Supporting information

Molecular engineering and structure-property relationship based on D-A chlorophyll derivative and the application in organic solar cells

Kaiyan Zhang[1,2], Ting Li[1], Peng Song[3*], Fengcai Ma[3], Yuanzuo Li[1,2*]

[1]   *College of Science, Northeast Forestry University, Harbin 150040, Heilongjiang, China*

[2]   *College of Materials Science and Engineering, Northeast Forestry University, Harbin 150040, Heilongjiang, China*

[3]   *Department of Physics, Liaoning University, Shenyang 110036, Liaoning, China*

----

*Corresponding author:

E-mail Address: yzli@nefu.edu.cn; Songpeng@lnu.edu.cn; liyuanzuo5203@126.com

Section S.1. Computational details

S.1.1. Electrochemical parameters

Some important electrochemical parameters can be calculated by following formula details, including ionization potential (*IP*), electron affinity (*EA*), electrophilicity index (ω), electronic acceptance ability (ω^+), absolute hardness (η) and reorganization energy.

IP and *EA* are directly related to the optimization energy of ionic state structure and ground state structure [1]:

$$IP = E(N-1) - E(N) \tag{S1}$$

$$EA = E(N) - E(N+1) \tag{S2}$$

Where *E(N)* is the energy of optimized ground state structure, *E(N-1)* is the energy of optimized cationic structure, and *E(N+1)* is the energy of optimized anionic structure.

Absolute hardness (η) is one of the critical parameters for evaluating the stability of organic molecules, which can be expressed by the following equation [2]:

$$\eta = \frac{IP - EA}{2} \tag{S3}$$

The electrophilic index ω is an important index to evaluate the electrophilic ability of molecules. A smaller ω indicates that electrons have good electron donating ability, and ω^+ indicates the electron receiving ability, which is used to characterize the size of the molecule's ability to acquire electrons. It can be calculated by the following formula[3]:

$$\omega = \frac{\left(IP + EA\right)^2}{4\left(IP - EA\right)} \tag{S4}$$

$$\omega^+ = \frac{\left(IP + 3EA\right)^2}{16\left(IP - EA\right)} \tag{S5}$$

According to Marcus theory, the reorganization energy can usually be adopted to predict the molecular transport capacity. The organization energy consists of λ_h (the reorganization energy of the hole) and λ_e (the reorganization energy of the electron) [4, 5]:

$$\lambda_h = E_0^+ - E_+ + E_+^0 - E_0 \qquad (S6)$$

$$\lambda_e = E_0^- - E_- + E_-^0 - E_0 \qquad (S7)$$

Where E_0^+ (E_0^-) stands for the energy of cation (anion) under the neutral structure, E_- (E_+) means the energy after optimizing the structure of anion/cation, E_-^0 (E_+^0) is the neutral energy calculated based on the ion geometry structure, and E_0 represents the neutral structure energy.

S.1.2. D/A interface charge transfer performance

Based on Marcus theory, the values of charge reorganization rate K_{CR} and exciton separation rate K_{CS} can be obtained through electronic coupling (V_{DA}) and reorganization energy (λ), Gibbs free energy change (ΔG). The detailed calculation process of these parameters is as follows.

V_{DA} indicates the charge transfer integral, which may be evaluated by utilizing the recognized Mulliken-Hush model of two states [6-9]:

$$V_{DA} = \frac{\mu_{tr}\Delta E}{\sqrt{(\Delta\mu)^2 + 4(\mu_{tr})^2}} \qquad (S8)$$

where μ_{tr} is the transition dipole moment, which can be assessed by the electron dipole moment of the initial state and the complete ICT state [6]:

$$\mu_{tr} = \sqrt{x^2 + y^2 + z^2} \qquad (S9)$$

ΔE represents the ICT state's vertical excitation energy, and *Δμ* reflects the dipole moment difference, which is usually evaluated through the finite field difference method under the Hellmann-Feynman theorem [10]:

$$E_{ext}(F) = E_{ext}(0) - \Delta\mu F - \frac{1}{2}\Delta\alpha F^2 \qquad (S10)$$

here E is the excitation energy. The F and 0 donate the electrostatic field and zero-electric field respectively. The $\Delta\alpha$ is the change rate of polarizability.

The recombination energy of an interface includes both external recombination energy λ_o and internal recombination energy λ_i. Because λ_o is challenging to be calculated theoretically, a value of 0.3 eV is used here for the results of the recombination energy study in the experiment [11]. The expression for the λ_i of the interface is as follows [4, 12]:

$$\lambda_1 = E_0^+(D) - E_+(D) + E_-^0(A) - E_0(A) \tag{S11}$$

where $E_0^+(D)$ means the neutral structural energy of the donor molecule carrying a positive charge, $E_+(D)$ is the optimized donor cation structural energy, $E_-^0(A)$ refers to the energy of the anion structure of the acceptor without charge, and $E_0(A)$ is the neutral acceptor's energy.

The changes in free energy during charge recombination and exciton separation are denoted as ΔG_{CR} and ΔG_{CS}, respectively. The expression of ΔG_{CR} has been shown below [13]:

$$\Delta G_{CR} = E_{IP}(D) - E_{EA}(A) \tag{S12}$$

The equation of ΔG_{CS} is as follows [14]:

$$\Delta G_{CS} = -\Delta G_{CR} - E_{D1} + E_C \tag{S13}$$

where E_{D1} refers to the excitation energy of the donor molecular lowest singlet state, and E_C represents the Coulomb interaction energy of the ICT state.

Coulomb attraction energy (E_C) can be obtained by Multiwfn software [15, 16], which is based on the under-expression (atomic unit system) [17, 18]:

$$E_C = \iint \frac{\rho^{hole}(r_1)\rho^{ele}(r_2)}{|r_1 - r_2|} dr_1 r_2 \tag{S14}$$

Where ρ^{ele} and ρ^{hole} represent the electron and hole density of the transition orbitals, separately, and r_1 and r_2 are the charges' coordinates.

Section S.2. Supporting Tables

Table S1. Statistics of bond length (Å) and dihedral angle (°) of the investigated donor molecules.

Molecules	d_1 (Å)	d_2 (Å)	d_3 (Å)	θ_1 (°)	θ_2 (°)	θ_3 (°)
ZnChl-1	1.43	1.43	1.22	6.16	110.22	0.91
B-ZnChl-1	1.54	1.43	1.23	-23.68	89.36	14.16
C-ZnChl-1	1.53	1.44	1.23	-22.59	-89.60	12.99
D-ZnChl-1	1.50	1.43	1.23	10.28	94.04	0.55
T-ZnChl-1	1.58	1.44	1.23	-17.53	-83.60	13.69

Table S2. Molecular overall surface area, positive surface area, extreme value of ESP, total average ESP, molecular polarity index (MPI) and polar surface area of ZnChl-1, B-ZnChl-1, C-ZnChl-1, D-ZnChl-1 and T-ZnChl-1 (isosurface=0.001 a.u.).

Molecules	ZnChl-1	B-ZnChl-1	C-ZnChl-1	D-ZnChl-1	T-ZnChl-1
Overall surface area /Å^2	671.93	710.99	710.28	752.11	791.84
Positive surface area /Å^2	392.83	410.74	416.09	439.73	442.33
Minimal value /kcal mol^{-1}	-49.40	-48.07	-48.68	-50.01	-50.06
Maximal value /kcal mol^{-1}	52.21	51.42	55.69	53.15	50.04
Overall average value /kcal mol^{-1}	1.43	1.09	0.84	1.12	0.76
MPI /kcal mol^{-1}	13.16	11.66	11.99	12.63	10.08
Polar surface area (|ESP|>10 kcal/mol) /%	50.35	46.51	46.01	49.80	40.73

Table S3. The calculated excited state transition energy, oscillator strength f and main transition configuration of the ZnChl-1 molecule.

Molecules	State	Transition energy (eV/nm)	Strength f	Contribution MOs
ZnChl-1	S_1	2.029/611.22	0.3809	H→L/0.65199
	S_2	2.343/529.16	0.2059	H-1→L/0.62336
	S_3	3.247/381.82	1.2783	H→L+1/0.61650
	S_4	3.415/363.06	1.5148	H-1→L+1/0.62547
	S_5	3.682/336.78	0.0315	H-3→L/0.39306
	S_6	3.725/332.84	0.0098	H-3→L/0.53541
	S_7	3.789/327.19	0.0012	H-6→L/0.53788
	S_8	3.961/313.05	0.2284	H-5→L/0.45890
	S_9	4.094/302.85	0.0119	H-8→L/0.54861
	S_{10}	4.127/300.45	0.0648	H→L+2/0.48369

Table S4. The calculated excited state transition energy, oscillator strength f and main transition configuration of the B-ZnChl-1 molecule.

Molecules	State	Transition energy (eV/nm)	Strength f	Contribution MOs
B-ZnChl-1	S_1	2.042/607.21	0.3706	H→L/0.66401
	S_2	2.419/512.45	0.1116	H-1→L/ 0.61918
	S_3	3.295/376.26	1.3457	H→L+1/0.62130
	S_4	3.537/350.53	1.2506	H-1→L+1/0.62161
	S_5	3.655/339.27	0.0586	H-2→L/0.42650
	S_6	3.703/334.78	0.0228	H-2→L/0.49600
	S_7	3.733/332.16	0.0064	H-4→L/0.51503
	S_8	3.780/328.01	0.0071	H-7→L/0.54596
	S_9	4.040/306.90	0.0129	H-10→L/0.42933
	S_{10}	4.052/305.97	0.3004	H-6→L/0.60611

Table S5. The calculated excited state transition energy, oscillator strength f and main transition configuration of the C-ZnChl-1 molecule.

Molecules	State	Transition energy (eV/nm)	Strength f	Contribution MOs
	S_1	2.049/605.20	0.3519	H→L/0.66136
	S_2	2.398/517.04	0.0922	H-1→L/0.61695
	S_3	3.285/377.44	1.2884	H→L+1/0.61692
	S_4	3.515/352.72	1.2532	H-1→L+1/0.64054
C-ZnChl-1	S_5	3.698/335.25	0.0425	H-5→L/ 0.54115
	S_6	3.774/328.54	0.0153	H-4→L/0.58174
	S_7	3.796/326.66	0.0038	H-7→L/0.54145
	S_8	3.905/317.53	0.0059	H-2→L/0.61290
	S_9	3.999/310.15	0.0371	H-3→L/0.50643
	S_{10}	4.070/304.66	0.0665	H-10→L/0.42318

Table S6. The calculated excited state transition energy, oscillator strength f and main transition configuration of the D-ZnChl-1 molecule.

Molecules	State	Transition energy (eV/nm)	Strength f	Contribution MOs
D-ZnChl-1	S_1	2.052/604.23	0.3645	H→L/0.66052
	S_2	2.395/517.72	0.0920	H-1→L/0.61578
	S_3	3.288/377.09	1.3874	H→L+1/0.61571
	S_4	3.515/352.77	1.4051	H-1→L+1/0.63811
	S_5	3.727/332.70	0.0350	H-4→L/0.54649
	S_6	3.773/328.64	0.0029	H-6→L/0.50463
	S_7	3.781/327.90	0.0077	H-3→L/0.53904
	S_8	4.027/307.91	0.6017	H-5→L/0.33568
	S_9	4.074/304.35	0.0601	H-9→L/0.49946
	S_{10}	4.122/300.79	0.0662	H-5→L/0.50850

Table S7. The calculated excited state transition energy, oscillator strength f and main transition configuration of the T-ZnChl-1 molecule.

Molecules	State	Transition energy (eV/nm)	Strength f	Contribution MOs
T-ZnChl-1	S_1	2.040/607.66	0.3517	H→L/ 0.66072
	S_2	2.388/519.23	0.0965	H-1→L/0.59313
	S_3	3.267/379.47	1.2464	H→L+1/0.60767
	S_4	3.474/356.90	0.6677	H-2→L/0.47584
	S_5	3.530/351.29	0.5854	H-1→L+1/0.48692
	S_6	3.708/334.33	0.0359	H-4→L/0.55927
	S_7	3.771/328.80	0.0183	H-3→L/0.55134
	S_8	3.787/327.41	0.0012	H-7→L/0.46512
	S_9	4.038/307.04	0.0170	H-10→L/0.52731
	S_{10}	4.089/303.22	0.2482	H-5→L/0.58496

Table S8. The HOMO, LUMO levels and energy gaps (in eV) of the D/A complexes.

	HOMO (eV)	LUMO (eV)	Δ_{H-L} (eV)
ZnChl-1/Y6	-4.97	-3.42	1.55
B-ZnChl-1/Y6	-5.05	-3.40	1.65
C-ZnChl-1/Y6	-4.98	-3.40	1.58
D-ZnChl-1/Y6	-5.00	-3.38	1.62
T-ZnChl-1/Y6	-4.94	-3.41	1.53

Table S9. The calculated excited state transition energy, oscillator strength f and main transition configuration of the ZnChl-1/Y6 interface.

Molecules	State	Transition energy (eV/nm)	Strength f	Contribution MOs
ZnChl-1/Y6	S_1	2.022/613.05	0.3046	H→L+2/0.64459
	S_2	2.077/597.04	2.3195	H-2→L/0.62463
	S_3	2.335/530.93	0.0051	H→L/0.64090
	S_4	2.339/530.07	0.3181	H-1→L+2/0.60546
	S_5	2.535/489.09	0.3181	H-2→L+1/0.55639
	S_6	2.573/481.86	0.0031	H-1→L/0.57914
	S_7	2.771/447.36	0.0000	H-1→L+2/0.60546
	S_8	3.003/412.81	0.0000	H-1→L+1/0.67005
	S_9	3.085/401.94	0.0349	H-2→L+3/0.53011
	S_{10}	3.169/391.26	0.0546	H-2→L+4/0.49387

Table S10. The calculated excited state transition energy, oscillator strength f and main transition configuration of the B-ZnChl-1/Y6 interface.

Molecules	State	Transition energy (eV/nm)	Strength f	Contribution MOs
B-ZnChl-1/Y6	S_1	2.021/613.37	0.4437	H→L+2/0.52615
	S_2	2.067/599.71	2.2350	H-2→L/0.50101
	S_3	2.304/538.18	0.0004	H→L/0.68892
	S_4	2.424/511.59	0.1051	H-1→L+2/0.61199
	S_5	2.513/493.31	0.5481	H-2→L+1/0.55208
	S_6	2.674/463.66	0.0004	H-1→L/0.60440
	S_7	2.760/449.30	0.0007	H→L+1/0.60041
	S_8	3.045/407.15	0.0010	H-1→L+1/0.49997
	S_9	3.064/404.59	0.0256	H-2→L+3/0.53234
	S_{10}	3.143/394.51	0.0549	H-2→L+4/0.49342

Table S11. The calculated excited state transition energy, oscillator strength f and main transition configuration of the C-ZnChl-1/Y6 interface.

Molecules	State	Transition energy (eV/nm)	Strength f	Contribution MOs
C-ZnChl-1/Y6	S_1	2.036/609.04	0.3855	H→L+2/0.54448
	S_2	2.080/596.13	2.3181	H-2→L/0.52004
	S_3	2.280/543.72	0.0013	H→L/0.68385
	S_4	2.405/515.49	0.0835	H-1→L+2/0.61550
	S_5	2.517/492.68	0.5748	H-2→L+1/0.55632
	S_6	2.646/468.55	0.0006	H-1→L/0.64876
	S_7	2.725/454.93	0.0002	H→L+1/0.63424
	S_8	3.053/406.14	0.0007	H-1→L+1/0.68654
	S_9	3.079/402.77	0.0168	H-2→L+3/0.53227
	S_{10}	3.165/391.80	0.0436	H-2→L+4/0.48681

Table S12. The calculated excited state transition energy, oscillator strength f and main transition configuration of the D-ZnChl-1/Y6 interface.

Molecules	State	Transition energy (eV/nm)	Strength f	Contribution MOs
D-ZnChl-1/Y6	S_1	2.020/613.75	0.2356	H→L+2/0.554040
	S_2	2.085/594.68	2.5633	H-2→L/0.551503
	S_3	2.336/530.71	0.0001	H→L/0.67854
	S_4	2.392/518.39	0.0646	H-1→L+2/0.61800
	S_5	2.515/492.97	0.5010	H-2→L+1/0.55538
	S_6	2.682/462.29	0.0002	H-1→L/0.60430
	S_7	2.763/448.68	0.0000	H→L+1/0.58827
	S_8	3.065/404.53	0.0156	H-2→L+3/0.53519
	S_9	3.089/401.44	0.0002	H-1→L+1/0.68562
	S_{10}	3.157/392.69	0.0360	H-2→L+4/0.45003

Table S13. The calculated excited state transition energy, oscillator strength f and main transition configuration of the T-ZnChl-1/Y6 interface.

Molecules	State	Transition energy(eV/nm)	Strength f	Contribution MOs
T-ZnChl-1/Y6	S_1	2.033/609.88	0.1951	H→L+2/0.60936
	S_2	2.075/597.41	2.4504	H-2→L/0.57710
	S_3	2.190/566.11	0.0379	H→L+1/0.68628
	S_4	2.391/518.62	0.0909	H-2→L+2/0.58529
	S_5	2.515/493.07	0.3774	H-3→L+1/0.46419
	S_6	2.529/490.28	0.1531	H-1→L/0.54315
	S_7	2.614/474.24	0.0020	H→L+1/0.63981
	S_8	2.798/443.10	0.0007	H-3→L/0.58092
	S_9	2.993/414.29	0.0020	H-1→L+1/0.61962
	S_{10}	3.070/403.90	0.0278	H-2→L+3/0.53007

Table S14. The charge transfer distance (Δd), transfer charge value (Δq), t index, Sr index and excited state property of important excited states of ZnChl-1/Y6 interfaces.

Molecule	State	Δd (Å)	Δq (e)	t index (Å)	Sr index (a.u.)	Property
ZnChl-1/Y6	S_1	0.155	-0.001	-2.653	0.8680	FE_1
	S_2	0.652	0.001	-1.747	0.7464	FE_2
	S_3	5.099	0.954	2.733	0.2064	CT_1
	S_4	0.951	0.043	-1.989	0.8673	FE_3
	S_5	0.665	0.004	-1.559	0.7213	FE_4
	S_6	5.583	0.995	3.013	0.0794	CT_2
	S_7	5.445	0.999	2.759	0.0294	CT_3
	S_8	6.222	0.999	2.326	0.0320	CT_4
	S_9	1.503	-0.002	-1.110	0.6564	FE_5
	S_{10}	2.114	0.001	-0.138	0.6784	FE_6

Table S15. The charge transfer distance (Δd), transfer charge value (Δq), t index, Sr index and excited state property of important excited states of B-ZnChl-1/Y6 interfaces.

Molecule	State	Δd (Å)	Δq (e)	t index (Å)	Sr index (a.u.)	Property
	S_1	0.276	0.001	-2.391	0.8171	-
	S_2	0.423	0.001	-2.591	0.7889	-
	S_3	4.404	0.999	2.321	0.0561	CT_1
	S_4	0.699	-0.002	-2.041	0.8808	FE_1
B-ZnChl-1/Y6	S_5	0.666	0.001	-1.864	0.7253	FE_2
	S_6	4.395	0.998	3.001	0.0489	CT_2
	S_7	4.616	0.998	2.195	0.0405	CT_3
	S_8	5.110	0.989	2.169	0.1078	CT_4
	S_9	1.755	0.005	-1.715	0.6551	FE_3
	S_{10}	2.152	0.012	-0.453	0.6783	FE_4

Table S16. The charge transfer distance (Δd), transfer charge value (Δq), t index, Sr index and excited state property of important excited states of C-ZnChl-1/Y6 interfaces.

Molecule	State	Δd (Å)	Δq (e)	t index (Å)	Sr index (a.u.)	Property
C-ZnChl-1/Y6	S_1	0.286	-0.001	-2.405	0.8293	-
	S_2	0.462	-0.001	-1.931	0.7863	-
	S_3	5.011	0.998	2.996	0.0315	CT_1
	S_4	0.585	-0.001	-1.976	0.8964	FE_1
	S_5	0.704	0.001	-1.154	0.7206	FE_2
	S_6	4.732	0.999	3.571	0.0299	CT_2
	S_7	5.587	0.999	2.563	0.0291	CT_3
	S_8	4.719	0.998	3.053	0.0604	CT_4
	S_9	1.786	0.001	-2.196	0.6572	FE_3
	S_{10}	2.110	0.004	-0.458	0.6895	FE_4

Table S17. The charge transfer distance (Δd), transfer charge value (Δq), t index, Sr index and excited state property of important excited states of D-ZnChl-1/Y6 interfaces.

Molecule	State	Δd (Å)	Δq (e)	t index (Å)	Sr index (a.u.)	Property
D-ZnChl-1/Y6	S_1	0.287	-0.001	-2.342	0.8229	-
	S_2	0.518	-0.000	-3.487	0.7876	-
	S_3	5.011	0.998	2.996	0.0315	CT_1
	S_4	0.585	-0.001	-1.976	0.8964	FE_1
	S_5	0.704	0.001	-1.154	0.7206	FE_2
	S_6	4.732	0.999	3.571	0.0299	CT_2
	S_7	5.587	0.999	2.563	0.0291	CT_3
	S_8	4.719	0.998	3.053	0.0604	CT_4
	S_9	1.786	0.001	-2.196	0.6572	FE_3
	S_{10}	2.110	0.004	-0.458	0.6895	FE_4

Table S18. The charge transfer distance (Δd), transfer charge value (Δq), t index, Sr index and excited state property of important excited states of T-ZnChl-1/Y6 interfaces.

Molecule	State	Δd (Å)	Δq (e)	t index (Å)	Sr index (a.u.)	Property
	S_1	0.150	-0.001	-2.686	0.8522	-
	S_2	0.583	0.012	-1.642	0.7608	-
	S_3	3.978	0.988	2.395	0.1303	CT_1
	S_4	0.601	-0.003	-2.082	0.8921	FE_1
T-ZnChl-1/Y6	S_5	1.201	0.286	-0.979	0.6707	-
	S_6	3.111	0.727	1.300	0.4448	CT_2
	S_7	3.939	0.996	2.683	0.0814	CT_3
	S_8	6.403	0.998	3.796	0.0505	CT_4
	S_9	4.774	0.998	1.185	0.0622	CT_5
	S_{10}	1.612	0.001	-1.145	0.6587	FE_2

HOMO

LUMO
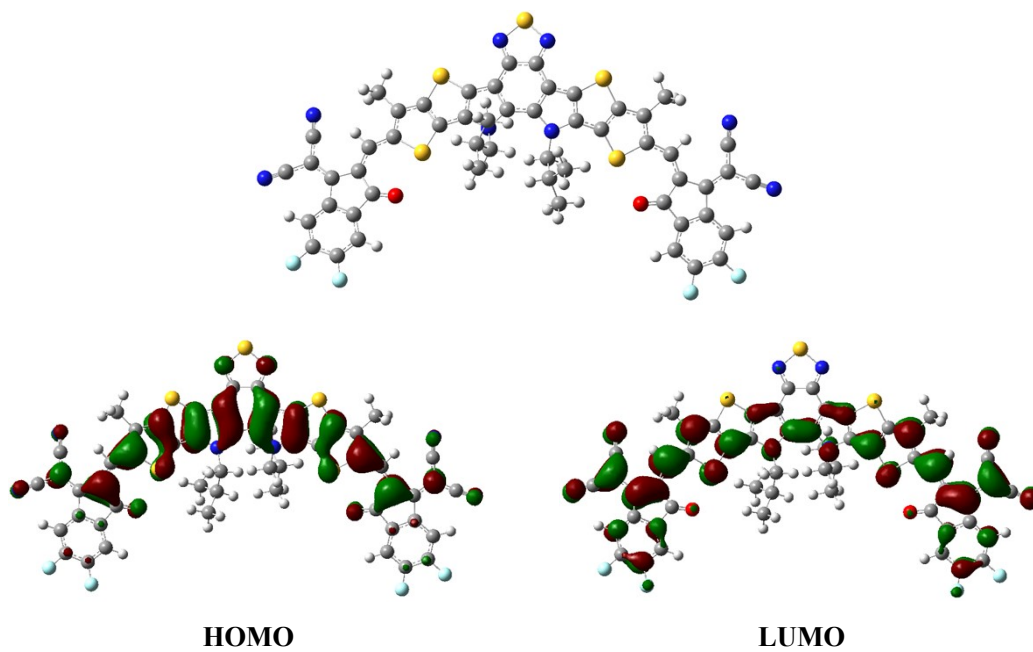
Figure S1. The optimized structure and frontier molecular orbitals (FMOs) of Y6 acceptor.
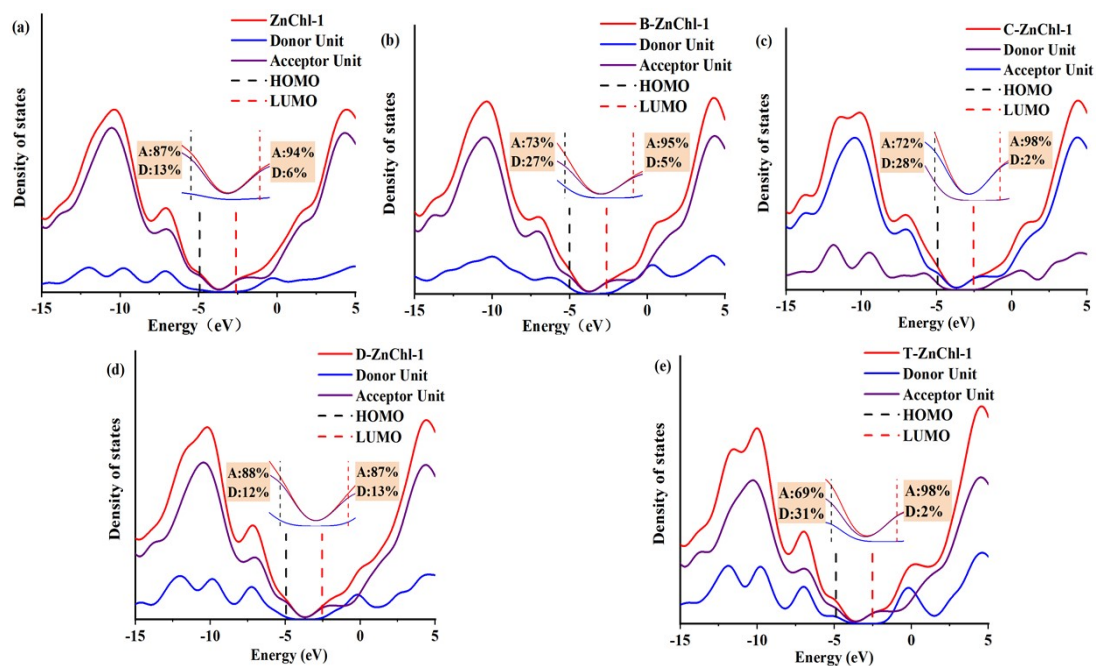
Figure S2. Density of states (DOS) of donor molecules ZnChl-1, B-ZnChl-1, C-ZnChl-1, D-ZnChl-1, T-ZnChl-1 (the percentage indicated is the contribution rate of donor unit (D) and acceptor unit (A) to HOMO and LUMO orbitals respectively).
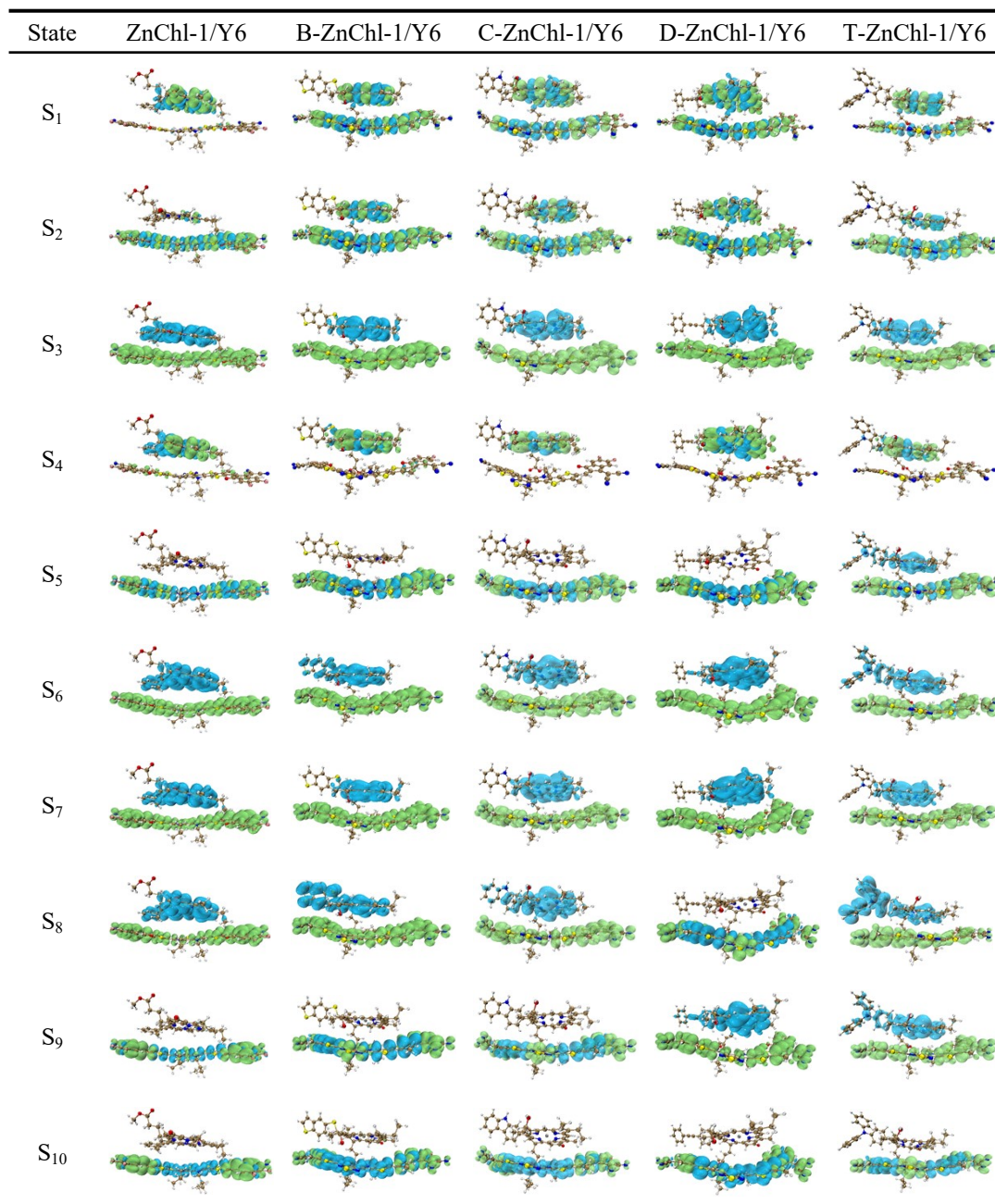
State	ZnChl-1/Y6	B-ZnChl-1/Y6	C-ZnChl-1/Y6	D-ZnChl-1/Y6	T-ZnChl-1/Y6

Figure S3. Charge differential density (CDD) of all D/A interfaces.

References of Supporting

[1]   Zhou B, Hu Z, Jiang Y, He X, Sun Z and Sun H. Benchmark study of ionization potentials and electron affinities of armchair single-walled carbon nanotubes using density functional theory. *Journal of Physics Condensed Matter* **2018**, 30, 215501.

[2]   Ompong D and Singh J. High Open-Circuit Voltage in Perovskite Solar Cells: The Role of Hole Transport Layer. *Organic Electronics*. **2018**, 63, 104-108.

[3]   Chattaraj PK, Sarkar U and Roy DR. Electrophilicity index. *Chemical Reviews*. **2006**, 106, 2065-2091.

[4]   Koese ME, Mitchell WJ, Kopidakis N, Chang CH, Shaheen SE, Kim K and Rumbles G. Theoretical studies on conjugated phenyl-cored thiophene dendrimers for photovoltaic applications. *Journal of the American Chemical Society*. **2007**, 129, 14257-14270.

[5]   Wang QG, Zeng ZY, Li YZ and Chen XR. Efficient strategies for improving the performance of EDOT derivatives and TPA derivatives-based hole transport materials for perovskite solar cells. *Solar energy*. **2020**, 208, 10-19.

[6]   Cave RJ and Newton MD. Generalization of the Mulliken-Hush treatment for the calculation of electron transfer matrix elements. *Chemical Physics Letters*. **1996**, 249, 15-19.

[7]   Liu XJ, Shao YY, Lu T, Chang DP, Li MJ and Lu WC. Accelerating the discovery of high-performance donor/acceptor pairs in photovoltaic materials via machine learning and density functional theory. *Materials & Design*. **2022**, 216, 110561.

[8]   Cossi M, Rega N, Scalmani G and Barone V. Energies, structures, and electronic properties of molecules in solution with the C-PCM solvation model. *Journal of Computational Chemistry*. **2003**, 6, 669-681.

[9]   Biswas S, Pramanik A, Pal S and Sarkar P. A theoretical perspective on the photovoltaic performance of S,N-heteroacenes: An even-odd effect on the charge separation dynamics. *Journal of Physical Chemistry C*. **2017**, 121, 2574-2587.

[10]   Zang ZF, Wang QG, Song P, Ma FC and Li YZ. Charge transfer processes via tandem modification of efficient non-fullerene acceptors for organic solar cells. *Solar Energy*. **2022**, 231, 503-515.

[11]   McMahon DP and Troisi A. Evaluation of the external reorganization energy of polyacenes. *Journal of Physical Chemistry Letters*. **2010**, 1, 941-946.

[12]   Kose ME and Schanze KS. Prediction of Internal reorganization energy in photoinduced electron transfer processes of molecular dyads. *Journal of Physical Chemistry A*. **2020**, 124, 9478-9486.

[13]   Zhao HF, Yin H, Liu XC, Li H, Shi Y, Liu CL, Jin MX, Gao JB, Luo Y and Ding DJ. Pressure-induced tunable electron transfer and auger recombination rates in CdSe/ZnS quantum dot-anthraquinone complexes. *Journal of Physical Chemistry Letters*. **2019**, 10, 3064-3070.

[14]   Shen FG, Peng AD, Chen Y, Dong Y, Jiang ZW, Wang YB, Fu HB and Yao JN. Photoinduced electron transfer in coaggregates of dicyanonaphthalene and pyrazoline. *Journal of Physical Chemistry A*. **2008**, 112, 2206-2210.

[15]   Lu T and Chen FW. Multiwfn: A multifunctional wavefunction analyzer. *Journal of*

Computational Chemistry. **2012**, 33, 580-592.

[16]   Lu T and Chen FW. Quantitative analysis of molecular surface based on improved Marching Tetrahedra algorithm. *Journal of Molecular Graphics & modelling.* **2012**, 38, 314-323.

[17]   Kraner S, Prampolini G and Cuniberti G. Exciton binding energy in molecular triads. *Journal of Physical Chemistry C.* **2017**, 121, 17088-17095.

[18]   Haroon M, Akhtar T, Khalid M, Mehmood H, Asghar MA, Baby R, Orfali R and Perveen S. Synthesis, characterization and exploration of photovoltaic behavior of hydrazide based scaffolds: a concise experimental and DFT study. *RSC Advances.* **2013**, 13, 7237-7249.