Electronic Supplementary Material (ESI) for Nanoscale Advances.

Theoretical study of the influence of doped oxygen group elements on the properties of organic semiconductors

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Table S1. Fukui (-), Fukui (+) indices for each atom of seven-membered benzothiophene

Position	Fukui(-)	Fukui(+)	Position	Fukui(-)	Fukui(+)	Position	Fukui(-)	Fukui(+)
C(1)	-0.002	0.004	C(10)	0.026	0.043	C(19)	0.011	0.027
C(2)	0.009	0.005	C(11)	0.010	0017	C(20)	0.029	0.036
C(3)	0.011	0.027	C(12)	-0.001	-0.003	C(21)	0.009	0.005
C(4)	0.006	-0.003	C(13)	0.029	0.036	C(22)	-0.002	0.004
S(5)	**0.103**	**0.065**	**S(14)**	**0.132**	**0.069**	**S(23)**	**0.103**	**0.065**
C(6)	0.017	0.016	C(15)	-0.001	-0.003	C(24)	0.017	0.016
C(7)	0.016	0.030	C(16)	0.010	0.017	C(25)	0.016	0.030
C(8)	0.019	0.009	C(17)	0.026	0.043	C(26)	0.019	0.009
C(9)	0.011	0.024	C(18)	0.006	-0.003	C(27)	0.011	0.024

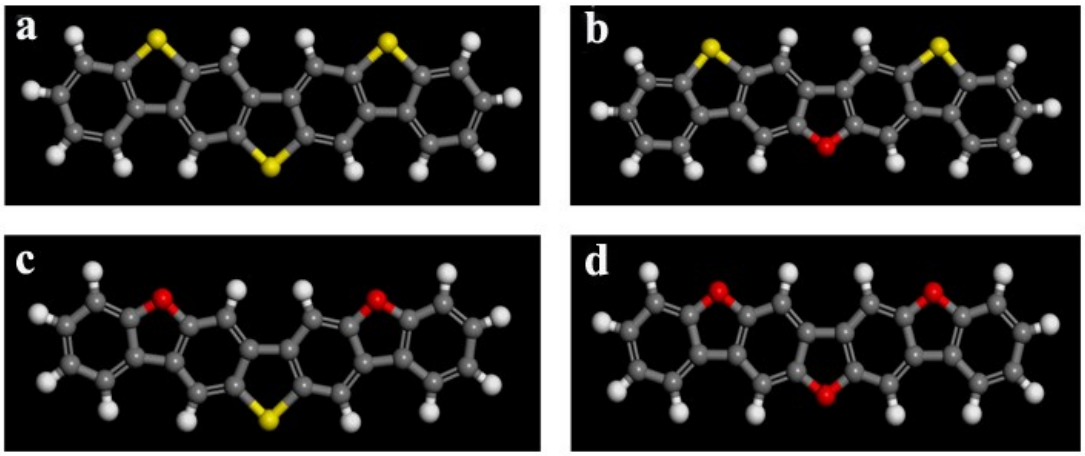
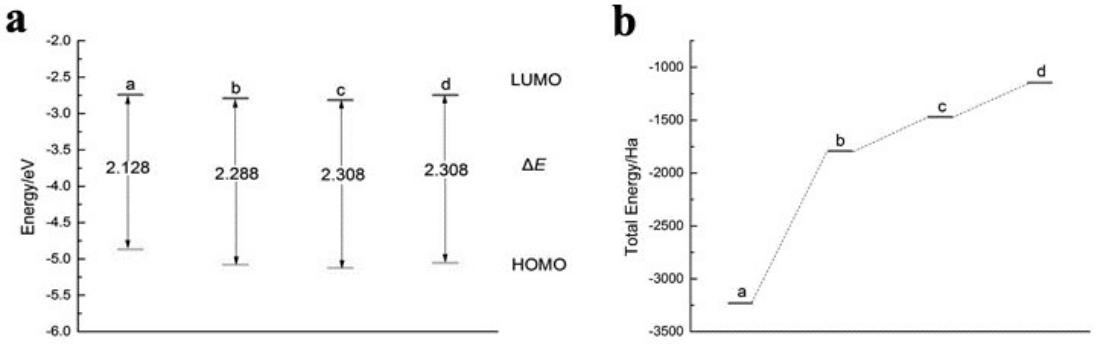


Fig. S1. Schematic diagram of the structure of the doping site of the oxygen group elemenst at the seven-membered benzothiophene (a: seven-membered benzothiophene; b: mono oxygen group elements doped benzothiophene; c: binary oxygen group elements doped benzothiophene; d: ternary oxygen group elements doped benzothiophene.



gray: C, white: H, yellow: S, red: Oxygen group elements)

Fig. S2. (a) E_{LUMO}, E_{HOMO}, and ΔE of seven-membered benzothiophene doped with O atom; (b) Schematic diagram of total energy of each substance (a: seven-membered benzothiophene;

b: mono O-doped seven-membered benzothiophene ; c: binary O-doped seven-membered benzothiophene; d: ternary O-doped seven-membered benzothiophene)

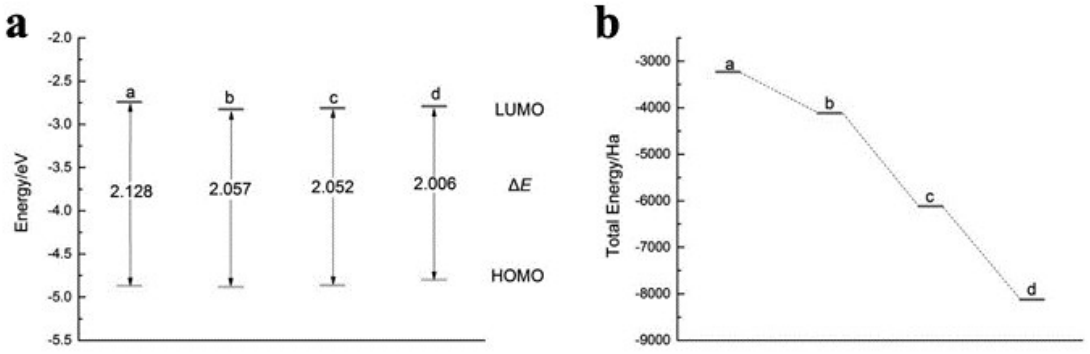


Fig. S3. (a) E_{LUMO}, E_{HOMO}, and ΔE of seven-membered benzothiophene doped with Se atom; (b) Schematic diagram of total energy of each substance (a: seven-membered benzothiophene; b: mono Se-doped seven-membered benzothiophene ; c: binary Se-doped seven-membered benzothiophene; d: ternary Se-doped seven-membered benzothiophene)

Table S2. E_{HOMO}, E_{LUMO}, ΔE and total energy of undoped and Te-doped seven-membered benzothiophene

Molecule	E_{HOMO}/eV	E_{LUMO}/eV	ΔE/eV	Total energy/Ha
seven-membered benzothiophene	-4.869	-2.741	2.128	-3230.788
mono Te-doped seven-membered benzothiophene	-4.823	-2.870	1.953	-8330.948
binary Te-doped seven-membered benzothiophene	-4.790	-2.846	1.944	-14546.716
ternary Te-doped seven-membered benzothiophene	**-4.658**	**-2.810**	**1.848**	**-20762.485**

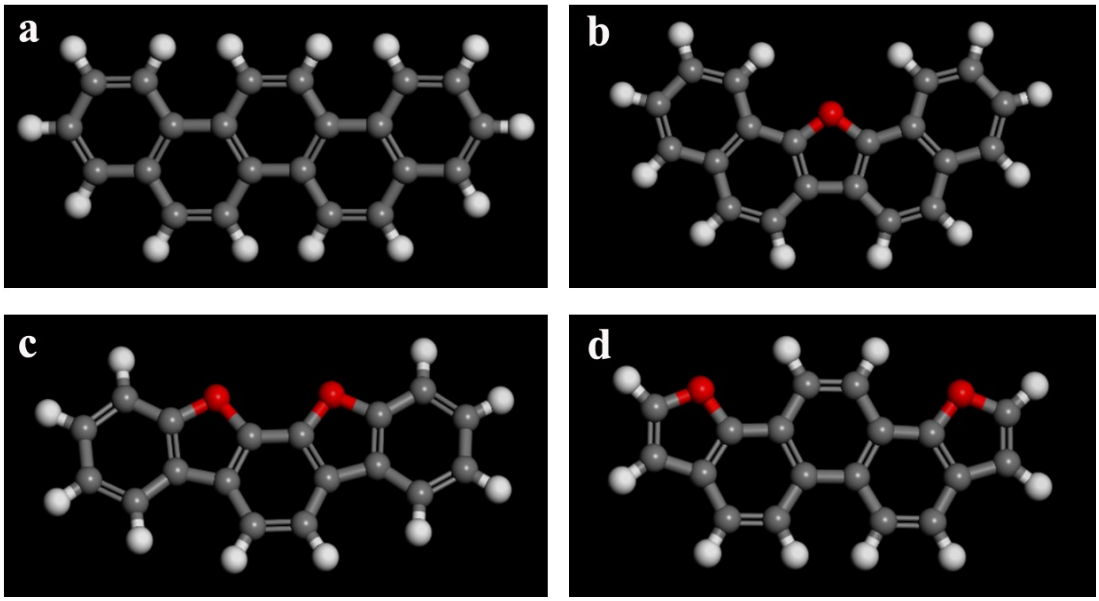


Fig. S4. Schematic diagram of the structure of the doping site of the oxygen group elements at the o-pentacene (a: o-pentacene; b: mono oxygen group elements doped o-pentacene; c: binary oxygen group elements doped o-pentacene (two-four ring); d: binary oxygen group elements doped o-pentacene(one-five ring). gray: C, white: H, red: Oxygen group elements)

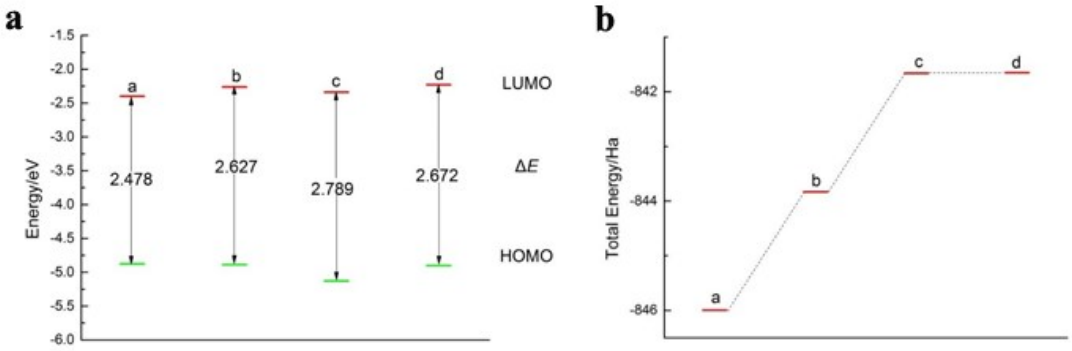


Fig. S5. (a) E_{LUMO}, E_{HOMO}, and ΔE of o-pentacene doped with O atoms; (b) Schematic diagram of total energy of each substance (a: o-pentacene; b: mono-O doped o-pentacene; c: binary O-doped o-pentacene (two-four ring); d: binary O-doped o-pentacene (one-five ring))

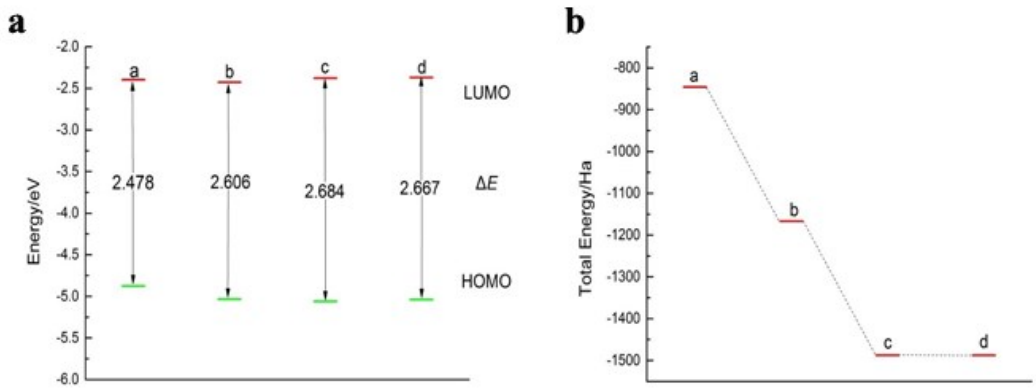


Fig. S6. (a) E_{LUMO}, E_{HOMO}, and ΔE of o-pentacene doped with S atoms;
(b) Schematic diagram of total energy of each substance
(a: o-pentacene; b: mono-S doped o-pentacene; c: binary S-doped o-pentacene (two-four ring); d: binary S-doped o-pentacene (one-five ring))

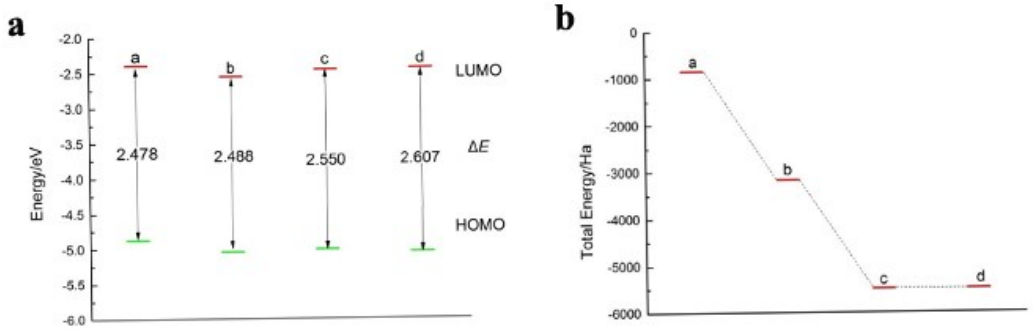


Fig. S7. (a) E_{LUMO}, E_{HOMO}, and ΔE of o-pentacene doped with Se atoms;
(b) Schematic diagram of total energy of each substance
(a: o-pentacene; b: mono-Se doped o-pentacene; c: binary Se-doped o-pentacene (two-four ring); d: binary Se-doped o-pentacene (one-five ring))

Table S3. E_{HOMO}, E_{LUMO}, ΔE and total energy of undoped and Te-doped o-pentacene

Molecule	E_{HOMO}/eV	E_{LUMO}/eV	ΔE/eV	Total energy/Ha
o-pentacene	-4.877	-2.399	2.478	-845.997
mono-Te doped o-pentacene	-4.977	-2.678	2.299	-7382.528
binary Te-doped o-pentacene (two-four ring);	**-4.893**	**-2.539**	**2.354**	**-13919.001**
binary Te-doped o-pentacene (one-five ring)	-5.004	-2.510	2.494	-13918.987

Table S4. Fukui (-), Fukui (+) indices for each atom of DP-DTT

Position	Fukui(-)	Fukui(+)	Position	Fukui(-)	Fukui(+)	Position	Fukui(-)	Fukui(+)
C(1)	0.021	0.011	C(9)	0.022	0.026	C(17)	0.011	0.010
C(2)	0.021	0.014	C(10)	0.039	0.029	C(18)	0.019	0.020
C(3)	0.021	0.014	**S(11)**	**0.071**	**0.079**	C(19)	0.017	0.019
C(4)	0.021	0.011	C(12)	-0.003	0.004	C(20)	0.011	0.011
S(5)	**0.087**	**0.087**	C(13)	-0.003	0.004	C(21)	0.032	0.035
C(6)	0.022	0.026	C(14)	0.017	0.019	C(22)	0.011	0.010
C(7)	0.039	0.029	C(15)	0.011	0.011	C(23)	0.019	0.020
S(8)	**0.074**	**0.080**	C(16)	0.032	0.035			

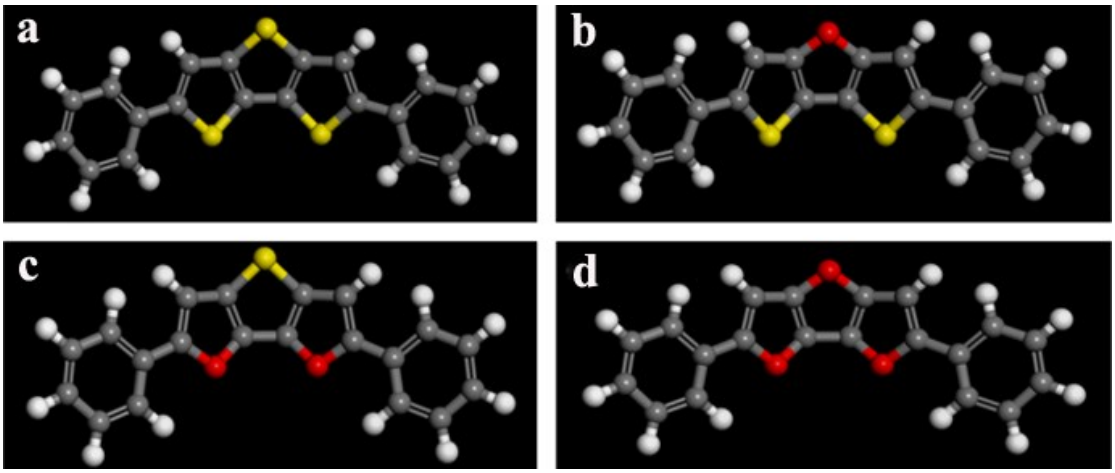
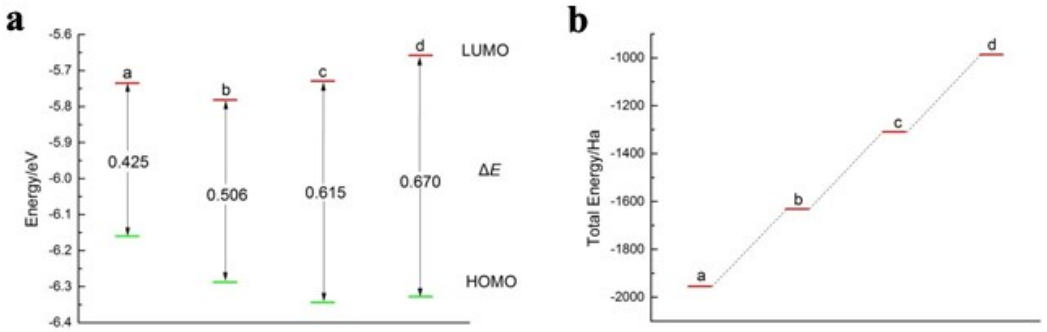


Fig. S8. Schematic diagram of the structure of the oxygen group element at the doping site of DP-DTT (a: DP-DTT; b: mono oxygen group elements doped DP-DTT; c: binary oxygen group elements doped DP-DTT; d: ternary oxygen group elements doped DP-DTT.



gray: C, white: H, red: Oxygen group elements)

Fig. S9. (a) E_{LUMO}, E_{HOMO}, and ΔE of DP-DTT doped with O atom; (b) Schematic diagram of total energy of each substance (a: DP-DTT; b: mono O-doped DP-DTT; c: binary O-doped DP-DTT; d: ternary O-doped DP-DTT)

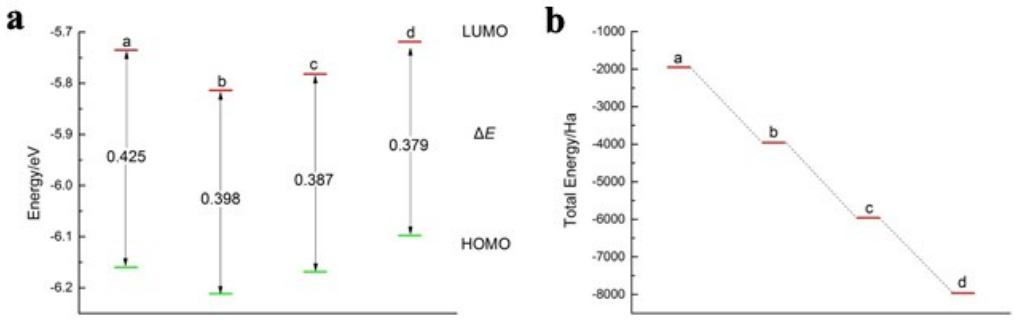


Fig. S10. (a) E_{LUMO}, E_{HOMO}, and ΔE of DP-DTT doped with Se atom; (b) Schematic diagram of total energy of each substance (a: DP-DTT; b: mono Se-doped DP-DTT; c: binary Se-doped DP-DTT; d: ternary Se-doped DP-DTT)

Table S5. E_{HOMO}, E_{LUMO}, ΔE and total energy of undoped and Te-doped DP-DTT

Molecule	E_{HOMO}/eV	E_{LUMO}/eV	ΔE/eV	Total energy/Ha
DP-DTT	-6.160	-5.735	0.425	-1954.536
mono Te-doped DP-DTT	-6.171	-5.821	0.350	-8170.734
binary Te-doped DP-DTT	**-6.075**	**-5.762**	**0.313**	**-14386.396**
ternary Te-doped DP-DTT	-5.931	-5.664	0.267	-20602.174

Table S6. Fukui (-), Fukui (+) indices for each atom of pentacene

Position	**Fukui(-)**	**Fukui(+)**	**Position**	**Fukui(-)**	**Fukui(+)**	**Position**	**Fukui(-)**	**Fukui(+)**
C(1)	0.030	0.022	**S(8)**	**0.098**	**0.106**	C(15)	0.020	0.021
C(2)	0.020	0.015	C(9)	0.020	0.021	C(16)	0.053	0.053
C(3)	0.020	0.015	C(10)	0.053	0.053	**S(17)**	**0.096**	**0.105**
C(4)	0.030	0.022	**S(11)**	**0.096**	**0.105**	H(18)	0.048	0.048
S(5)	**0.095**	**0.104**	C(12)	0.009	0.007	H(19)	0.055	0.054
C(6)	0.009	0.007	C(13)	0.023	0.018	H(20)	0.048	0.048
C(7)	0.023	0.018	**S(14)**	**0.098**	**0.106**	H(21)	0.055	0.054

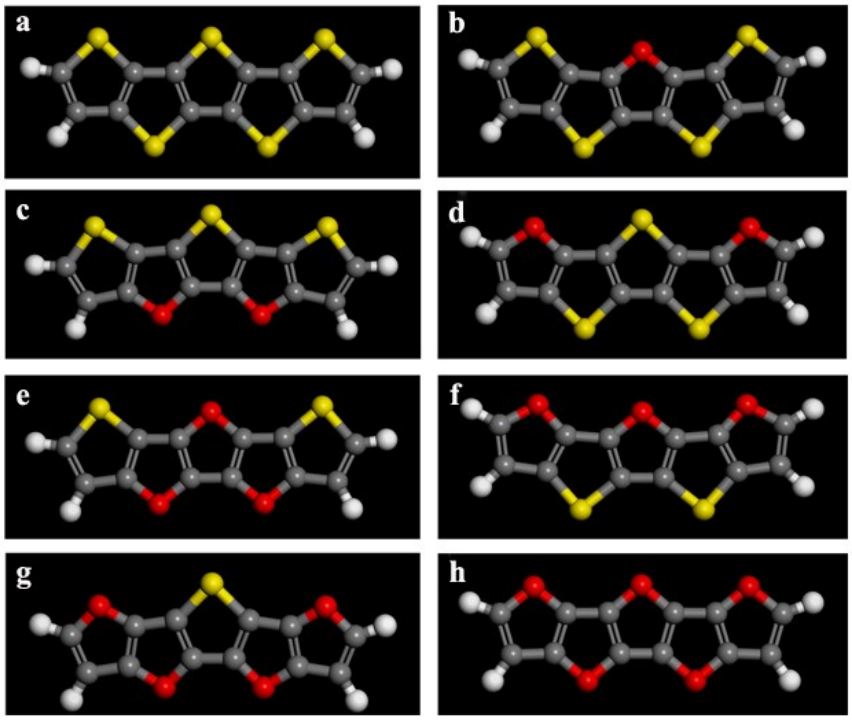
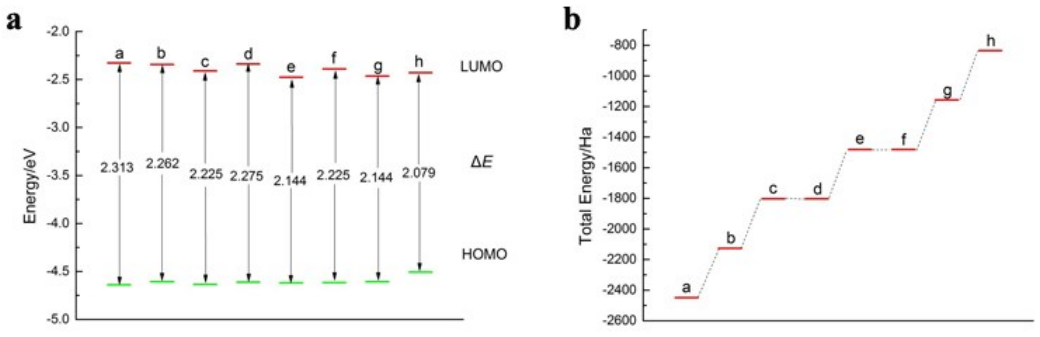


Fig. S11. Schematic diagram of the structure of the doping site of the oxygen group elements at the pentacene (a: pentacene; b: mono oxygen group elements doped pentacene; c: binary oxygen group elements doped pentacene (two-four ring); d: binary oxygen group elements doped pentacene (one-five ring); e: ternary oxygen group elements doped pentacene (two-three-four ring); f: ternary oxygen group elements doped pentacene (one-three-five-ring); g: quaternary oxygen group elements doped pentacene; h: five membered oxygen group-doped pentacene. gray: C, white: H, red: Oxygen group element)

Fig. 12. (a) E_{LUMO}, E_{HOMO}, and ΔE of pentacene doped with O atom; (b) Schematic diagram of total energy of each substance (a: pentacene; b: mono O-doped pentacene; c: binary O-doped pentacene (two-four ring); d: binary O-doped pentacene (one-five ring); e: ternary O-doped pentacene (two-three-four ring); f: ternary O-doped pentacene (one-three-five-ring); g: quaternary O-doped pentacene; h: five membered O-doped pentacene)



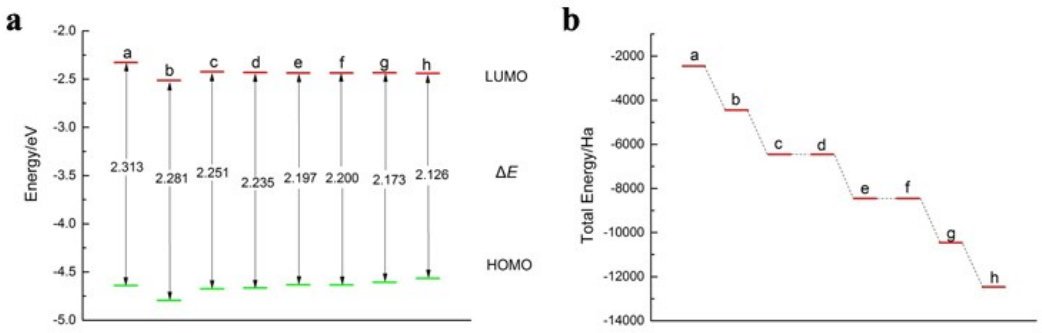


Fig. S13. (a) E_{LUMO}, E_{HOMO}, and ΔE of pentacene doped with Se atom; (b) Schematic diagram of total energy of each substance (a: pentacene; b: mono Se-doped pentacene; c: binary Se-doped pentacene (two-four ring); d: binary Se-doped pentacene (one-five ring); e: ternary Se-doped pentacene (two-three-four ring); f: ternary Se-doped pentacene (one-three-five-ring); g: quaternary Se-doped pentacene; h: five membered Se-doped pentacene)

Table S7. E_{HOMO}, E_{LUMO}, ΔE and total energy of undoped and Te-doped pentacene

Molecule	E_{HOMO}/eV	E_{LUMO}/eV	ΔE/eV	Total energy/Ha
pentacene	-4.640	-2.327	2.313	-2449.494
mono Se-doped pentacene	-4.849	-2.612	2.237	-8665.292
binary Se-doped pentacene (two-four ring)	-4.707	-2.522	2.185	-14881.068
binary Se-doped pentacene (one-five ring)	-4.699	-2.552	2.147	-14881.058
ternary Se-doped pentacene (two-three-four ring)	-4.650	-2.570	2.080	-21096.843
ternary Se-doped pentacene (one-three-five-ring)	-4.649	-2.568	2.081	-21096.834
quaternary Se-doped pentacene	-4.593	-2.585	2.008	-27312.609
five membered Se-doped pentacene	**-4.557**	**-2.629**	**1.928**	**-33528.383**