Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information for

Theoretical design of asymmetric A-$D_1A'D_2$-A acceptors for organic solar cells

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Contents

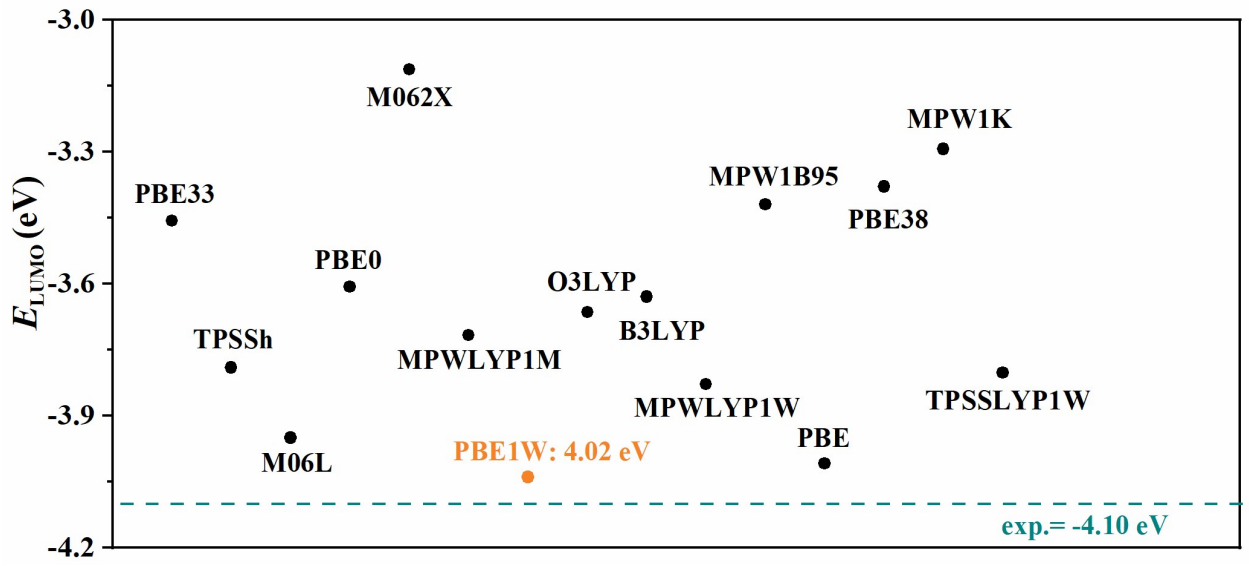

Figure S1. The calculated energy of LUMO (E_{LUMO}, eV) of acceptor Y6 using different DFT functionals and the experiment E_{LUMO} of Y6.[1]

1. J. Yuan, Y. Zhang, L. Zhou, G. Zhang, H.-L. Yip, T.-K. Lau, X. Lu, C. Zhu, H. Peng, P. A. Johnson, M. Leclerc, Y. Cao, J. Ulanski, Y. Li and Y. Zou, *Joule*, 2019, **3**, 1140-1151.

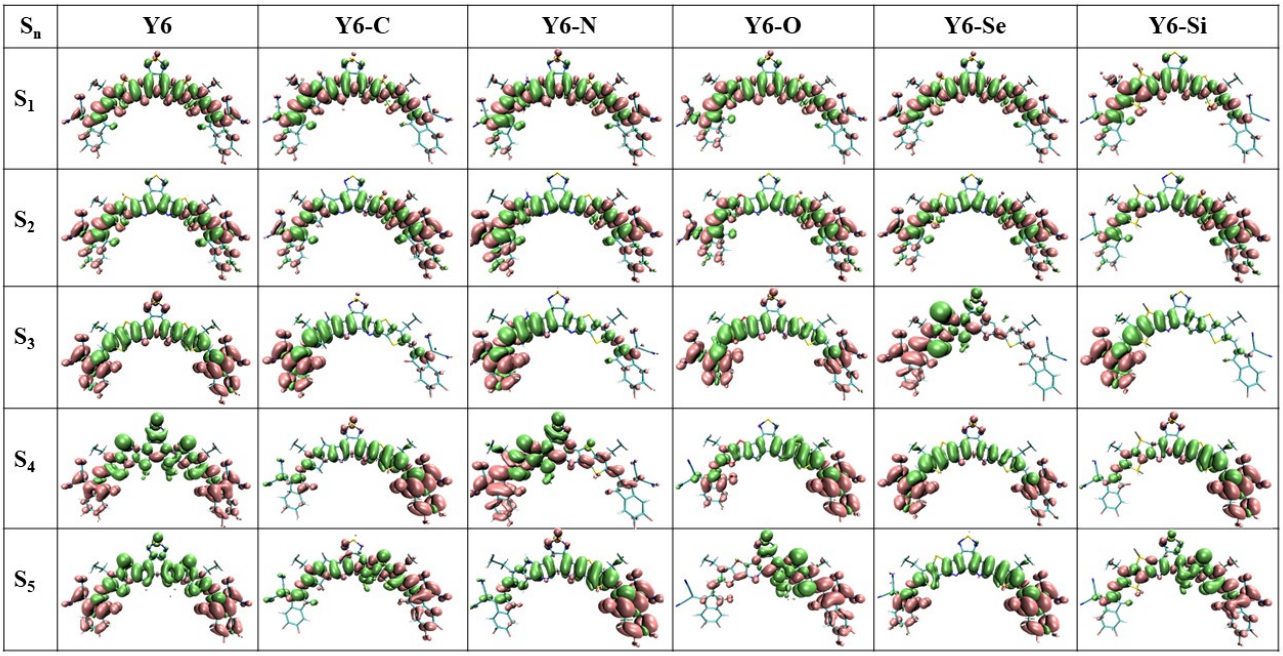

Figure S2. The charge difference density (CDD) maps of the five lowest excited states for the investigate acceptors at TD-CAM-B3LYP /6-311G (d, p) level.

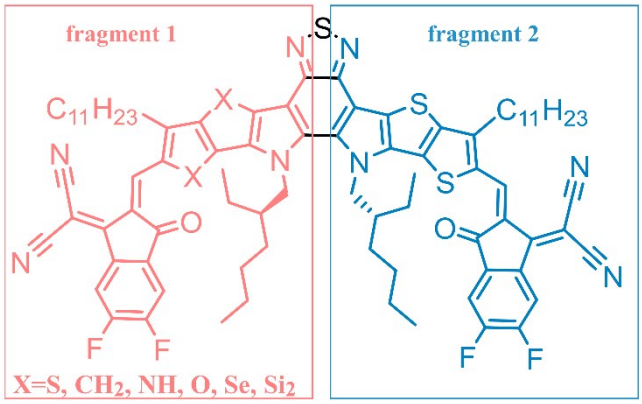

Figure S3. The fragment 1 and fragment 2 of studied molecules.

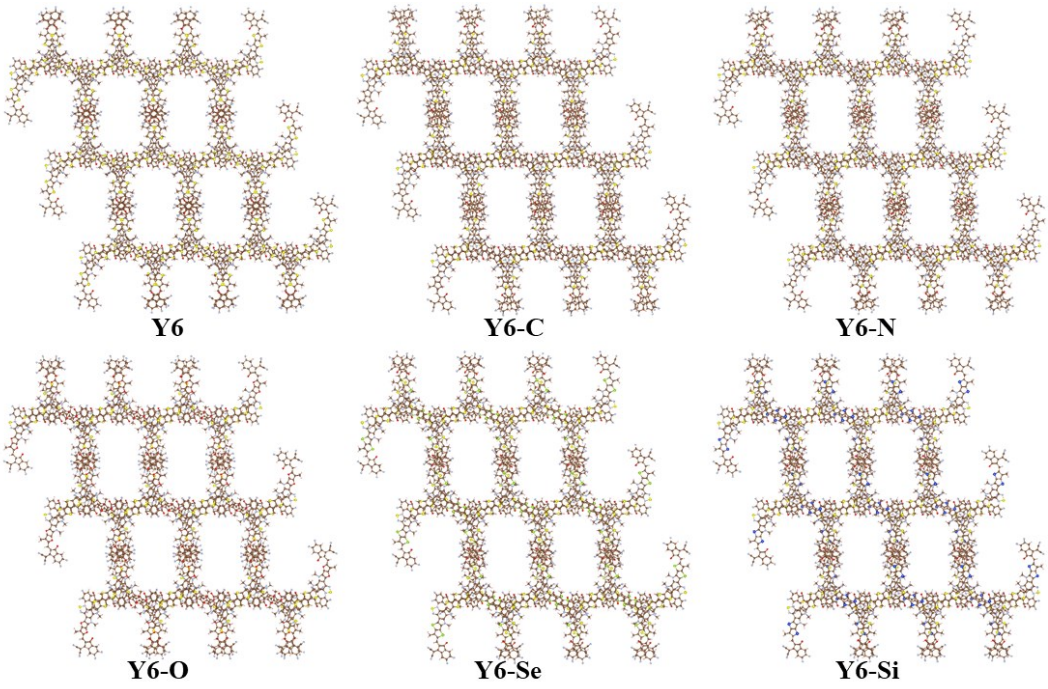

Figure S4. The grid-like packing of the studied molecules (the long branched side chains have been omitted for the sake of clarity).

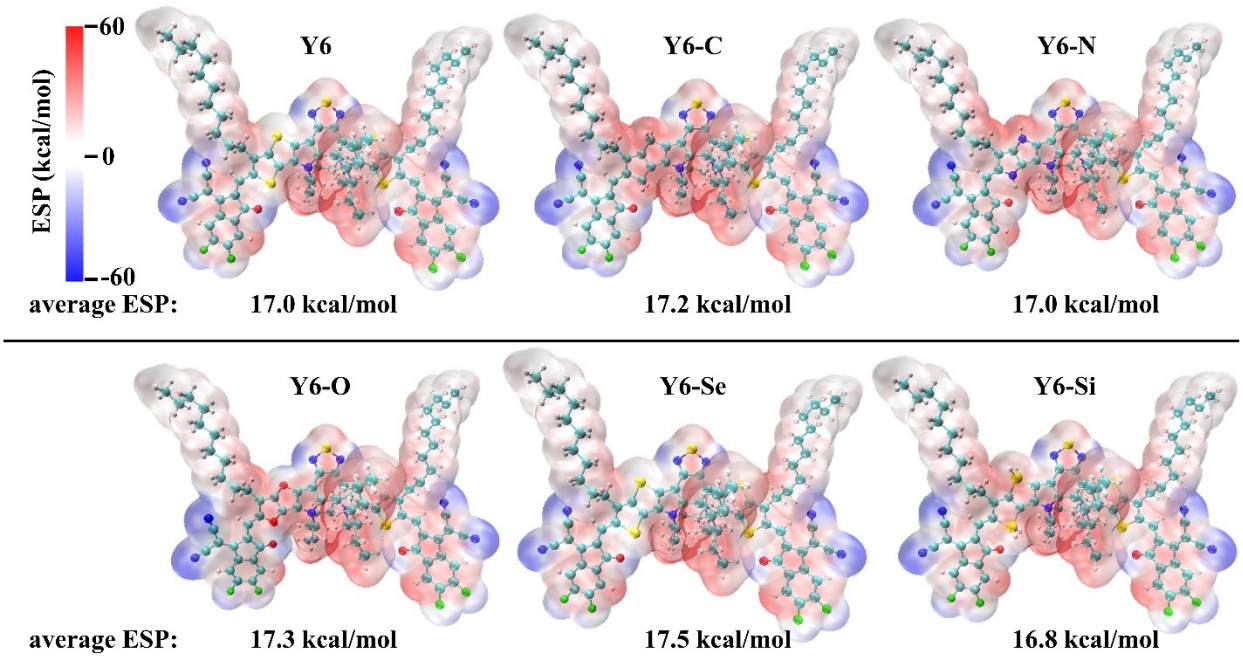

Figure S5. The electrostatic potential (ESP) mapped onto a surface of total electrons for the Y6 and the newly designed acceptors.

Table S1. The amount of charge transferring from fragment 1 to fragment 2 for the lowest 20 excited states of the studied molecules.

S_n	Y6/|e|	Y6-C/|e|	Y6-N/|e|	Y6-O/|e|	Y6-Se/|e|	Y6-Si/|e|
S_1	0.00	0.02	0.07	0.01	-0.01	-0.03
S_2	0.00	0.07	0.02	0.02	0.02	0.07
S_3	0.00	-0.04	-0.04	-0.04	0.06	-0.06
S_4	0.00	0.09	0.10	0.04	-0.04	0.02
S_5	0.00	0.21	0.10	-0.06	0.04	-0.01
S_6	0.00	-0.01	0.03	-0.04	-0.04	-0.11
S_7	0.02	0.03	0.29	0.13	0.00	0.06
S_8	0.00	0.02	0.10	0.02	0.02	0.14
S_9	-0.01	-0.06	0.13	-0.03	0.03	-0.12
S_{10}	-0.01	0.01	0.01	0.00	0.04	0.04
S_{11}	0.01	-0.01	-0.01	-0.01	-0.01	-0.02
S_{12}	0.00	0.07	0.06	0.00	0.01	-0.01
S_{13}	0.00	0.00	0.09	0.03	0.12	0.06
S_{14}	-0.01	0.11	0.07	-0.08	0.02	-0.10
S_{15}	0.00	0.02	0.05	-0.02	0.05	-0.01
S_{16}	0.04	0.26	0.06	-0.11	-0.11	-0.05
S_{17}	-0.07	-0.08	0.13	0.02	0.13	-0.40
S_{18}	0.05	-0.03	0.25	0.19	-0.08	-0.30
S_{19}	0.02	0.04	0.14	0.12	-0.03	-0.05
S_{20}	-0.03	-0.02	-0.02	-0.02	-0.01	0.35

Table S2. The HOMO level E_{HOMO} (eV) of acceptors and the differences of HOMO level ΔE_{HOMO} (eV) between PM6 and acceptors.

molecule	E_{HOMO} (eV)	ΔE_{HOMO} (eV)
PM6	-5.56	-
Y6	-5.20	-0.36
Y6-C	-5.01	-0.55
Y6-N	-5.01	-0.55
Y6-O	-5.19	-0.37
Y6-Se	-5.18	-0.38
Y6-Si	-5.13	-0.43