Supplementary data for

Boosting performance of D-A-D type hole-transporting materials for perovskite solar cells via tuning the acceptor group

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Computational details

The ground-state geometry optimizations are carried out with density functional theory (DFT) at the B3LYP/6-31G** level.[1] On the basis of the optimized geometries, the light absorption spectra are calculated by time-dependent DFT (TD-DFT) method at the CAM-B3LYP/6-31G** level.[2] The dichloromethane (DCM) solvent effects are simulated with the C-PCM method,[3] and the frequency calculations are performed to confirm the energetic minima. To evaluate the charge transfer properties from ground-state to the first singlet excited-state, the transferred charge amounts and distance, and charge density difference (CDD) maps are obtained with the method of Ciofini *et al*.[4] Based on the optimized ground-geometries, the transferred charges are calculated at the CAM-B3LYP/6-31G** level to keep consistent with the absorption calculations, and the CDD maps are depicted by the Multiwfn 3.3.8.[5] Particularly, the SMD model, coupled with the M05-2X/6-31G** method are used to calculate the solvation Gibbs free energies.[6] All above calculations are implemented with Gaussian 09 package.[7]

As we known, the organic small molecules usually display a weak electronic coupling between adjacent molecules, and thus the thermally activated hopping and diffusion model is employed to describe the charge transportation of designed system in this work. With Einstein relation,[8] the hole mobility can be expressed as:

$$\mu = \frac{eD}{k_B T}$$

where e means the unit charge, and D is the diffusion coefficient, with formula as

$$D = \frac{1}{2d}\sum_i r_i^2 k_i p_i$$

where i is the hole transfer pathway, r_i is the centroid to centroid distance, d is the spatial dimensionality and taken as 1 in this work,[9,10] and p_i ($p_i = k_i / \sum_i k_i$) is the relative probability for hole hopping to the *i*th pathway.

With Marcus theory of electron transfer, the hole hopping rate (κ) is calculated using the formula as follows:[11]

$$\kappa = \frac{2\pi}{\hbar} V_{ab}^2 \frac{1}{\sqrt{4\pi\lambda k_B T}} exp\left[-\lambda / 4k_B T \right]$$

where V_{ab} denotes the hole transfer integral, λ represents the reorganization energy, $\hbar$ is the Planck's constant, k_B is the Boltzmann's constant, and T is the temperature in Kelvin, respectively.

The reorganization energy is evaluated with an adiabatic potential energy surface approach,[12] and the transfer integral is calculated with a direct coupling method:[13]

$$V_{ab} = \left\langle \psi_{HOMO}^{0,a} \middle| F \middle| \psi_{HOMO}^{0,b} \right\rangle$$

where $\psi_{HOMO}^{0,a}$ and $\psi_{HOMO}^{0,b}$ are the HOMOs of two adjacent molecules *a* and *b* with no intermolecular interaction is present, and F is the Fock operator for the dimer.

To obtain the stable dimers for hole transfer, the 30 ps molecular dynamics (MD) simulations are carried out firstly with the DFTB+ 1.2.2 package.[14] The 3ob-3-1 SK parameters for C, N, O, S and H, and the NVE ensemble were employed. Based on the rough dimers, which come from dynamic simulations with the lowest energies, the energy optimizations are further implemented with the Gaussian 09 package at the B3LYP/6-31G** level to get accurate dimeric geometries. The dispersion corrections are also considered with the B3LYP-D3 method. Finally, the hole transfer integrals

are calculated with the PW91PW91/6-31G** method,[15] which has been shown as a better choice for describing of intermolecular electronic coupling at the DFT level.

References

1. A. D. Becke, *J. Chem. Phys.*, 1993, **98**, 5648-5652.
2. Z. Z. Sun, S. Feng, C. Gu, N. Cheng and J. Liu, *Phys. Chem. Chem. Phys.*, 2019, **21**, 15206-15214.
3. J. Tomasi, B. Mennucci and R. Cammi, *Chem. Rev.*, 2005, **105**, 2999-3093.
4. T. Le Bahers, C. Adamo and I. Ciofini, *J. Chem. Theory Comput.*, 2011, **7**, 2498-2506.
5. T. Lu and F. W. Chen, *J. Comput. Chem.*, 2012, **33**, 580-592.
6. J. Ho, A. Klamt and M. L. Coote, *J. Phys. Chem. A*, 2010, **114**, 13442-13444.
7. M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, *Gaussian 09, Revision D.01*, Gaussian, Inc., Wallingford, CT, 2009.
8. L. B. Schein and A. R. McGhie, *Phys. Rev. B*, 1979, **20**, 1631-1639.
9. W. J. Chi, Q. S. Li and Z. S. Li, *Nanoscale*, 2016, **8**, 6146-6154.
10. W. J. Chi, P. P. Sun and Z. S. Li, *Phys. Chem. Chem. Phys.*, 2016, **18**, 27073-27077.
11. R.A. Marcus, N. Sutin, *Biochim. Biophys. Acta*, 1985, **811**, 265-322.
12. Z. Z. Sun, S. Feng and W. L. Ding, *Synth. Met.*, 2020, **259**, 116219.
13. G. J. Nan, L. J. Wang, X. D. Yang, Z. G. Shuai and Y. Zhao, *J. Chem. Phys.*, 2009, **130**, 024704.
14. B. Aradi, B. Hourahine and T. Frauenheim, *J. Phys. Chem. A*, 2007, **111**, 5678-5684.
15. J. Huang and M. Kertesz, *Chem. Phys. Lett.*, 2004, **390**, 110-115.

Table S1 Calculated frontier molecular orbital energies of the designed HTMs.

HTMs	E_{HOMO}[a]				E_{LUMO}[b]			
	B3LYP	B3LYP -semi	PBE33	PBE38	B3LYP	B3LYP -semi	PBE33	PBE38
SM-1	-4.69	-5.31	-5.27	-5.43	-2.35	-3.37	-2.13	-2.04
SM-2	-4.75	-5.38	-5.34	-5.50	-2.13	-3.10	-1.89	-1.78
SM-3	-4.74	-5.36	-5.33	-5.49	-2.49	-3.45	-2.28	-2.18

[a] Calculated HOMO energies (in eV). [b] Calculated LOMO energies (in eV).

Table S2 Calculated frontier molecular orbital energies, adiabatic ionization potential (IP) and adiabatic electron affinity (EA) of electron-donor and acceptor groups with the B3LYP/6-31G** method.

HTMs	E_{H^a}	E_{L^b}	E_{IP}	E_{EA}
MeOTPA	-4.78	-0.47	4.69	0.54
BT	-6.63	-2.40	6.70	2.38
PT	-6.34	-2.14	6.29	2.19
TBT	-6.09	-2.51	6.02	2.62

[a] Calculated HOMO energies (in eV). [b] Calculated LOMO energies (in eV). [c]Adiabatic ionization potentials (in eV). [d] Adiabatic electron affinities (in eV).

Table S3 Calculated ground and excited-state properties of the designed HTMs with the CAM-B3LYP/6-31G** method.

HTMs	E_{H}[a]	E_{L}[b]	E_{H-L}[c]	λ_{abs}[d]	ΔE[e]	f[f]	$Assignment$[g]
SM-1	-5.91	-1.30	4.62	446	2.78	0.89	$H \rightarrow L$ (83%)
SM-2	-5.99	-1.02	4.97	367	3.38	1.49	$H \rightarrow L$(65%)
SM-3	-5.97	-1.44	4.54	400	3.10	0.08	$H \rightarrow L$(73%)

[a] Calculated HOMO energies (in eV). [b] Calculated LOMO energies (in eV). [c] Energy gaps (in eV). [d] Maximum absorption wavelengths (in nm). [e] Excitation energies (in eV). [f] Oscillator strengths. [g] Main orbital contributions (H = HOMO, L = LUMO).

Table S4 Calculated ground and excited-state properties of the designed HTMs with the MPW1K/6-31G** method.

HTMs	E_{H}[a]	E_{L}[b]	E_{H-L}[c]	λ_{abs}[d]	ΔE[e]	f[f]	Assignment[g]
SM-1	-5.65	-1.93	3.72	481	2.58	0.78	$H \rightarrow L$ (92%)
SM-2	-5.73	-1.67	4.06	398	3.11	0.91	$H \rightarrow L$ (85%)
SM-3	-5.71	-2.07	3.63	447	2.77	0.05	$H \rightarrow L$ (89%)

[a] Calculated HOMO energies (in eV). [b] Calculated LOMO energies (in eV). [c] Energy gaps (in eV). [d] Maximum absorption wavelengths (in nm). [e] Excitation energies (in eV). [f] Oscillator strengths. [g] Main orbital contributions (H = HOMO, L = LUMO).

Table S5 Calculated ground and excited-state properties of the designed HTMs with the BMK/6-31G** method.

HTMs	E_{H}[a]	E_{L}[b]	E_{H-L}[c]	λ_{abs}[d]	ΔE[e]	f[f]	$Assignment$[g]
SM-1	-5.38	-1.79	3.59	494	2.51	0.78	$H \rightarrow L$ (94%)
SM-2	-5.46	-1.53	3.93	408	3.04	0.87	$H \rightarrow L$ (88%)
SM-3	-5.44	-1.94	3.50	462	2.68	0.04	$H \rightarrow L$ (91%)

[a] Calculated HOMO energies (in eV). [b] Calculated LOMO energies (in eV). [c] Energy gaps (in eV). [d] Maximum absorption wavelengths (in nm). [e] Excitation energies (in eV). [f] Oscillator strengths. [g] Main orbital contributions (H = HOMO, L = LUMO).

Table S6 Calculated the five lowest excited-states of the SM-3 with the CAM-B3LYP /6-31G** method.

Excited states	λ_{abs}[a]	ΔE[b]	f[c]	$Assignment$[d]	
1	400	3.10	0.08	H-0->L+0(73%)	H-2->L+0(21%)
2	360	3.44	0.43	H-1->L+0(41%)	H-0->L+1(21%)
3	343	3.62	1.31	H-3->L+0(82%)	
4	340	3.65	0.76	H-1->L+0(48%)	H-0->L+2(24%)
5	327	3.80	0.78	H-0->L+1(56%)	H-0->L+2(27%)

[a] Absorption wavelengths (in nm). [b] Excitation energies (in eV). [c] Oscillator strengths. [d] Main orbital contributions (H = HOMO, L = LUMO).

Table S7 Calculated the six lowest excited-states of SM-3 with the MPW1K/6-31G** method.

Excited states	λ_{abs}[a]	ΔE[b]	f[c]	$Assignment$[d]	
1	447	2.77	0.05	H-0->L+0(89%)	
2	411	3.02	0.13	H-1->L+0(73%)	H-0->L+1(22%)
3	392	3.17	0.07	H-0->L+1(71%)	H-1->L+0(24%)
4	369	3.36	0.00	H-1->L+1(96%)	
5	355	3.50	0.68	H-0->L+2(55%)	H-3->L+0(27%)
6	349	3.55	2.11	H-3->L+0(66%)	H-0->L+2(24%)

[a] Absorption wavelengths (in nm). [b] Excitation energies (in eV). [c] Oscillator strengths. [d] Main orbital contributions (H = HOMO, L = LUMO).

Table S8 Calculated the six lowest excited-states of the SM-3 with the BMK/6-31G** method.

Excited states	λ_{abs}[a]	ΔE[b]	f[c]	$Assignment$[d]
1	462	2.68	0.04	H-0->L+0(91%)
2	427	2.90	0.11	H-1->L+0(81%)
3	404	3.07	0.08	H-0->L+1(79%)
4	382	3.25	0.00	H-1->L+1(96%)
5	361	3.43	1.97	H-0->L+2(81%)
6	350	3.54	0.72	H-3->L+0(94%)

[a] Absorption wavelengths (in nm). [b] Excitation energies (in eV). [c] Oscillator strengths. [d] Main orbital contributions (H = HOMO, L = LUMO).

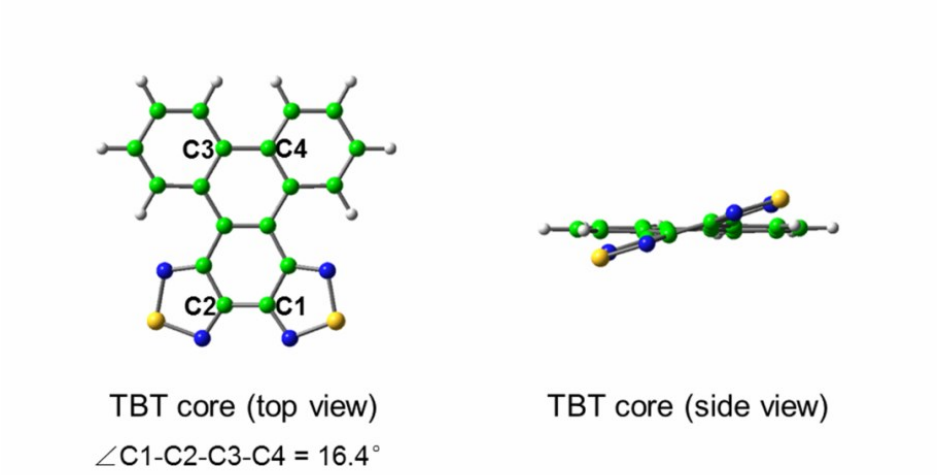

Fig. S1 Core configuration of the SM-3 and the measured dihedral angle.

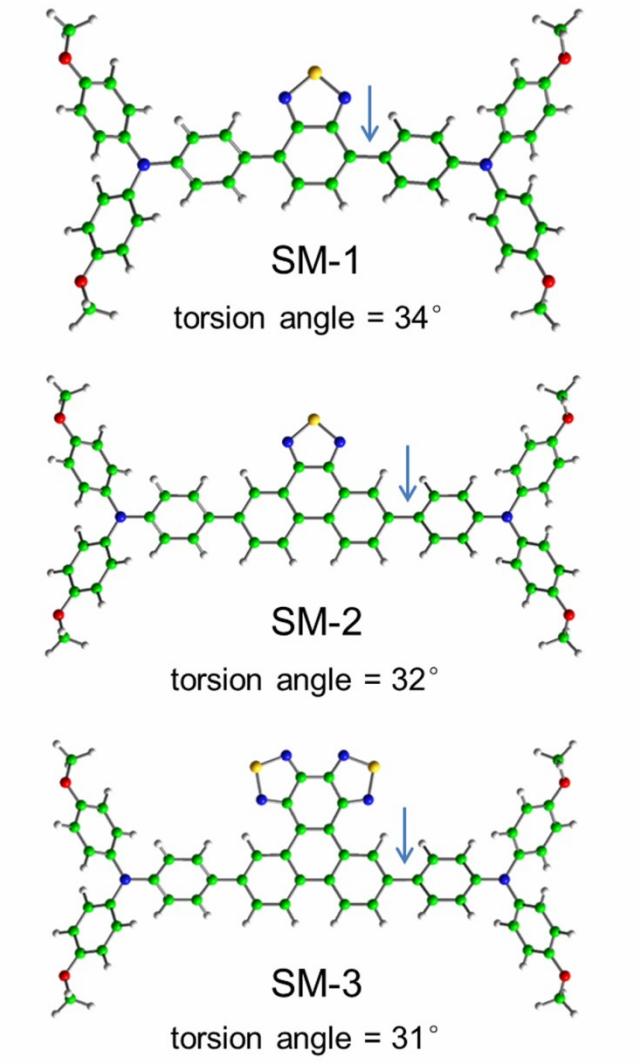

Fig. S2 Optimized geometries of investigated HTMs, and torsion angles between the MeOTPA-donors and central cores.

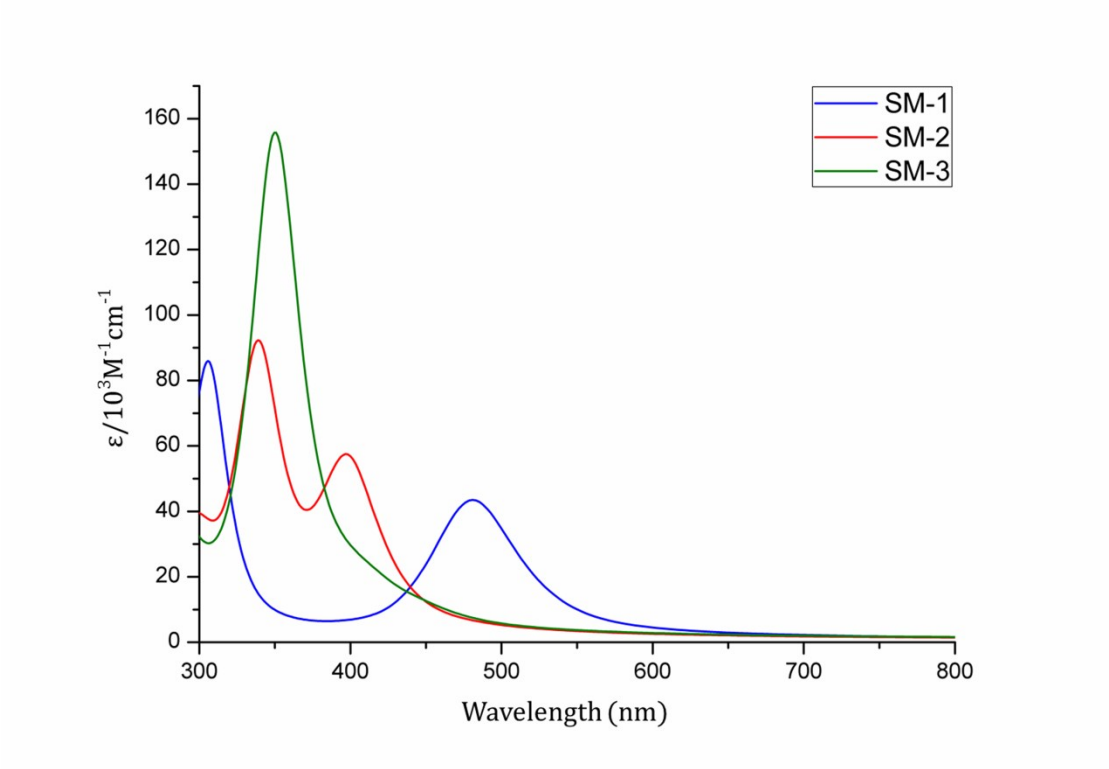

Fig. S3 Calculated absorption spectra of designed HTMs with the MPW1K/6-31G** method.

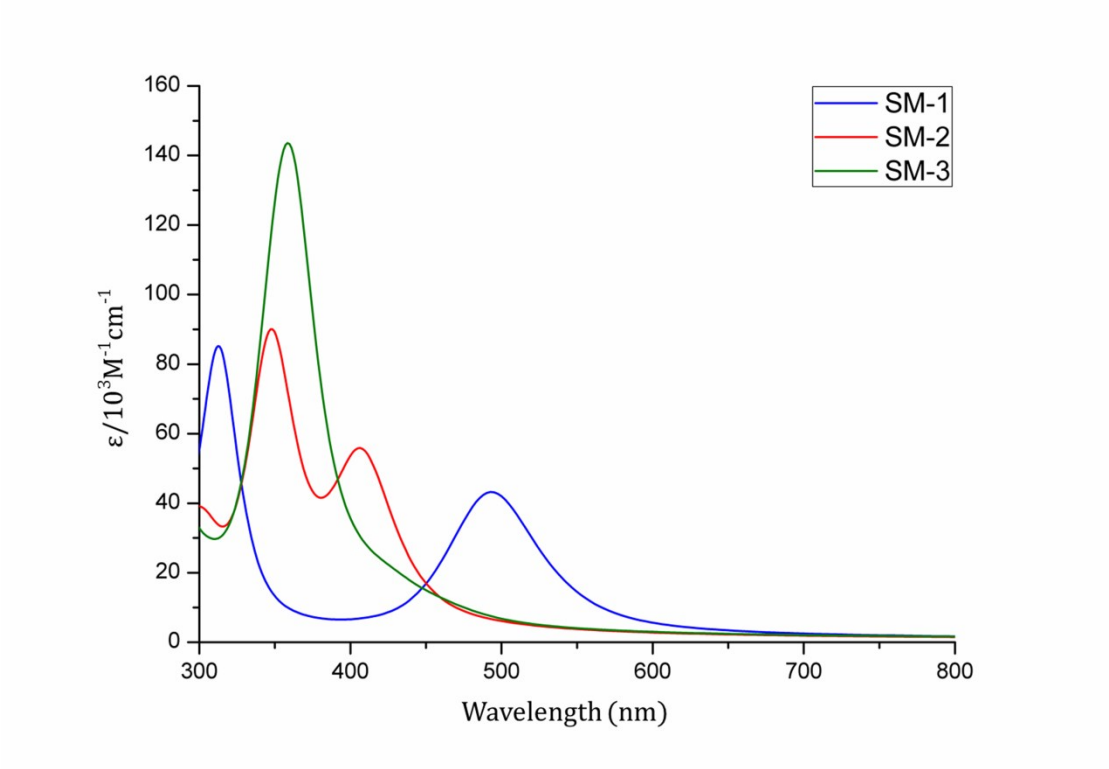

Fig. S4 Calculated absorption spectra of the designed HTMs with the BMK/6-31G** method.

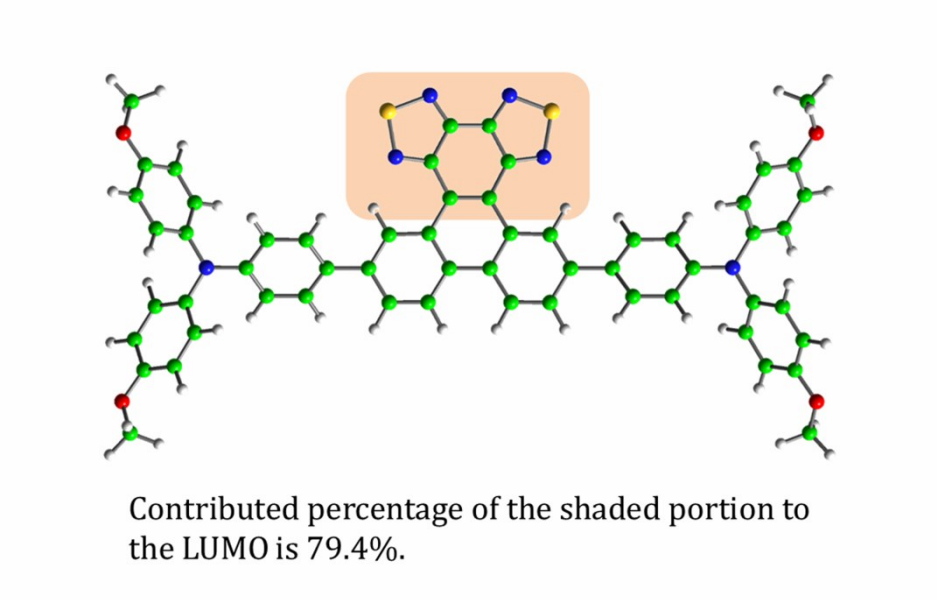

Fig. S5 Calculated orbital contributed percentage of bithiadiazole unit to the LUMO.

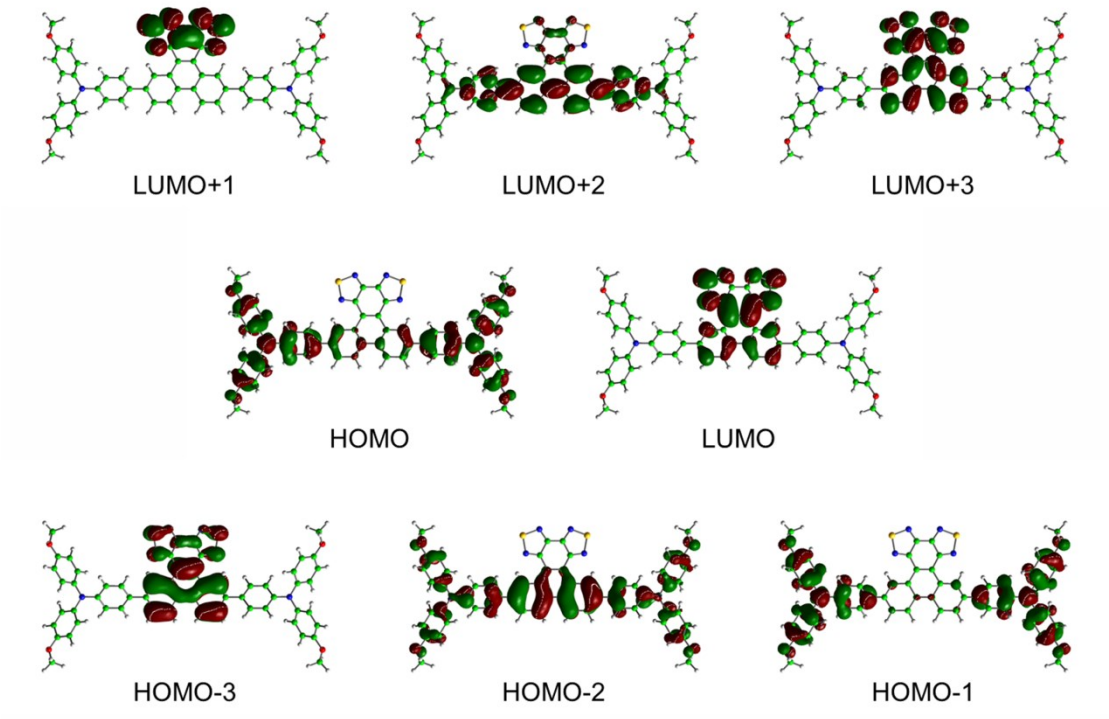

Fig. S6 Calculated orbital spatial distributions of the SM-3.

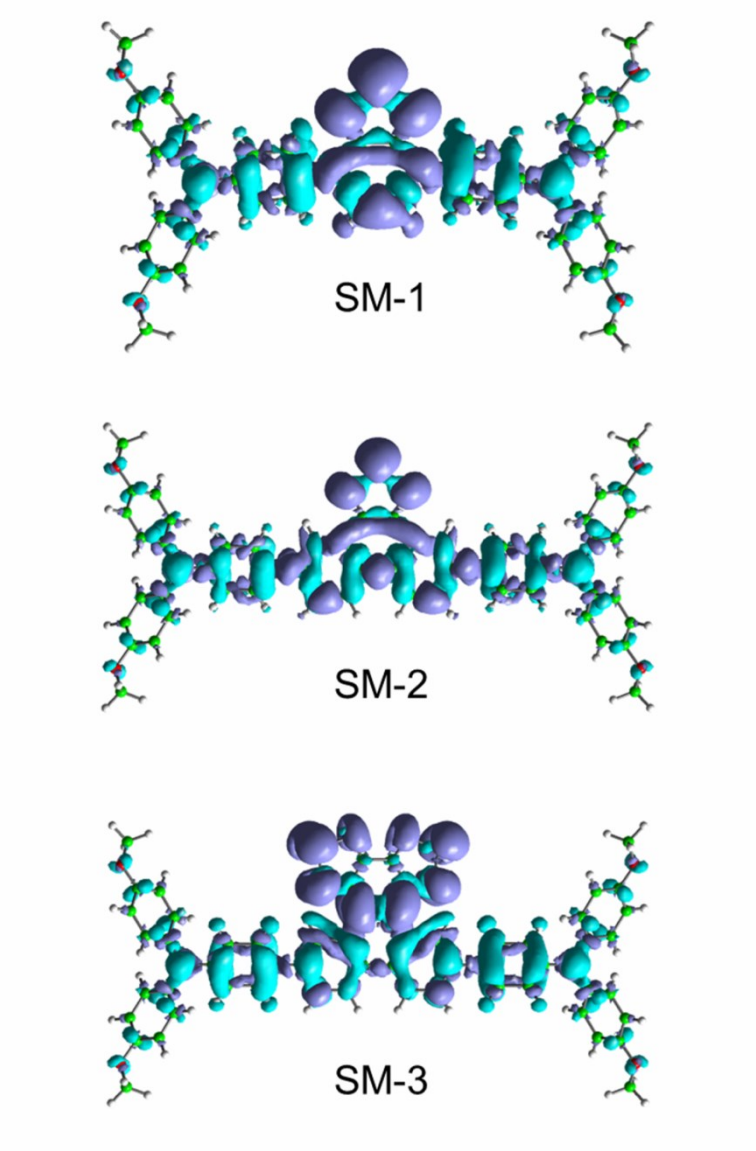

Fig. S7 CDD maps of the investigated HTMs, the purple and the blue represent where the electrons are increased and reduced, respectively.

Molecular coordinate

SM-1

C	1.47825100	-0.10286300	-0.00302400
C	0.73013500	-1.33390800	-0.00127800
C	0.70971800	1.04766300	0.00207300
C	-0.73009200	-1.33393400	0.00118900
C	-0.70975800	1.04763800	-0.00299500
H	1.21008000	2.01048900	0.02289300
C	-1.47825700	-0.10291100	0.00247700
H	-1.21015000	2.01044100	-0.02413900
S	0.00007500	-3.62505900	0.00022900
N	1.25560300	-2.56543000	-0.01225600
N	-1.25550000	-2.56547900	0.01263400
N	7.20347900	0.24708800	-0.02856100
C	7.84633100	1.51553000	-0.15579100
C	8.89159400	1.69218700	-1.07804000
C	7.47038000	2.59990200	0.64473200
C	9.54039700	2.91464100	-1.18849600
H	9.19520500	0.86135900	-1.70660300
C	8.10252600	3.83927400	0.52487900
H	6.67135400	2.47796400	1.36872800
C	9.14853100	4.00184600	-0.39192500
H	10.34932400	3.05270300	-1.89864500
H	7.78273300	4.65697400	1.15919300
C	8.02238100	-0.91315600	0.11935500
C	9.06584900	-0.93129300	1.06003500
C	7.82084900	-2.04523600	-0.67807000
C	9.88129500	-2.04701400	1.19266600
H	9.23571600	-0.06132400	1.68592200
C	8.62183900	-3.18025500	-0.53595400
H	7.02625000	-2.04417300	-1.41717100
C	9.66324300	-3.18489500	0.40042800
H	10.68875700	-2.06264700	1.91757400
H	8.43381500	-4.03980100	-1.16764700
O	9.84253200	5.16233400	-0.58360100
O	10.51222000	-4.23256900	0.61635900
C	10.33679500	-5.41212600	-0.16327700
H	11.10504500	-6.11006500	0.17080800
H	9.34805700	-5.85746900	-0.00167800
H	10.47091500	-5.21108100	-1.23268600
C	9.48978100	6.29454300	0.20614600
H	10.15815700	7.09787800	-0.10507700
H	8.45128000	6.59934400	0.03079800

H	9.63224000	6.09888500	1.27543200
C	2.95382700	-0.05298900	-0.02595800
C	3.62107800	0.97410200	-0.72156600
C	3.75615500	-0.98454800	0.66019800
C	5.00568100	1.07346300	-0.73254100
H	3.04472600	1.69002600	-1.29980900
C	5.14190100	-0.88555400	0.66842400
H	3.28654000	-1.78662200	1.21679800
C	5.79995700	0.14643500	-0.02896200
H	5.48081400	1.86492700	-1.30095800
H	5.72398500	-1.60809500	1.22907000
N	-7.20348900	0.24709400	0.02737200
C	-8.02257200	-0.91312000	-0.11955900
C	-9.06697400	-0.93123500	-1.05922700
C	-7.82040600	-2.04517500	0.67775300
C	-9.88266400	-2.04687900	-1.19099500
H	-9.23737100	-0.06129800	-1.68501800
C	-8.62165400	-3.18012000	0.53647400
H	-7.02511200	-2.04418600	1.41610900
C	-9.66395500	-3.18474200	-0.39891000
H	-10.69082400	-2.06246600	-1.91513200
H	-8.43308600	-4.03964000	1.16804400
C	-7.84617400	1.51560600	0.15499400
C	-8.89037000	1.69266000	1.07836300
C	-7.47097000	2.59966300	-0.64629600
C	-9.53892300	2.91522200	1.18913700
H	-9.19335500	0.86206100	1.70753500
C	-8.10284300	3.83914200	-0.52615700
H	-6.67275300	2.47736200	-1.37113000
C	-9.14782700	4.00211300	0.39175100
H	-10.34704400	3.05361500	1.90014000
H	-7.78366600	4.65660800	-1.16108800
O	-10.51323000	-4.23236600	-0.61397000
O	-9.84149100	5.16272800	0.58379400
C	-9.48952700	6.29461900	-0.20677100
H	-10.15754700	7.09809700	0.10484300
H	-8.45082900	6.59944600	-0.03262800
H	-9.63311600	6.09854500	-1.27583200
C	-10.33711200	-5.41190400	0.16554200
H	-11.10574500	-6.10980600	-0.16774900
H	-9.34856000	-5.85732000	0.00298100
H	-10.47015500	-5.21080800	1.23508000
C	-2.95383600	-0.05305900	0.02533000
C	-3.75612900	-0.98485700	-0.66055900

C	-3.62113700	0.97425600	0.72054900
C	-5.14186500	-0.88586400	-0.66890100
H	-3.28648200	-1.78710400	-1.21687800
C	-5.00574800	1.07362700	0.73140700
H	-3.04482500	1.69039200	1.29857000
C	-5.79997800	0.14635300	0.02811200
H	-5.72391500	-1.60858200	-1.22935600
H	-5.48090200	1.86530200	1.29950800

SM-2

C	-0.72057300	-2.06775300	-0.00804100
C	0.72055200	-2.06778400	-0.00857400
S	-0.00006200	-4.36201900	-0.00789300
N	-1.25736500	-3.28178700	-0.00787000
N	1.25728800	-3.28184200	-0.00834000
C	-1.46919400	-0.82132700	-0.01160500
C	-0.73665600	0.39667100	-0.01085700
C	-2.87099400	-0.82216400	-0.00725300
C	-1.49203500	1.58787500	-0.01512300
C	-3.60685100	0.36532600	-0.01256000
H	-3.37825800	-1.78020700	0.02280900
C	-2.87677100	1.57501200	-0.01906300
H	-0.99263900	2.54927300	-0.02893600
H	-3.40800400	2.52075500	-0.05219200
C	1.46922700	-0.82139000	-0.00530600
C	0.73675500	0.39664300	-0.00748000
C	2.87102600	-0.82229500	-0.00809400
C	1.49219400	1.58781500	-0.00381100
C	3.60694200	0.36516100	-0.00255900
H	3.37828000	-1.78038800	-0.03669500
C	2.87693000	1.57489200	0.00167600
H	0.99283400	2.54925100	0.00860600
H	3.40817100	2.52064100	0.03458100
N	9.34624400	0.33527000	0.00203100
C	10.06959100	-0.89503000	0.02644100
C	11.12258300	-1.08350900	0.93758900
C	9.76272700	-1.92997400	-0.86395400
C	11.84538000	-2.26883900	0.95007200
H	11.37358100	-0.29132800	1.63542300
C	10.46978600	-3.13402300	-0.84334000
H	8.95876900	-1.79750900	-1.58063900
C	11.52254900	-3.30793200	0.06351600
H	12.66026400	-2.41565700	1.65161000
H	10.20157000	-3.91414600	-1.54532000

C	10.08429600	1.55667600	-0.02107500
C	11.14368600	1.73093300	-0.92767700
C	9.78648100	2.59660600	0.86664200
C	11.88124900	2.90716800	-0.93840600
H	11.38816300	0.93470200	-1.62319600
C	10.50854600	3.79173400	0.84761600
H	8.97797700	2.47509300	1.58014500
C	11.56744600	3.95139500	-0.05468200
H	12.70110000	3.04277700	-1.63640900
H	10.24698500	4.57601600	1.54747600
O	12.28698800	-4.43537800	0.16262700
O	12.34620000	5.06926900	-0.15166900
C	12.00537100	-5.51804100	-0.71971000
H	10.98709700	-5.89866600	-0.57721800
H	12.13773400	-5.22703000	-1.76842200
H	12.72090500	-6.30226400	-0.47081000
C	12.07445900	6.15591900	0.72882000
H	11.06166100	6.54927300	0.58178400
H	12.19863500	5.86392300	1.77826800
H	12.80084700	6.93095000	0.48256800
C	5.08679900	0.35843000	0.00010300
C	5.82758200	1.37835200	-0.62461800
C	5.81620900	-0.66865300	0.62675400
C	7.21693300	1.37345200	-0.63279200
H	5.30977000	2.17420600	-1.15138700
C	7.20522200	-0.67903500	0.63541600
H	5.28846100	-1.45794300	1.15349800
C	7.93811500	0.34321400	0.00131100
H	7.75211500	2.16498800	-1.14498500
H	7.73145900	-1.47586800	1.14865200
N	-9.34612700	0.33466900	0.00042200
C	-10.08384000	1.55631200	0.02616900
C	-11.13645700	1.73302400	0.94011800
C	-9.79208700	2.59404900	-0.86607600
C	-11.87351100	2.90955600	0.95352100
H	-11.37604100	0.93848900	1.63928300
C	-10.51357500	3.78947700	-0.84459400
H	-8.98880000	2.47054200	-1.58513000
C	-11.56582400	3.95158500	0.06504200
H	-12.68815300	3.04713900	1.65721400
H	-10.25682700	4.57203900	-1.54815200
C	-10.06987400	-0.89540600	-0.01956400
C	-11.12917300	-1.08299700	-0.92358400
C	-9.75752700	-1.93091200	0.86830600

C	-11.85260800	-2.26796700	-0.93168000
H	-11.38459000	-0.29037800	-1.61930300
C	-10.46530800	-3.13461200	0.85192800
H	-8.94870400	-1.79919300	1.57961700
C	-11.52426400	-3.30762900	-0.04784000
H	-12.67234400	-2.41404100	-1.62770000
H	-10.19275200	-3.91518000	1.55173400
O	-12.34344500	5.06993500	0.16508700
O	-12.28993400	-4.43467400	-0.14230300
C	-12.07744600	6.15464900	-0.71955500
H	-11.06348300	6.54787300	-0.58042900
H	-12.20910700	5.86052600	-1.76749100
H	-12.80177900	6.93048400	-0.46981900
C	-12.00310400	-5.51775900	0.73781100
H	-10.98596900	-5.89884700	0.58857000
H	-12.12848100	-5.22704300	1.78746700
H	-12.72062900	-6.30155600	0.49332800
C	-5.08671000	0.35868500	-0.01176600
C	-5.81790700	-0.66906300	-0.63525100
C	-5.82571300	1.37918500	0.61410000
C	-7.20694700	-0.67971800	-0.63947300
H	-5.29168200	-1.45879000	-1.16286600
C	-7.21502000	1.37404200	0.62669800
H	-5.30638900	2.17565900	1.13843200
C	-7.93802000	0.34289000	-0.00382400
H	-7.73466400	-1.47714800	-1.15025900
H	-7.74871000	2.16601300	1.13976200

SM-3

C	-0.69082700	-4.12202800	-0.25379600
C	-1.36809200	-2.85271600	-0.39575000
S	-2.90319700	-4.63123200	-0.98920000
C	1.36449300	-2.85325900	0.29846600
C	0.68442700	-4.12208700	0.16325700
S	2.89650600	-4.63254400	0.89869000
C	-0.69578900	-1.56455000	-0.15576300
C	0.69464900	-1.56476400	0.05198800
N	-2.62257000	-3.01415400	-0.81498000
N	-1.41455500	-5.19115000	-0.53936500
N	1.40621600	-5.19130700	0.45318700
N	2.61909200	-3.01578500	0.71688200
C	-1.43845100	-0.30750300	-0.14302100
C	-0.72382900	0.92449100	-0.07403500
C	-2.85343400	-0.26413700	-0.11770200

C	-1.46721400	2.12696400	-0.01853400
C	-3.57423200	0.92615200	-0.06444000
H	-3.39804000	-1.19382400	-0.11236800
C	-2.84476200	2.13634900	-0.02381600
H	-0.95242200	3.07768500	0.03587400
H	-3.36863800	3.08655300	-0.00561400
C	1.43849200	-0.30825000	0.03080400
C	0.72556900	0.92344000	-0.06195500
C	2.85366900	-0.26538300	0.02210100
C	1.47034800	2.12417900	-0.13329800
C	3.57572800	0.92376100	-0.04024600
H	3.39782900	-1.19509800	0.03972100
C	2.84780400	2.13320600	-0.11353600
H	0.95665200	3.07402000	-0.20930600
H	3.37245500	3.08270800	-0.14289100
N	9.31697400	0.90106800	-0.01772600
C	10.05179200	2.12270500	-0.07645500
C	11.12628200	2.26549100	-0.97094900
C	9.73536600	3.19614700	0.76388000
C	11.85996900	3.44337400	-1.01557300
H	11.38567100	1.44360800	-1.63024500
C	10.45356600	4.39247700	0.70971600
H	8.91508600	3.10006500	1.46771100
C	11.52752900	4.52063200	-0.17965800
H	12.69133700	3.55436300	-1.70427100
H	10.17709500	5.20278900	1.37325000
C	10.04017000	-0.32706300	0.05310700
C	11.09463500	-0.48168400	0.96913300
C	9.73070800	-1.39564900	-0.79582700
C	11.81605200	-1.66658000	1.02622500
H	11.34794600	0.33636600	1.63554900
C	10.43624500	-2.59889000	-0.72964900
H	8.92580200	-1.29018400	-1.51593200
C	11.49049100	-2.73897200	0.18131500
H	12.63193800	-1.78700000	1.73165300
H	10.16573400	-3.40522300	-1.40044400
O	12.30412000	5.63713200	-0.30731300
O	12.25357100	-3.86299600	0.32255100
C	12.01501700	6.75512500	0.52714100
H	11.00364300	7.13931100	0.34915500
H	12.12276800	6.50307600	1.58870600
H	12.74314600	7.52287600	0.26378800
C	11.96939100	-4.97767400	-0.51808900
H	10.95097500	-5.35171000	-0.35977900

H	12.10008400	-4.72623400	-1.57720500
H	12.68461000	-5.75277600	-0.24125500
C	5.05654800	0.91819700	-0.03645800
C	5.78519600	-0.07494600	0.64412400
C	5.79861400	1.90556400	-0.71002700
C	7.17423500	-0.08328400	0.65744000
H	5.25522900	-0.83737200	1.20696600
C	7.18830300	1.90167100	-0.71355700
H	5.28247500	2.67363900	-1.27804200
C	7.90789000	0.90642000	-0.02506700
H	7.70015500	-0.85201100	1.21241200
H	7.72488000	2.66675500	-1.26331500
N	-9.31431000	0.89919600	0.04821700
C	-10.04031100	-0.32866700	0.01847700
C	-11.13178300	-0.48900700	-0.85219000
C	-9.69904900	-1.39040100	0.86399000
C	-11.85757300	-1.67243900	-0.86894500
H	-11.41052500	0.32369600	-1.51494600
C	-10.40956400	-2.59231900	0.83760800
H	-8.86525400	-1.28079600	1.54968200
C	-11.50032800	-2.73795000	-0.02825100
H	-12.70200000	-1.79695500	-1.53918500
H	-10.11385500	-3.39329100	1.50415900
C	-10.04695900	2.12215600	0.11658300
C	-11.07678900	2.28476400	1.05871600
C	-9.77102100	3.17701100	-0.76049200
C	-11.80735700	3.46418300	1.11384100
H	-11.30369400	1.47713800	1.74704100
C	-10.48556500	4.37506300	-0.69723300
H	-8.98547900	3.06480900	-1.50075700
C	-11.51536700	4.52309500	0.24012400
H	-12.60435000	3.59089900	1.83946900
H	-10.24127200	5.17086200	-1.39029300
O	-12.27141000	-3.86113200	-0.12799800
O	-12.28447400	5.64287300	0.38151400
C	-11.95770900	-4.96800900	0.71232700
H	-10.94732600	-5.34696500	0.51830200
H	-12.04621900	-4.70535200	1.77309600
H	-12.68533600	-5.74365400	0.47168000
C	-12.03293000	6.74447900	-0.48637000
H	-11.01404800	7.12994700	-0.36221500
H	-12.18965200	6.47274500	-1.53689700
H	-12.74743400	7.51835200	-0.20433100
C	-5.05480100	0.92125400	-0.03927800

C	-5.78187500	1.92048600	0.63304600
C	-5.79831400	-0.08419700	-0.68487100
C	-7.17099500	1.91545400	0.67030700
H	-5.25330600	2.69919500	1.17449300
C	-7.18730100	-0.09412600	-0.66429700
H	-5.28104100	-0.85629100	-1.24638800
C	-7.90572100	0.90636500	0.01896100
H	-7.69495800	2.69014700	1.21870600
H	-7.72540700	-0.87326900	-1.19239000