE_5	2.70	0.07	0.28	0.98
S_{21}	FE_{10}	2.83	0.12	0.61	2.10	S_{21}	CT_{16}	2.72	0.09	0.26	1.59
S_{22}	FE_{11}	2.86	0.01	0.24	3.54	S_{22}	FE_6	2.79	0.01	0.14	0.44
S_{23}	FE_{12}	2.89	0.01	0.18	0.64	S_{23}	CT_{17}	2.82	0.20	0.43	2.03
S_{24}	FE_{13}	2.91	0.05	0.43	1.26	S_{24}	FE_7	2.87	0.01	0.08	0.52
S_{25}	FE_{14}	2.92	0.15	0.17	0.31	S_{25}	CT_{18}	2.90	0.13	0.51	1.54
S_{26}	CT_{12}	3.00	0.03	0.58	2.01	S_{26}	CT_{19}	2.93	0.04	0.73	4.24
S_{27}	CT_{13}	3.02	0.00	0.62	1.63	S_{27}	CT_{20}	2.94	0.05	0.69	3.88
S_{28}	FE_{15}	3.04	0.27	0.04	0.93	S_{28}	FE_8	2.98	0.01	0.00	3.53
S_{29}	FE_{16}	3.06	0.11	0.14	1.77	S_{29}	CT_{21}	3.00	0.14	0.51	1.78
S_{30}	CT_{14}	3.09	0.01	0.49	1.30	S_{30}	FE_9	3.05	0.11	0.39	1.05
S_{31}	CT_{15}	3.12	0.01	0.62	8.28	S_{31}	FE_{10}	3.05	0.05	0.06	0.86

S_{32}	FE_{17}	3.14	0.01	0.14	2.07	S_{32}	CT_{22}	3.07	0.02	0.26	2.81
S_{33}	CT_{16}	3.17	0.01	0.32	5.39	S_{33}	FE_{11}	3.08	0.02	0.17	0.73
S_{34}	CT_{17}	3.19	0.00	0.57	2.40	S_{34}	FE_{12}	3.08	0.09	0.48	1.65
S_{35}	FE_{18}	3.22	0.02	0.04	3.04	S_{35}	CT_{23}	3.08	0.01	0.69	2.13
S_{36}	FE_{19}	3.24	0.02	0.17	1.30	S_{36}	FE_{13}	3.13	0.02	0.29	1.32
S_{37}	CT_{18}	3.24	0.01	0.42	2.70	S_{37}	FE_{14}	3.14	0.01	0.53	1.44
S_{38}	FE_{20}	3.26	0.01	0.03	1.22	S_{38}	FE_{15}	3.16	0.01	0.08	0.79
S_{39}	FE_{21}	3.27	0.00	0.03	2.36	S_{39}	CT_{24}	3.16	0.00	0.16	2.47
S_{40}	FE_{22}	3.29	0.01	0.37	0.86	S_{40}	CT_{25}	3.18	0.01	0.66	2.80
S_{41}	FE_{23}	3.30	0.03	0.31	2.56	S_{41}	FE_{16}	3.19	0.03	0.31	4.67
S_{42}	CT_{19}	3.31	0.00	0.25	1.39	S_{42}	CT_{26}	3.20	0.00	0.22	2.41
S_{43}	CT_{20}	3.32	0.01	0.49	1.22	S_{43}	CT_{27}	3.21	0.00	0.41	2.79
S_{44}	FE_{24}	3.32	0.01	0.27	2.68	S_{44}	CT_{28}	3.24	0.00	0.37	2.30
S_{45}	CT_{21}	3.34	0.00	0.76	2.61	S_{45}	CT_{29}	3.25	0.01	0.51	1.65
S_{46}	FE_{25}	3.36	0.35	0.18	0.61	S_{46}	CT_{30}	3.26	0.03	0.31	1.78
S_{47}	FE_{26}	3.36	0.06	0.47	4.04	S_{47}	FE_{17}	3.27	0.05	0.46	1.00
S_{48}	CT_{22}	3.39	0.01	0.35	1.12	S_{48}	CT_{31}	3.29	0.01	0.65	4.42
S_{49}	CT_{23}	3.39	0.08	0.76	1.98	S_{49}	CT_{32}	3.30	0.02	0.66	2.05
S_{50}	CT_{24}	3.41	0.04	0.41	1.44	S_{50}	CT_{33}	3.30	0.03	0.73	2.28
S_{51}	CT_{25}	3.41	0.06	0.60	1.50	S_{51}	CT_{34}	3.32	0.00	0.49	2.84
S_{52}	FE_{27}	3.42	0.02	0.12	0.94	S_{52}	CT_{35}	3.33	0.10	0.61	2.10
S_{53}	CT_{26}	3.44	0.02	0.49	0.43	S_{53}	FE_{18}	3.34	0.16	0.30	1.61
S_{54}	FE_{28}	3.44	0.02	0.32	0.93	S_{54}	CT_{36}	3.36	0.19	0.50	3.17
S_{55}	CT_{27}	3.45	0.01	0.78	5.29	S_{55}	CT_{37}	3.36	0.03	0.38	2.03
S_{56}	CT_{28}	3.46	0.10	0.42	1.23	S_{56}	CT_{38}	3.38	0.05	0.34	1.00
S_{57}	CT_{29}	3.48	0.01	0.50	1.67	S_{57}	CT_{39}	3.38	0.07	0.14	3.10
S_{58}	CT_{30}	3.49	0.01	0.16	2.39	S_{58}	FE_{19}	3.40	0.07	0.29	1.73
S_{59}	FE_{29}	3.50	0.03	0.30	1.91	S_{59}	CT_{40}	3.42	0.02	0.31	1.19
S_{60}	FE_{30}	3.51	0.02	0.41	1.70	S_{60}	FE_{20}	3.43	0.04	0.09	0.78