Incorporation of a Boron–Nitrogen Covalent Bond Improves the Charge-Transport and Charge-Transfer Characteristics of Organoboron Small-Molecule Acceptors for Organic Solar Cells

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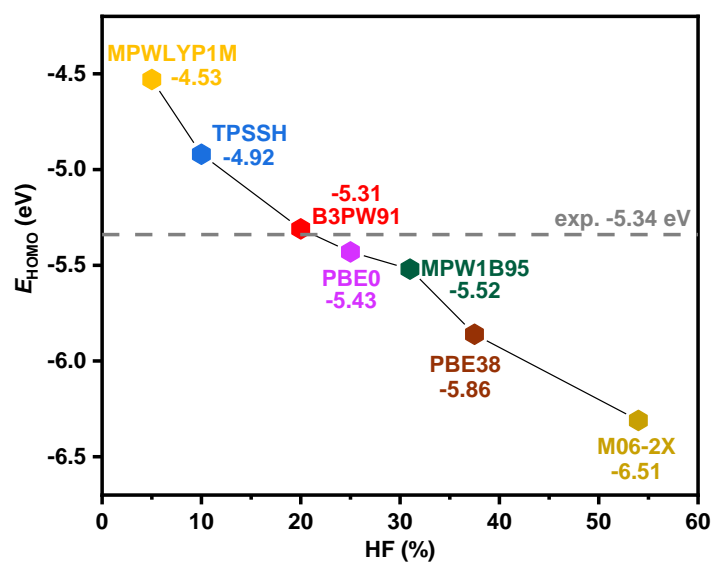* Correspondence: liquansong@bit.edu.cn (Q.-S.L.); zeshengli@bit.edu.cn (Z.-S.L.)

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Figure S1. The relationship between the calculated the highest occupied orbital energy level (E_{HOMO}) of $M_{B \leftarrow N}$ and the Hartree-Fock ratio of the employed DFT functionals. The dashed line indicates the experimental value.
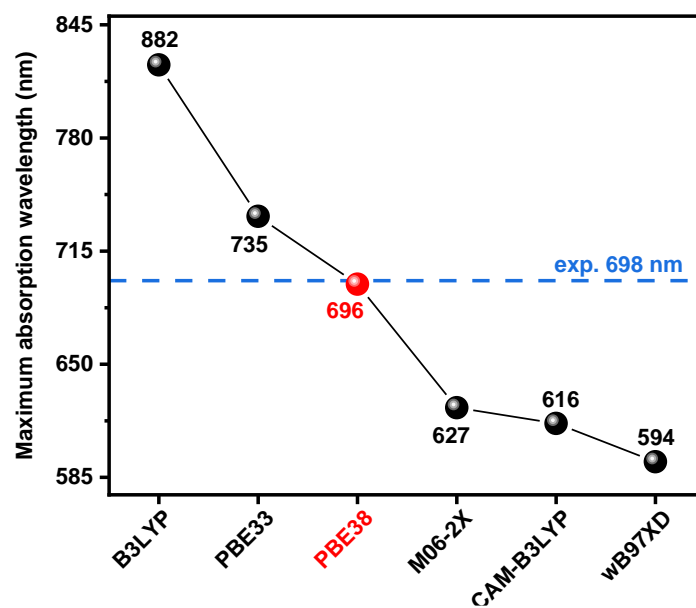
Figure S2. Calculated values of maximum absorption wavelength of $M_{B \leftarrow N}$ employed different DFT functionals along with the experiment value of 698 nm.
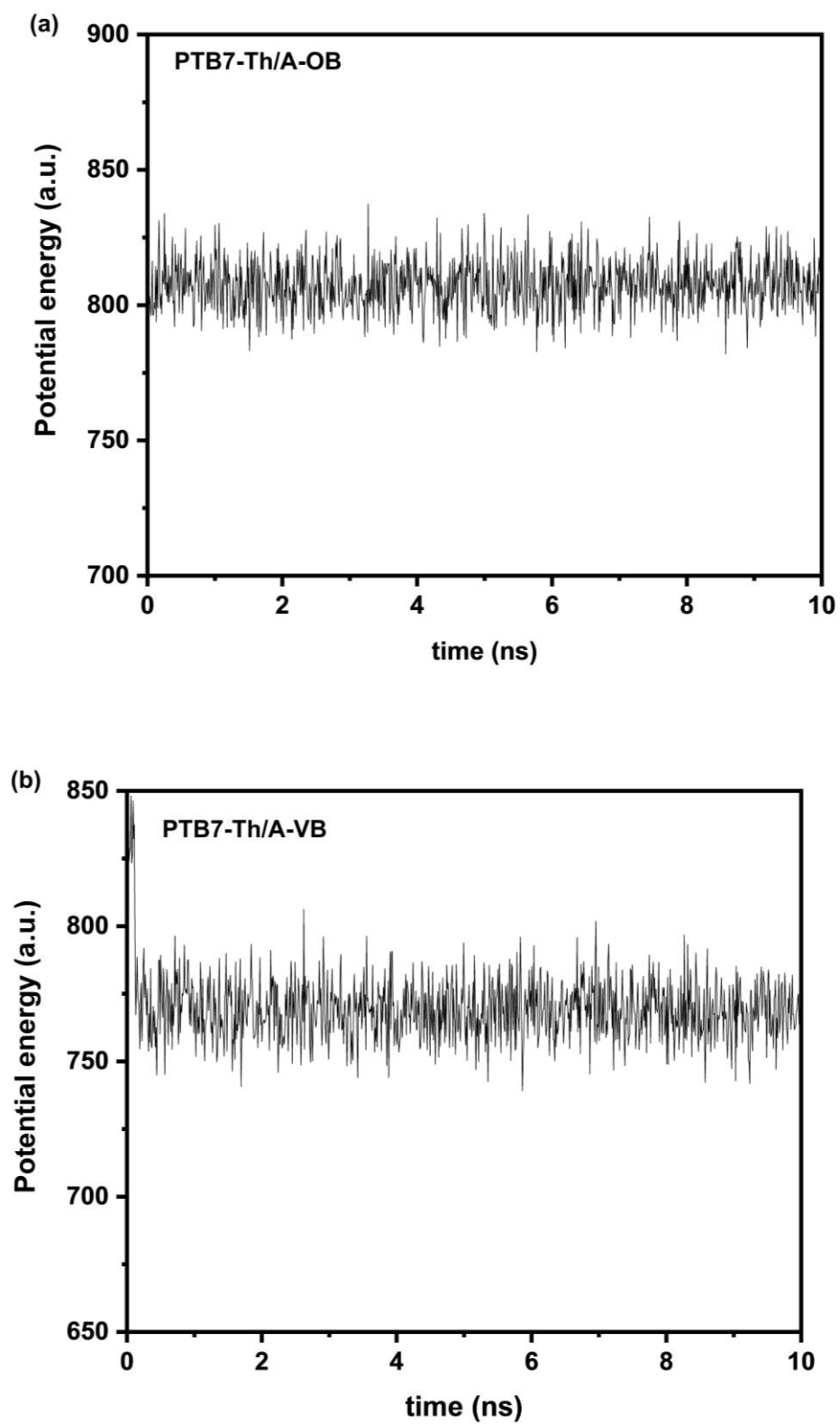
Figure S3. The potential energy evolutions of (a) PTB7-Th/$M_{B \leftarrow N}$ and (b) PTB7-Th/M_{B-N} as a function of simulation time after equilibration.

M_{C-N}: 145.14°
$M_{B\leftarrow N}$: 176.60°
M_{B-N}: 150.07°
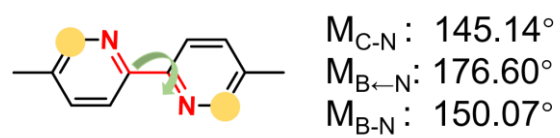
Figure S4. The dihedral angles of studied molecules.

Table S1. The values of electron transfer integral v_i (eV) in the nearest six pathways of the investigated molecules (The bold fonts represent the largest transfer integrals v_{max}).

Path	$M_{B\leftarrow N}$	M_{B-N}	M_{C-N}
v_1	1.68×10^{-4}	2.51×10^{-5}	$\mathbf{3.68\times10^{-4}}$
v_2	1.67×10^{-4}	2.31×10^{-5}	3.67×10^{-4}
v_3	1.04×10^{-4}	2.50×10^{-6}	4.23×10^{-5}
v_4	1.04×10^{-4}	3.66×10^{-3}	1.09×10^{-4}
v_5	$\mathbf{1.23\times10^{-3}}$	3.65×10^{-3}	7.13×10^{-5}
v_6	$\mathbf{1.23\times10^{-3}}$	$\mathbf{5.36\times10^{-3}}$	4.84×10^{-5}

Table S2. Net transferred charge Δq (|e|) and D index (Å) of the lowest sixty excited states of PTB7-Th/$M_{B \leftarrow N}$ and PTB7-Th/$M_{B\text{-}N}$ interfaces.

PTB7-Th/$M_{B \leftarrow N}$						PTB7-Th/$M_{B\text{-}N}$					
S_n	Δq	D	S_n	Δq	D	S_n	Δq	D	S_n	Δq	D
S_1	0.78	2.37	S_{31}	0.62	8.28	S_1	0.14	0.54	S_{31}	0.02	4.34
S_2	0.31	0.75	S_{32}	0.14	2.07	S_2	0.89	3.14	S_{32}	0.83	4.91
S_3	0.81	2.58	S_{33}	0.32	5.39	S_3	0.91	2.81	S_{33}	0.00	0.32
S_4	0.01	0.58	S_{34}	0.57	2.40	S_4	0.01	0.77	S_{34}	0.85	3.13
S_5	0.93	3.07	S_{35}	0.04	3.04	S_5	0.07	0.62	S_{35}	0.04	6.04
S_6	0.48	2.39	S_{36}	0.17	1.30	S_6	0.87	2.98	S_{36}	0.63	2.54
S_7	0.46	2.95	S_{37}	0.42	2.70	S_7	0.90	4.07	S_{37}	0.87	9.72
S_8	0.35	1.70	S_{38}	0.03	1.22	S_8	0.14	0.42	S_{38}	0.23	2.67
S_9	0.48	3.16	S_{39}	0.03	2.36	S_9	0.69	4.82	S_{39}	0.53	2.06
S_{10}	0.09	0.69	S_{40}	0.37	0.86	S_{10}	0.14	2.67	S_{40}	0.80	12.20
S_{11}	0.87	2.83	S_{41}	0.31	2.56	S_{11}	0.79	3.27	S_{41}	0.31	1.13
S_{12}	0.73	2.32	S_{42}	0.25	1.39	S_{12}	0.85	5.95	S_{42}	0.00	1.44
S_{13}	0.74	5.48	S_{43}	0.49	1.22	S_{13}	0.95	3.21	S_{43}	0.36	2.02
S_{14}	0.21	1.98	S_{44}	0.27	2.68	S_{14}	0.07	0.89	S_{44}	0.82	3.49
S_{15}	0.78	2.02	S_{45}	0.76	2.61	S_{15}	0.82	2.44	S_{45}	0.55	4.80
S_{16}	0.06	1.14	S_{46}	0.18	0.61	S_{16}	0.14	1.34	S_{46}	0.58	2.58
S_{17}	0.33	1.03	S_{47}	0.47	4.04	S_{17}	0.06	1.42	S_{47}	0.02	1.26
S_{18}	0.11	0.67	S_{48}	0.35	1.12	S_{18}	0.66	2.72	S_{48}	0.34	3.84
S_{19}	0.09	0.33	S_{49}	0.76	1.98	S_{19}	0.86	4.23	S_{49}	0.70	3.74
S_{20}	0.76	5.04	S_{50}	0.41	1.44	S_{20}	0.26	0.84	S_{50}	0.23	3.10
S_{21}	0.61	2.10	S_{51}	0.60	1.50	S_{21}	0.28	0.96	S_{51}	0.17	3.00
S_{22}	0.24	3.54	S_{52}	0.12	0.94	S_{22}	0.35	1.37	S_{52}	0.53	1.59
S_{23}	0.18	0.64	S_{53}	0.49	0.43	S_{23}	0.50	2.27	S_{53}	0.39	4.52
S_{24}	0.43	1.26	S_{54}	0.32	0.93	S_{24}	0.23	3.07	S_{54}	0.04	1.22
S_{25}	0.17	0.31	S_{55}	0.78	5.29	S_{25}	0.02	1.50	S_{55}	0.12	2.71
S_{26}	0.58	2.01	S_{56}	0.42	1.23	S_{26}	0.41	5.45	S_{56}	0.29	1.45
S_{27}	0.62	1.63	S_{57}	0.50	1.67	S_{27}	0.03	1.89	S_{57}	0.45	2.51
S_{28}	0.04	0.93	S_{58}	0.16	2.39	S_{28}	0.60	3.16	S_{58}	0.56	3.12
S_{29}	0.14	1.77	S_{59}	0.30	1.91	S_{29}	0.14	2.04	S_{59}	0.12	1.39
S_{30}	0.49	1.30	S_{60}	0.41	1.70	S_{30}	0.00	0.89	S_{60}	0.81	2.59

Table S3. Charge difference density (CDD) maps of the lowest sixty excited states of PTB7-Th/M$_{B\leftarrow N}$ and PTB7-Th/M$_{B-N}$ interfaces.

PTB7-Th/M$_{B\leftarrow N}$						PTB7-Th/M$_{B-N}$					
S$_n$	CDD	S$_n$	CDD	S$_n$	CDD	S$_n$	CDD	S$_n$	CDD	S$_n$	CDD
S$_1$		S$_{21}$		S$_{41}$		S$_1$		S$_{21}$		S$_{41}$	
S$_2$		S$_{22}$		S$_{42}$		S$_2$		S$_{22}$		S$_{42}$	
S$_3$		S$_{23}$		S$_{43}$		S$_3$		S$_{23}$		S$_{43}$	
S$_4$		S$_{24}$		S$_{44}$		S$_4$		S$_{24}$		S$_{44}$	
S$_5$		S$_{25}$		S$_{45}$		S$_5$		S$_{25}$		S$_{45}$	
S$_6$		S$_{26}$		S$_{46}$		S$_6$		S$_{26}$		S$_{46}$	
S$_7$		S$_{27}$		S$_{47}$		S$_7$		S$_{27}$		S$_{47}$	
S$_8$		S$_{28}$		S$_{48}$		S$_8$		S$_{28}$		S$_{48}$	
S$_9$		S$_{29}$		S$_{49}$		S$_9$		S$_{29}$		S$_{49}$	
S$_{10}$		S$_{30}$		S$_{50}$		S$_{10}$		S$_{30}$		S$_{50}$	
S$_{11}$		S$_{31}$		S$_{51}$		S$_{11}$		S$_{31}$		S$_{51}$	
S$_{12}$		S$_{32}$		S$_{52}$		S$_{12}$		S$_{32}$		S$_{52}$	
S$_{13}$		S$_{33}$		S$_{53}$		S$_{13}$		S$_{33}$		S$_{53}$	
S$_{14}$		S$_{34}$		S$_{54}$		S$_{14}$		S$_{34}$		S$_{54}$	
S$_{15}$		S$_{35}$		S$_{55}$		S$_{15}$		S$_{35}$		S$_{55}$	
S$_{16}$		S$_{36}$		S$_{56}$		S$_{16}$		S$_{36}$		S$_{56}$	
S$_{17}$		S$_{37}$		S$_{57}$		S$_{17}$		S$_{37}$		S$_{57}$	
S$_{18}$		S$_{38}$		S$_{58}$		S$_{18}$		S$_{38}$		S$_{58}$	
S$_{19}$		S$_{39}$		S$_{59}$		S$_{19}$		S$_{39}$		S$_{59}$	
S$_{20}$		S$_{40}$		S$_{60}$		S$_{20}$		S$_{40}$		S$_{60}$	