Electronic Supplementary Information for

Promising alkoxy-wrapped porphyrins with novel push–pull moieties for dye-sensitized solar cells

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Dedicated to Professor Xinquan Xin on the occasion of his 80th birthday

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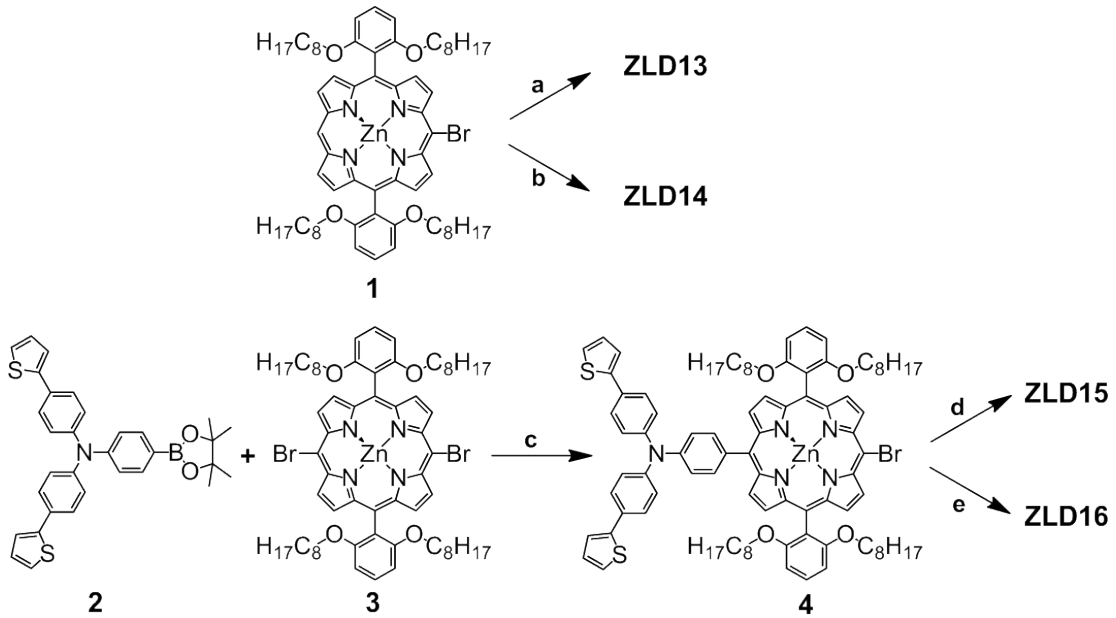
Experimental Section

Synthesis and characterizations of dyes

[5-Bromo-10,20-bis(2,6-di-octoxyphenyl)porphinato] zinc (II) (**1**), 4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-N,N-bis(4-(thiophen-2-yl)phenyl)aniline (**2**) and [5,15-dibromo-10,20-bis(2,6-di-octoxyphenyl)porphinato] zinc(II) (**3**) were synthesized according to references [S1-S3] respectively. Synthetic routes of ZLD13, ZLD14, ZLD15 and ZLD16 are depicted in Scheme S1.



Scheme S1: Synthetic Routes of Dyes ZLD13, ZLD14, ZLD15 and ZLD16 [1]

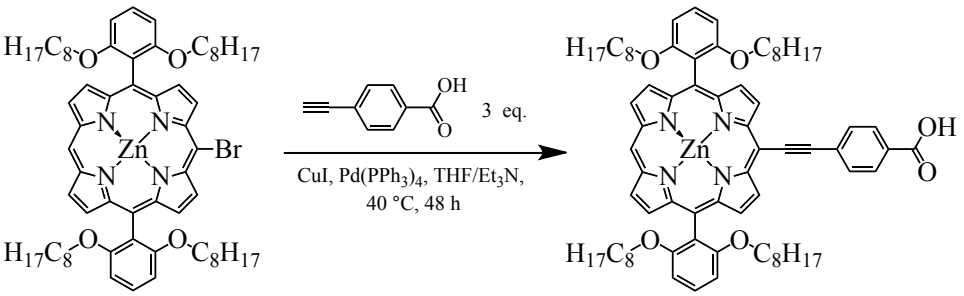
[1] Reagents and conditions: (a) 4-ethylnylbenzoic acid, CuI, $Pd(PPh_3)_4$, THF/Et_3N, 40 °C, 48 h; (b) 5-ethynylthiophene-2-carboxylic acid, CuI, $Pd(PPh_3)_4$, THF/Et_3N, 40 °C, 48 h; (c) K_2CO_3, $Pd(PPh_3)_4$, H_2O, THF, reflux, 18 h; (d) 4-ethylnylbenzoic acid, CuI, $Pd(PPh_3)_4$, THF/Et_3N, 40 °C, 48 h; (e) 5-ethynylthiophene-2-carboxylic acid, CuI, $Pd(PPh_3)_4$, THF/Et_3N, 40 °C, 48 h;

Materials: All reagents and chemicals were purchased from commercial suppliers. *N*, *N*-Dimethylformamide (DMF), 1,2-dichroloethane and Tetrahydrofuran (THF) were distilled with CaH_2, while acetonitrile was distilled with P_2O_5. Other chemicals and reagents were used as received without further purifications.

Characterizations: The molecular structures of TTC104, TTC105 and intermediates were confirmed by ^1H NMR, ^{13}C NMR, and mass spectra. The attenuated total reflection Fourier transform infrared

(ATR-FTIR) spectra were measured with a Thermo Scientific Nicolet iS10 FT-IR Spectrometer. The ^{1}H NMR and ^{13}C NMR spectra were recorded in solution of $CDCl_3$ or DMSO-d_6 on a Bruker DRX (500 MHz) NMR spectrometer with tetramethylsilane (TMS) as the internal standard. MALDI-TOF (matrix-assisted laser desorption ionization time-of-flight) analysis was performed on Bruker Daltonics Ultraflex MALDI TOF/TOF Mass Spectrometer, using α-Cyano-4-hydroxycinnamic acid as matrix. Electron spray mass spectrometry was measured in Thermo LCQ Fleet Electro-Spray Mass Spectrometer.

Synthesis of ZLD13:

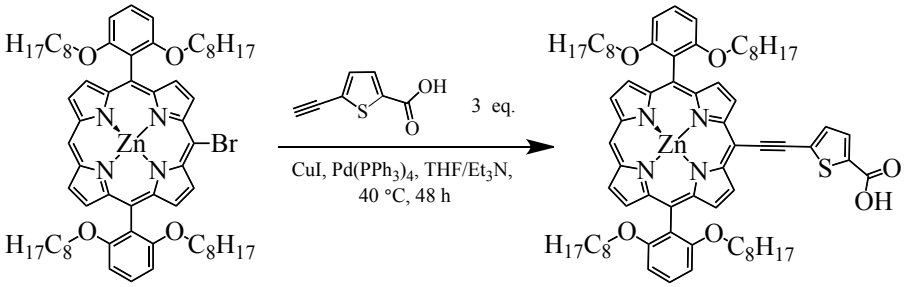


1 **ZLD13**

ZLD13 was prepared under modified conditions of a literature precedure. [S4]

Compound **1** (111.00 mg, 0.1 mmol), 4-ethynylbenzoic acid (43.80 mg, 0.30 mmol) in THF (30 mL) and triethylamine (5 mL) were degassed with a steady stream of N_2 for 15 min at room temperature. Then, $Pd(PPh_3)_4$ (11.56 mg, 0.01 mmol) and CuI (1.90 mg, 0.01 mmol) were added to the solution under an inert atmosphere. The reaction was stirred at 40 ^{o}C for 48 h. The progress of the reaction was monitored with TLC. The solvent was removed under diminished pressure. The residue was purified on a column chromatograph (silica gel) using CH_2Cl_2 / MeOH = 9/1 as eluent. The product was recrystallized from CH_2Cl_2 / MeOH to yield ZLD13 (65.00 mg, yield = 55 %). ^{1}H NMR (DMSO-d_6, 500 MHz): δ, [ppm]: 10.02 (s, 1H), 9.76 (d, J = 4.5 Hz, 2H), 9.22 (d, J = 4.5 Hz, 2H), 9.01 (d, J = 4.5 Hz, 2H), 8.97 (d, J = 4.5 Hz, 2H), 8.27 (d, J = 8.0 Hz, 2H), 8.07 (d, J = 8.0 Hz, 2H), 7.75 (t, J = 8.0 Hz, 2H), 7.65-7.80 (m, 3H), 7.06 (d, J = 8.0 Hz, 4H), 3.83 (t, J = 6.0 Hz, 8H), 0.80-1.00 (m, 16H), 0.66-0.78 (m, 8H), 0.55-0.65 (m, 20H), 0.30-0.45 (m, 8H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ, [ppm]: 168.62, 160.09, 151.66, 151.14, 150.32, 149.10, 132.44, 131.61, 131.46, 131.38, 131.02, 130.19, 130.09, 129.69, 129.43, 121.45, 113.91, 106.69, 105.35, 97.50, 97.22, 94.38, 68.60, 31.39, 28.71, 28.60, 25.16, 22.33, 13.89. MS (MALDI-Tof): Calcd for $C_{73}H_{88}N_4O_6Zn$, 1182.88; found, 1182.179.

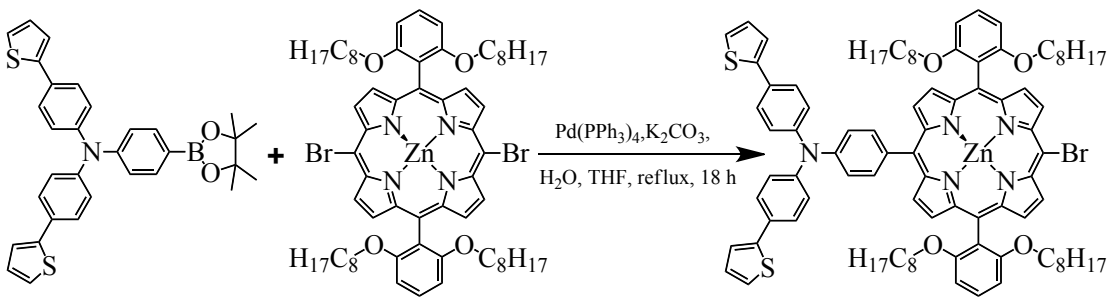
Synthesis of ZLD14:



1 **ZLD14**

Compound **1** (111.00 mg, 0.1 mmol), 5-ethynylthiophene-2-carboxylic acid (45.60 mg, 0.30 mmol) in THF (30 mL) and triethylamine (5 mL) were degassed with a steady stream of N_2 for 15 min at room temperature. Then, $Pd(PPh_3)_4$ (11.56 mg, 0.01 mmol) and CuI (1.90 mg, 0.01 mmol) were added to the solution under an inert atmosphere. The reaction was stirred at 40 °C for 48 h. The progress of the reaction was monitored with TLC. The solvent was removed under diminished pressure. The residue was purified on a column chromatograph (silica gel) using CH_2Cl_2 / MeOH = 9/1 as eluent. The product was recrystallized from CH_2Cl_2 / MeOH to yield ZLD14 (61.80 mg, yield = 52%). ^{1}H NMR (DMSO-d_6, 500 MHz): δ, [ppm]: 10.10 (s, 1H), 9.69 (d, J = 4.5 Hz, 2H), 9.27 (d, J = 4.5 Hz, 2H), 9.03 (d, J = 4.5 Hz, 2H), 8.98 (d, J = 4.5 Hz, 2H), 7.96 (s, 1H), 7.77 (s, 1H), 7.74 (d, J = 8.0 Hz, 4H), 7.60 (s, 1H), 7.05 (d, J = 8.0 Hz, 4H), 3.88 (t, J = 6.0 Hz, 8H), 0.96-1.10 (m, 8H), 0.75-0.85 (m, 8H), 0.56-0.65 (m, 8H), 0.45-0.56 (m, 28H), 0.35-0.45 (m, 8H). ^{13}C NMR (DMSO-d_6, 125 MHz): δ, [ppm]: 162.76, 159.99, 151.42, 151.27, 150.82, 149.20, 135.00, 134.83, 132.42, 131.72, 131.65, 131.46, 130.03, 129.88, 125.33, 121.75, 120.93, 114.41, 112.34, 107.13, 105.32, 68.68, 31.27, 28.62, 28.57, 25.20, 22.24, 13.77. MS (MALDI -Tof): Calcd for $C_{71}H_{86}N_4O_6SZn$, 1188.91; found, 1189.279.

Synthesis of compound 4:



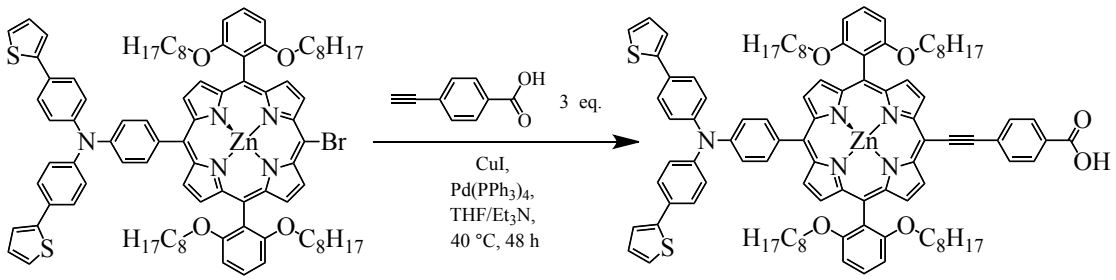
2 **3** **4**

Compound **4** was prepared under modified conditions of a literature precedure.[S5]

A mixture of compound **2** (0.536 g, 1.0 mmol), compound **3** (1.196 g, 1.0 mmol), $Pd(PPh_3)_4$ (0.058 g, 0.05 mmol), 0.5 mM K_2CO_3 (3.0 mL, 1.5 mmol) and THF (30 mL) were degassed with a steady stream of N_2 for 15 min at room temperature. The reaction mixture was then heated to reflux for

18 h under N_2. After cooling to room temperature, the reaction mixture was extracted by $CHCl_3$ (3×30 mL). The combined organic layers were washed with brine, dried over $MgSO_4$, and evaporated in vacuo. The residue was purified by silica gel column chromatography with CH_2Cl_2 : hexane (v : v, 1 : 10) as eluent to give the target compound **4** (0.747 g, 49%). ^{1}H NMR ($CDCl_3$, 500 MHz): δ, [ppm]: 9.71 (d, J = 3.5 Hz, 2H), 9.05 (d, J = 4.5 Hz, 2H), 8.97 (d, J = 4.5 Hz, 2H), 8.93 (d, J = 4.5 Hz, 2H), 8.15 (d, J = 8.0 Hz, 2H), 7.74 (t, J = 8.5 Hz, 2H), 7.67 (t, J = 8.5 Hz, 4H), 7.53 (d, J = 8.0 Hz, 2H), 7.45 (t, J = 8.5 Hz, 4H), 7.32 (d, J = 4.5 Hz, 2H), 7.27 (d, J = 4.5 Hz, 2H), 7.09 (d, J = 4.5 Hz, 2H), 7.05 (t, J = 8.5 Hz, 4H), 3.87 (t, J = 6.0 Hz, 8H), 0.90-1.05 (m, 8H), 0.75-0.85 (m, 8H), 0.57-0.65 (m, 8H), 0.45-0.56 (m, 28H), 0.35-0.45 (m, 8H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ, [ppm]: 160.05, 151.10, 150.93, 150.32, 149.25, 146.97, 146.40, 144.16, 137.94, 135.46, 132.39, 131.81, 131.57, 129.84, 129.31, 127.97, 127.03, 124.64, 124.58, 124.18, 122.40, 121.98, 121.22, 114.23, 105.26, 68.66, 31.32, 29.75, 28.61, 25.23, 22.22, 13.81. MS (MALDI-Tof): Calcd for $C_{90}H_{100}BrN_5O_4S_2Zn$, 1525.20; found, 1525.684.

Synthesis of ZLD15:

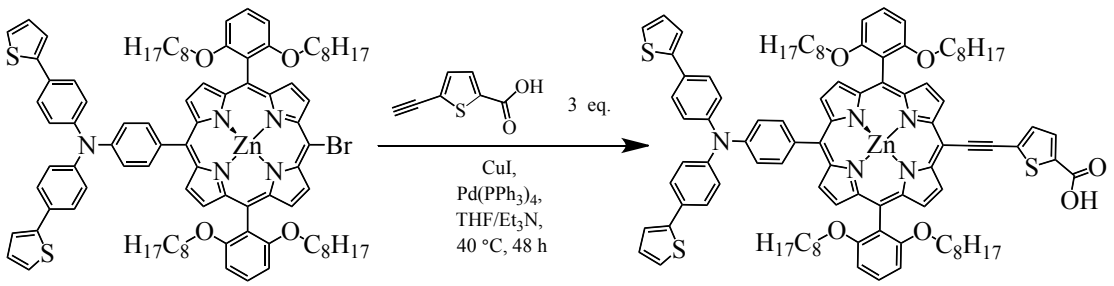


ZLD15 was prepared under modified conditions of a literature precedure. [S4]

Compound **4** (152.50 mg, 0.1 mmol), 4-ethynylbenzoic acid (43.80 mg, 0.30 mmol) in THF (30 mL) and triethylamine (5 mL) were degassed with a steady stream of N_2 for 15 min at room temperature. Then, $Pd(PPh_3)_4$ (11.56 mg, 0.01 mmol) and CuI (1.90 mg, 0.01 mmol) were added to the solution under an inert atmosphere. The reaction was stirred at 40 °C for 48 h. The progress of the reaction was monitored with TLC. The solvent was removed under diminished pressure. The residue was purified on a column chromatograph (silica gel) using CH_2Cl_2 / MeOH = 9/1 as eluent. The product was recrystallized from CH_2Cl_2 / MeOH to yield ZLD15 (77.90 mg, yield = 49 %). ^{1}H NMR ($CDCl_3$, 500 MHz): δ, [ppm]: 9.76 (d, J = 3.5 Hz, 2H), 9.03 (d, J = 6.0 Hz, 2H), 8.97 (d, J = 4.0 Hz, 2H), 8.92 (d, J = 4.0 Hz, 2H), 8.05-8.15 (m, 4H), 8.00 (t, J = 7.5 Hz, 2H), 7.78 (t, J = 8.5 Hz, 2H), 7.64 (d, J = 8.5 Hz, 4H), 7.52 (d, J = 8.0 Hz, 2H), 7.44 (s, J = 8.5 Hz, 4H), 7.24 (d, J = 3.5 Hz, 2H), 7.18 (d,

J = 5.0 Hz, 2H), 7.10 (d, J = 8.5 Hz, 4H), 6.99 (d, J = 4.5 Hz, 2H), 3.93 (t, J = 6.0 Hz, 8H), 1.00-1.10 (m, 8H), 0.80-0.79 (m, 8H), 0.61-0.70 (m, 8H), 0.43-0.61 (m, 36H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ, [ppm]: 170.87, 160.04, 152.12, 151.17, 150.37, 149.62, 146.95, 146.43, 144.14, 137.83, 135.46, 132.37, 132.28, 131.87, 131.71, 131.65, 131.10, 130.25, 129.87, 129.29, 127.94, 127.77, 127.01, 124.64, 124.15, 122.38, 121.94, 121.59, 121.17, 114.87, 105.31, 97.43, 94.48, 68.71, 31.34, 28.68, 28.63, 25.26, 22.24, 13.81. MS (MALDI-Tof): Calcd for $C_{99}H_{105}N_5O_6S_2Zn$, 1590.43; found, 1590.046.

Synthesis of ZLD16:



4 **ZLD16**

Compound **4** (152.50 mg, 0.1 mmol), 5-ethynylthiophene-2-carboxylic acid (45.60 mg, 0.30 mmol) in THF (30 mL) and triethylamine (5 mL) were degassed with a steady stream of N_2 for 15 min at room temperature. Then, $Pd(PPh_3)_4$ (11.56 mg, 0.01 mmol) and CuI (1.90 mg, 0.01 mmol) were added to the solution under an inert atmosphere. The reaction was stirred at 40 °C for 48 h. The progress of the reaction was monitored with TLC. The solvent was removed under diminished pressure. The residue was purified on a column chromatograph (silica gel) using CH_2Cl_2 / MeOH = 9/1 as eluent. The product was recrystallized from CH_2Cl_2 / MeOH to yield ZLD16 (79.80 mg, yield = 50%). ^{1}H NMR ($CDCl_3$, 500 MHz): δ, [ppm]: 9.68 (d, J = 3.5 Hz, 2H), 9.03 (d, J = 4.5 Hz, 2H), 8.98 (d, J = 4.5 Hz, 2H), 8.92 (d, J = 4.5 Hz, 2H), 8.13 (d, J = 8.0 Hz, 2H), 7.78 (t, J = 8.5 Hz, 2H), 7.62 (t, J = 8.5 Hz, 4H), 7.52-7.58 (m, 3H), 7.50 (s, 1H), 7.45 (t, J = 8.5 Hz, 4H), 7.19 (t, J = 2.5 Hz, 2H), 7.14 (t, J = 4.5 Hz, 2H), 7.09 (t, J = 8.5 Hz, 4H), 6.94 (t, J = 4.5 Hz, 2H), 3.94 (t, J = 6.0 Hz, 8H), 1.00-1.10 (m, 8H), 0.80-0.90 (m, 8H), 0.64-0.73 (m, 8H), 0.44-0.65 (m, 36H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ, [ppm]: 165.85, 160.01, 151.92, 151.24, 150.34, 149.64, 146.94, 146.48, 144.09, 137.80, 135.47, 134.99, 133.17, 132.52, 131.95, 131.72, 131.65, 131.32, 131.08, 130.10, 129.91, 129.28, 127.88, 127.00, 124.65, 124.12, 122.33, 121.90, 121.14, 114.96, 105.33, 101.10, 96.65, 87.72, 68.75, 31.36, 28.70, 28.65, 25.27, 22.27, 13.84. MS (MALDI-Tof): Calcd for $C_{97}H_{103}N_5O_6S_3Zn$, 1596.46; found, 1596.417.

Fabrication of DSSCs

The porphyrin-sensitized solar cells (PSSC) devices were fabricated with working electrodes based on TiO_2 nanoparticles (NP) and Pt-coated counter electrodes reported elsewhere.[S6] For the working electrode, a paste composed of 22-nm-sized TiO_2 nanoparticles prepared with a sol-gel method for the transparent nanocrystalline layer was coated on a $TiCl_4$-treated FTO glass substrate to obtain the required thickness on repetitive screen printing.[S7] Crystallization of TiO_2 films was performed with a programmed procedure: (1) heating at 80 °C for 15 min; (2) heating at 135 °C for 10 min; (3) heating at 325 °C for 30 min; (4) heating at 375 °C for 5 min; (5) heating at 450 °C for 15 min, and (6) heating at 500 °C for 15 min. The resulting layer had a transparent layer (thickness ~ 17 μm), which were treated again with $TiCl_4$ at 70 °C for 30 min and sintered at 500 °C for 30 min. The electrode was then immersed in a dye solution (0.2 mM) with EtOH/Toluene = 1/1 at 25 °C for 2 h for dye loading onto the TiO_2 film. The Pt counter electrodes were prepared on spin-coating drops of H_2PtCl_6 solution onto FTO glass and heating at 385 °C for 15 min. The dye-adsorbed TiO_2 electrodes and the Pt counter electrodes were assembled into a sealed sandwich-type cell by heating with a Surlyn film as a spacer between the electrodes. A drop of the electrolyte solution was placed in the drilled hole of the counter electrode and was driven into the cell via vacuum backfilling. Finally, the hole was sealed using additional Surlyn and a cover glass (0.1 mm thickness). The electrolyte introduced into the cell is composed of 0.6 M 1,3-dimethylimidazolium iodide (DMII), 50 mM LiI, 30 mM I_2, 0.5 M tert-butylpyridine and 0.1 M guanidinium thiocyanate (GuNCS) in a solvent mixture of 85% acetonitrile with 15% valeronitrile by volume.[S8] An Al foil was taped at the back side of each counter electrode to reflect unabsorbed light back to the photoanode.

Characterizations of DSSCs

A Xenon light source (Oriel) was used to give an irradiance of 100 mW cm^{-2} at the surface of a testing cell using a Keithley 2400 source meter. The measurement delay time was fixed to 40 ms with 100 measurement points scanning from V_{oc} to J_{sc}.[S8] For the setup used in our measurements, there was no hysteresis in the I-V curves when reversing the scan direction.

Incident photon-to-current conversion efficiency (IPCE) of the DSSCs was measured by a DC method. The light source was a 300 W Xenon Lamp (Oriel 6258) coupled with a flux controller to improve the stability of the irradiance. The light passed through a monochromator (Cornerstone 260 Oriel 74125) to select a single wavelength with a resolution of 10 nm. The monochromatic light beam was then focused on the active region of the device. Light intensity was measured by a NREL

traceable Si detector (Oriel 71030NS) and the short circuit currents of the DSSCs were measured by an optical power meter (Oriel 70310).

UV-Vis spectroscopy, Photoluminescence, Electrochemical properties and Measurement of dye adsorbed amounts

UV-vis absorption spectroscopy was studied by a Shimadzu UV-3600 spectrometer for liquid phase. Fluorescence spectra were measured by a Perkin Elmer LS55 spectrophotometer at room temperature for liquid phase. TiO_2 nanoparticle films (thickness: 12 μm) were immersed into 0.4 mM dye solutions in 3:2 mixture of chloroform and ethanol for 24 h, and UV-vis absorption spectra of dyes sensitized on TiO_2 were tested by a Shimadzu MPC-3100 spectrometer for solid phase at room temperature. Quasi-reversible oxidation and reduction waves were recorded using a Chenhua CHI660D model Electrochemical Workstation (Shanghai), while Electrochemical Impedance Spectroscopy were studied using a Chenhua CHI660I model Electrochemical Workstation (Shanghai).

To estimate the dye adsorbed amounts on the TiO_2 films, the sensitized 4×4 mm electrodes were separately immersed into a 0.1 M NaOH solution in a mixed solvent (DMF : H_2O = 4 : 1), which resulted in the desorption of each dye. The absorbance of the resulting solution was measured by a Shimadzu UV-3600 spectrometer.

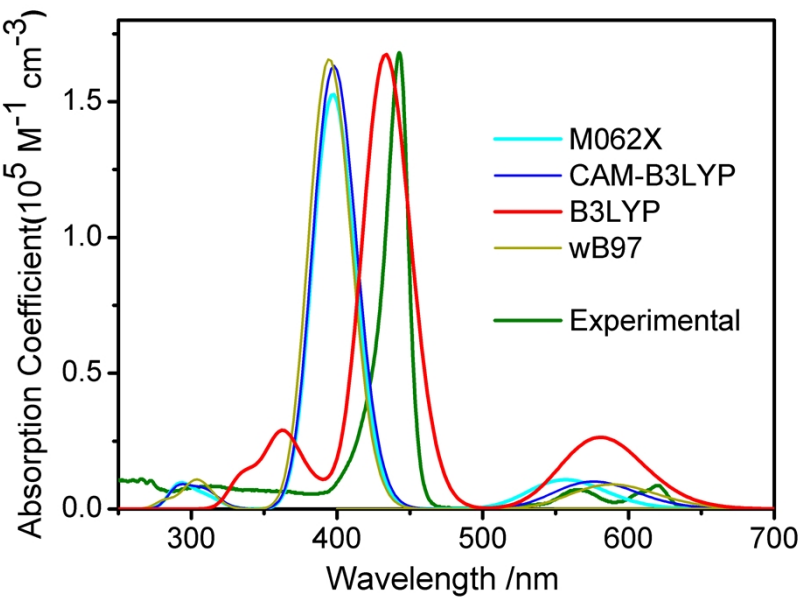
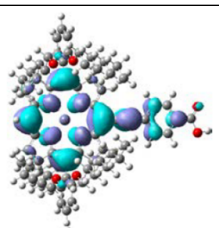
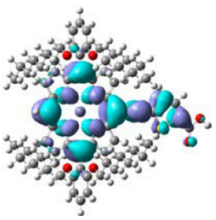
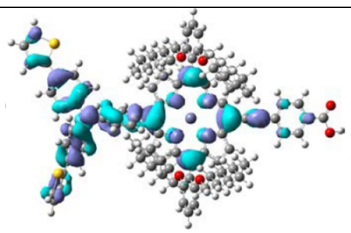
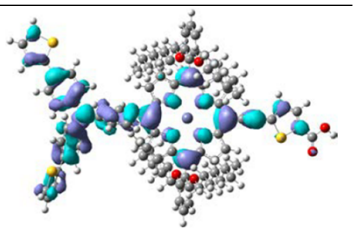
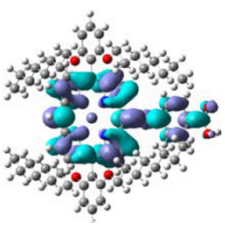
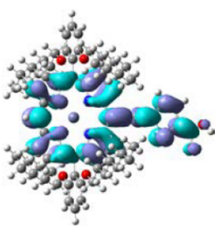
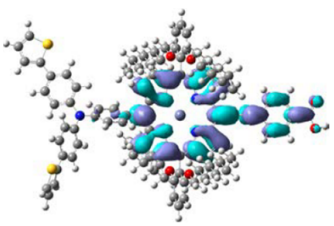
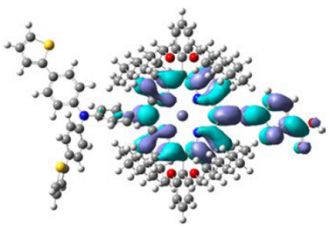


Fig. S1 UV-vis absorption spectra of ZLD13 via four mainstream theoretical calculation methods and experimental data tested in chloroform (1.0×10^{-6} M).

Theoretical calculations of dyes

All calculations were performed with the Gaussian 09 suite.1 Density functional theory (DFT) with B3LYP functional was used to perform geometry optimization of ZLD13~ZLD16 and ZLD13~ZLD16 absorbed on $[Ti_2O_2(OH)_2(H_2O)_4]^{2+}$. By time dependent DFT (TD-DFT) method, the UV-vis spectra were calculated, The basis set included the LANL2DZ basis for Zn and Ti, and 6-31G(d) basis for all other elements. Polarized continuum model (PCM) was adopted to consider solvent ($CHCl_3$) effect.

Table S1 Frontier molecular orbitals (LUMO, HOMO) of ZLD13~ZLD16 before absorbed on the $[Ti_2O_2(OH)_2(H_2O)_4]^{2+}$ model.[a]

Dye	ZLD13	ZLD14	ZLD15	ZLD16
HOMO				
LUMO				

[a] The calculations were carried out under vacuum using the 631-G(d) basis set and B3LYP functional

Table S2 HOMO and LUMO energy levels and band gaps of ZLD 13~ZLD16

Dye	ZLD13	ZLD14	ZLD15	ZLD16
E(HOMO) / eV	-4.76	-4.76	-4.69	-4.69
E(LUMO) / eV	-2.24	-2.31	-2.26	-2.33
Band gap (ΔE) / eV	2.52	2.45	2.43	2.36

Table S3 The exact results of Cyclic voltammograms of dyes.

Dye	$E_{0\text{-}0}{}^{a}$/eV	$E_{ox}{}^{b}$/V	$E_{red}{}^{b}$/V	$E_{ox}{}^{*c}$/V
ZLD13	1.938	1.100	-0.875	-0.838
ZLD14	1.911	1.125	-0.897	-0.786
ZLD15	1.897	1.113	-0.918	-0.780
ZLD16	1.877	1.142	-0.901	-0.735

[a]$E_{0\text{-}0}$ was estimated from the onset point of the absorption spectra; [b]0.08 M $TBAPF_6$ in DMF were used as supporting electrolytes. working electrode: glassy carbon; reference electrode: Ag/Ag^{+}; counter electrode: Pt; scan rate: 100 mV/s; [c]$E_{ox}{}^{*} = E_{ox} - E_{0\text{-}0}$.

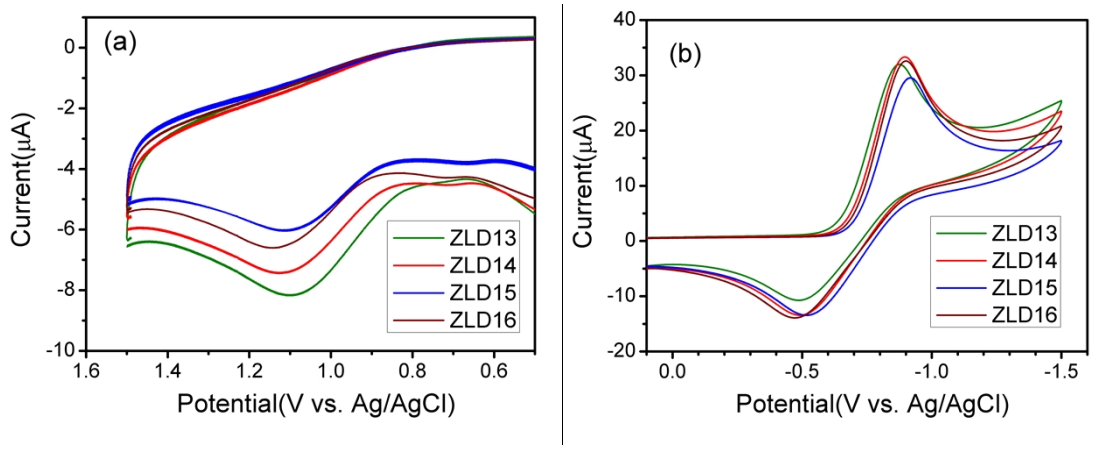


Fig. S2 Quasi-reversible oxidation (a) and reduction (b) waves for the dyes in the cyclic voltammetry (CV) measurements; 0.08 M $TBAPF_6$ in DMF were used as supporting electrolytes. A glassy carbon electrode was used as the working electrode; scan rate: 100 mV/s.

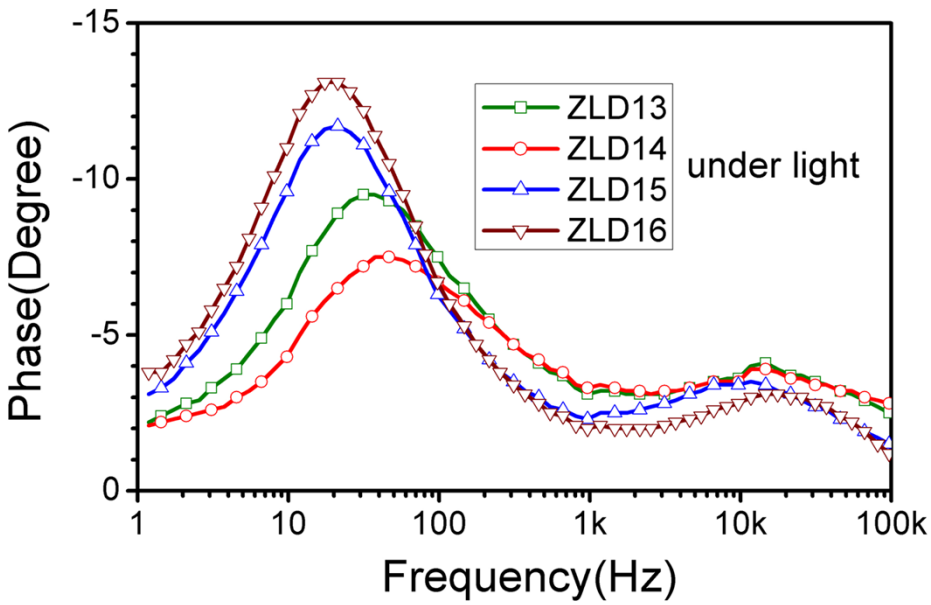


Fig. S3 Bode phase plots of Electrochemical impedance Spectroscopy (under AM 1.5G) of DSSCs based on ZLD13-ZLD16, scanned from 10^5 to 1 Hz. The applied potential and ac amplitude were set as -0.4 V and 10 mV, respectively.

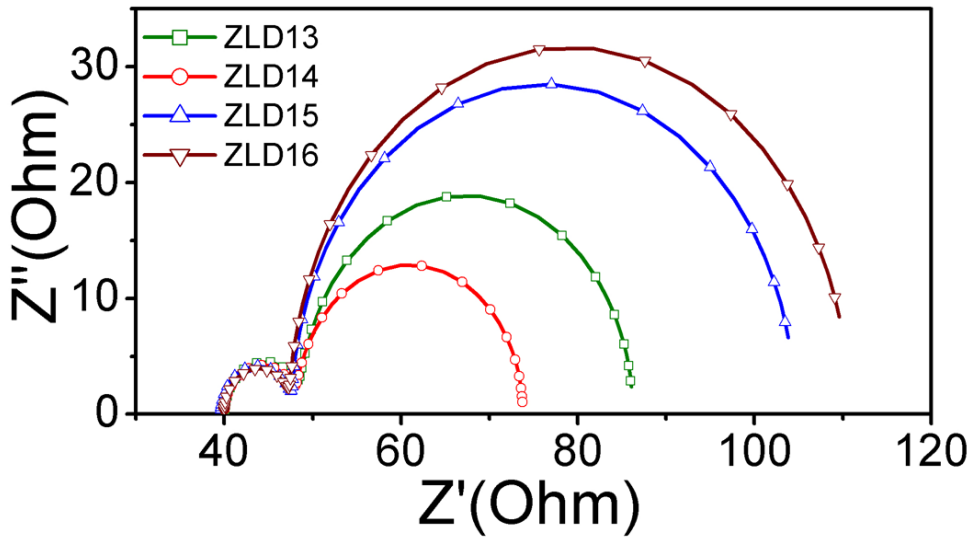


Fig. S4 Nyquist plots of Electrochemical impedance Spectroscopy (under dark) of DSSCs based on ZLD13-ZLD16, scanned from 10^5 to 1 Hz. The applied potential and ac amplitude were set as -0.4 V and 10 mV, respectively.

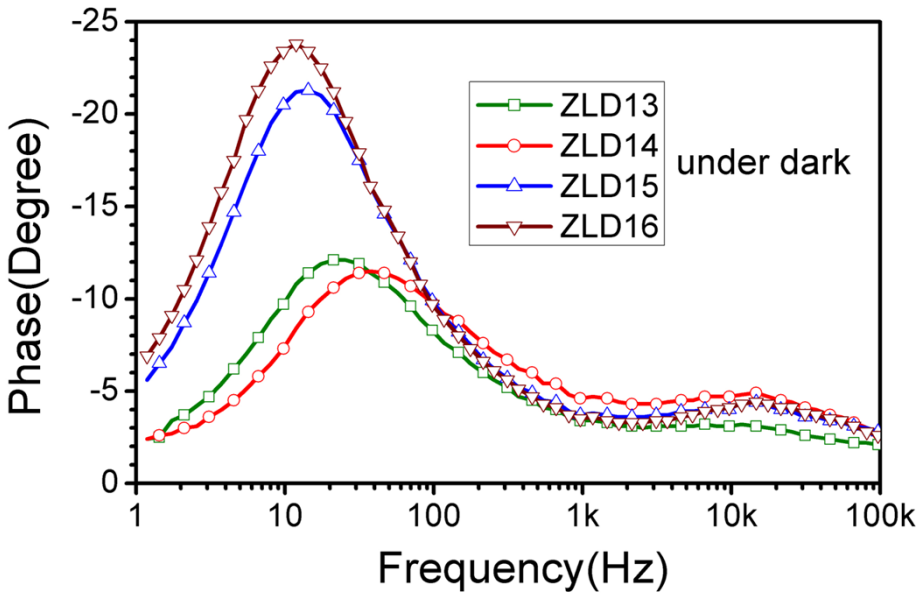
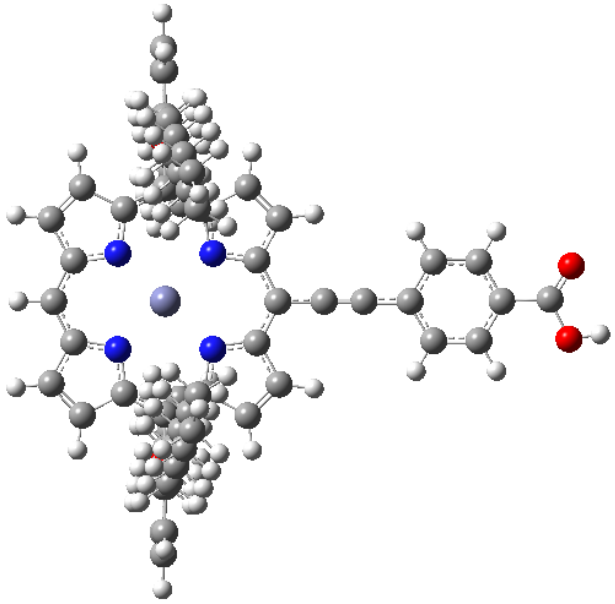


Fig. S5 Bode phase plots of Electrochemical impedance Spectroscopy (under dark) of DSSCs based on ZLD13-ZLD16, scanned from 10^5 to 1 Hz. The applied potential and ac amplitude were set as -0.4 V and 10 mV, respectively.

Coordinates for calculated geometries:

1. ZLD13



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N	0.02239600	-1.47174800	0.20732600
N	-0.15302900	-1.47674100	-2.70900700

C	-0.22610700	1.26046400	-4.06138000
C	-0.25862600	2.52978900	-4.75349800
C	-0.20327200	3.50421400	-3.79818200
C	-0.13703300	2.83647300	-2.51248100
C	-0.06725700	3.48232700	-1.25571400
C	0.00406800	2.83846300	-0.00548700
C	0.07095900	3.51342700	1.27462300
C	0.12935900	2.54848500	2.23696800
C	0.09772100	1.27234900	1.55522800
C	0.13569900	0.00207200	2.19872900
C	0.09737600	-1.26823000	1.55533000
C	0.12907000	-2.54433300	2.23711400
C	0.07082400	-3.50931000	1.27478200
C	0.00386600	-2.83438100	-0.00535300
C	-0.06740400	-3.47825800	-1.25557800
C	-0.13727100	-2.83243200	-2.51236400
C	-0.20372300	-3.50019800	-3.79804000
C	-0.25901700	-2.52579200	-4.75338000
C	-0.22626900	-1.25645100	-4.06130600
C	-0.26089700	0.00199200	-4.67606400
H	-0.31507300	2.65286800	-5.82797500
H	-0.20604800	4.57528500	-3.94507100
H	0.07225500	4.58541300	1.41455100
H	0.18700000	2.68126100	3.30837100
H	0.18674200	-2.67703000	3.30853300
H	0.07229700	-4.58129900	1.41471600
H	-0.20673500	-4.57127200	-3.94490400
H	-0.31559100	-2.64890000	-5.82784800
Zn	-0.06530500	0.00203700	-1.25330800
C	0.21707100	0.00228800	3.61769700
C	0.28751700	0.00280600	4.83563200
C	0.36941100	0.00525000	6.25335000
C	0.40401500	-1.20955100	6.97470900
C	0.41758100	1.22331500	6.96967800
C	0.48371100	-1.20528400	8.36122100
H	0.36755700	-2.15011100	6.43455200
C	0.49742600	1.21979700	8.35459900
H	0.39165100	2.16218200	6.42599100
C	0.53104500	0.00924300	9.06510400
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H	0.53479200	2.15330100	8.90597900
C	0.61624800	0.06497400	10.54485700
O	0.66205500	1.09342500	11.19976100
O	0.63886100	-1.15745500	11.12341100

H	0.69417600	-1.01231000	12.08721200
C	-0.07087400	4.98272600	-1.26232400
C	1.13943200	5.70281300	-1.29741100
C	-1.28602700	5.69542900	-1.24549100
C	1.13900000	7.10561900	-1.32373400
O	2.27234700	4.94304300	-1.30348500
C	-1.29564700	7.09809900	-1.27193800
O	-2.41302600	4.92830500	-1.20099000
C	-0.08071400	7.78107200	-1.31172600
H	2.06583600	7.66466200	-1.35651500
C	3.54863100	5.59522100	-1.29360000
H	-2.22658900	7.65121900	-1.26401500
C	-3.69264100	5.57098200	-1.13893800
H	-0.08452600	8.86747500	-1.33401400
C	4.61845500	4.51508700	-1.21117800
H	3.61181800	6.27156900	-0.43045800
H	3.66502700	6.19595700	-2.20611100
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H	-3.84932900	6.17401600	-2.04380000
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C	6.03838600	5.09704300	-1.19636400
H	4.44799400	3.92165300	-0.30330100
H	4.50130900	3.83366800	-2.06404700
C	-6.17248500	5.05020500	-0.93852400
H	-4.66339100	3.80851100	-1.88320700
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H	6.13343600	5.80885600	-0.36346000
C	-7.24187200	3.96027900	-0.78535600
H	-6.24033500	5.74586200	-0.08950400
H	-6.38310400	5.64326600	-1.84013700
H	6.95306900	3.44636400	-0.14299300
H	7.02492100	3.30297100	-1.89427100
C	8.54902800	4.58764000	-1.05336400
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H	-7.02656900	3.36805800	0.11613600
C	-8.67046100	4.51343200	-0.69847700
C	9.63257600	3.51190500	-0.90198500
H	8.64265800	5.31433400	-0.23257200
H	8.72367100	5.15151000	-1.98174900
C	-9.73685400	3.42311600	-0.53037400
H	-8.88905600	5.09934000	-1.60361600
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H	11.15328200	4.80533800	-0.07280400
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H	-11.23274800	4.67756800	0.39797500
H	-11.38852900	4.55316800	-1.34792300
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H	12.00362800	2.44083000	0.20680800
H	12.08773400	2.26727700	-1.55292500
H	-13.23409500	3.29648600	-0.21054300
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C	1.13970200	-5.69840800	-1.30076400
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C	1.13957000	-7.10121300	-1.32762800
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C	-0.07992800	-7.77699200	-1.31283400
H	-2.22570300	-7.64774200	-1.25984300
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C	3.54881000	-5.59028300	-1.31023600
H	-0.08349900	-8.86338800	-1.33548600
C	-4.74927100	-4.47906700	-1.01221600
H	-3.72560700	-6.24100500	-0.26492500
H	-3.84938000	-6.17092800	-2.03734900
C	4.61927200	-4.51028900	-1.23463900
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C	-6.17194100	-5.04850600	-0.93007400
H	-4.53465100	-3.87948600	-0.11785400
H	-4.66405100	-3.80570100	-1.87521800
C	6.03921300	-5.09241500	-1.23619100
H	4.49362100	-3.82601700	-2.08399900
H	4.45791500	-3.91991800	-0.32310300
C	-7.24178600	-3.95915600	-0.77605100

H	-6.38278100	-5.64144200	-1.83171700
H	-6.23896800	-5.74441100	-0.08119300
C	7.12594000	-4.01630400	-1.11024100
H	6.14203600	-5.80876700	-0.40810700
H	6.19933600	-5.66565700	-2.16071700
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H	-7.17362500	-3.26150300	-1.62370000
C	-8.67004500	-4.51307400	-0.68857900
H	7.01831900	-3.29358500	-1.93244100
H	6.96580900	-3.44920800	-0.18151500
C	8.55127800	-4.58444700	-1.11760800
C	-9.73692900	-3.42334400	-0.51981500
H	-8.73476000	-5.21746500	0.15412600
H	-8.88875500	-5.09895100	-1.59371000
C	9.63690800	-3.51035100	-0.96961500
H	8.71556000	-5.14103700	-2.05226300
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C	-11.16723800	-3.97204400	-0.43067800
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H	-9.67238800	-2.71774700	-1.36173700
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H	12.08552100	-2.26152700	-1.63839600
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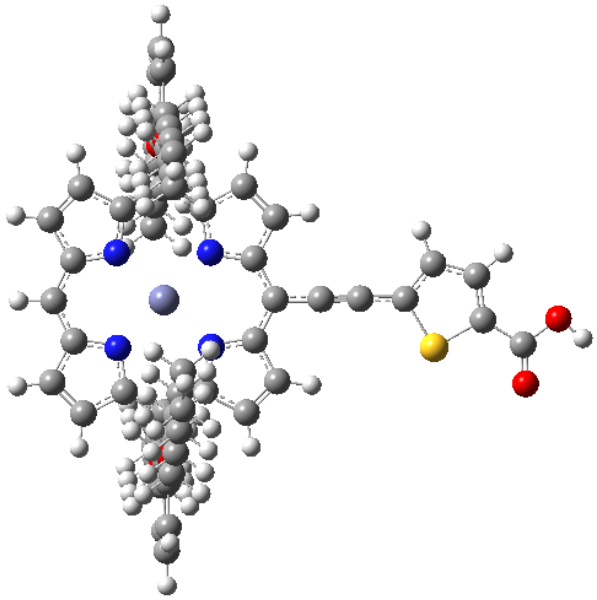
2. ZLD14



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C	-0.27930300	-0.57232500	-4.04118900
C	-0.30709100	-1.72192700	-4.91452900
C	-0.21706900	-2.82761800	-4.11967800
C	-0.13360000	-2.36123500	-2.75188600
C	-0.02702200	-3.18875200	-1.61329600
C	0.05817900	-2.73957700	-0.28471300
C	0.16824800	-3.59844400	0.87406800
C	0.22738700	-2.79126800	1.97033300
C	0.15329300	-1.42952300	1.49306300
C	0.17997200	-0.27485200	2.32246000
C	0.10558200	1.07428000	1.87919300
C	0.13023700	2.23043900	2.74476200
C	0.03708700	3.32815400	1.94231100
C	-0.04468700	2.85497200	0.57791000
C	-0.15076700	3.68002700	-0.55461300
C	-0.23396300	3.23047400	-1.88999000
C	-0.34169100	4.08344300	-3.05441100
C	-0.39733100	3.26571700	-4.14563300
C	-0.32394600	1.90838800	-3.65864700
C	-0.34798300	0.76085700	-4.45779000
H	-0.38458400	-1.68192200	-5.99405400
H	-0.20672200	-3.86506700	-4.42283900
H	0.19585700	-4.67841000	0.84517600
H	0.31248900	-3.08199200	3.00788800

H	0.20755600	2.19574700	3.82225000
H	0.02364600	4.36703300	2.24010400
H	-0.36992700	5.16367900	-3.03114400
H	-0.48009300	3.54963000	-5.18752600
Zn	-0.08717700	0.24510000	-1.08211500
C	0.29091800	-0.48978300	3.72013900
C	0.38669100	-0.67038100	4.92392700
C	-0.00515600	-4.67116900	-1.84240100
C	-1.20594900	-5.40397700	-1.90173000
C	1.21498600	-5.35562400	-1.99951500
C	-1.19183300	-6.79080800	-2.11306000
O	-2.34337600	-4.67132100	-1.73969700
C	1.23843700	-6.74216000	-2.21270700
O	2.33224600	-4.57878900	-1.92734200
C	0.03255200	-7.43837400	-2.26537800
H	-2.11338300	-7.35801300	-2.15706200
C	-3.60874100	-5.32826200	-1.77361500
H	2.17485400	-7.27226900	-2.33492200
C	3.61484900	-5.18953300	-2.05373200
H	0.04739200	-8.51274200	-2.42908600
C	-4.68231900	-4.26722900	-1.57012800
H	-3.65684500	-6.09015500	-0.98170800
H	-3.74181900	-5.83709100	-2.73981600
C	4.66467500	-4.09681900	-1.90084900
H	3.70184700	-5.67956800	-3.03486700
H	3.74014100	-5.96088700	-1.27966100
C	-6.10079300	-4.85187800	-1.58646400
H	-4.49418700	-3.75814500	-0.61626300
H	-4.57664400	-3.50925300	-2.35682400
C	6.09540400	-4.63646400	-2.02758500
H	4.48199100	-3.32671700	-2.66121900
H	4.52709100	-3.61394300	-0.92499500
C	-7.18874200	-3.78697800	-1.39261200
H	-6.27270800	-5.37551900	-2.53864800
H	-6.19469600	-5.61325500	-0.79800600
C	7.16531300	-3.54884100	-1.86208100
H	6.26004400	-5.42232000	-1.27546900
H	6.22048800	-5.12104000	-3.00733500
H	-7.01530700	-3.26150900	-0.44218800
H	-7.09421000	-3.02653000	-2.18157900
C	-8.61311800	-4.35729600	-1.40504500
H	6.99930300	-2.76041800	-2.61077700
H	7.04230300	-3.06695200	-0.88120600
C	8.59929100	-4.07909900	-1.99185300

C	-9.69930200	-3.28996100	-1.21750400
H	-8.70824500	-5.11526000	-0.61324000
H	-8.78452600	-4.88681700	-2.35418700
C	9.67096300	-2.99451800	-1.82095700
H	8.72179500	-4.55878300	-2.97448000
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C	-11.12557300	-3.85596800	-1.22768000
H	-9.52742300	-2.75892500	-0.26932100
H	-9.60482300	-2.53250600	-2.01002200
C	11.10551900	-3.52359600	-1.95096300
H	9.50857400	-2.20172300	-2.56654600
H	9.54951400	-2.51509600	-0.83811600
C	-12.20270800	-2.78156400	-1.04371700
H	-11.29690200	-4.38835400	-2.17423000
H	-11.22133400	-4.61024600	-0.43362000
C	12.16936800	-2.43415600	-1.77890200
H	11.26803600	-4.31501300	-1.20537400
H	11.22693100	-4.00250500	-2.93314100
H	-13.20881000	-3.21642200	-1.05410800
H	-12.07732700	-2.25437000	-0.08982700
H	-12.15522300	-2.03210600	-1.84349600
H	13.18162100	-2.84337400	-1.87553300
H	12.05513600	-1.64595400	-2.53345400
H	12.09439800	-1.95970800	-0.79258600
C	-0.17505500	5.16277400	-0.32765000
C	1.02463600	5.89674500	-0.25956300
C	-1.39690300	5.84688800	-0.18225000
C	1.00778200	7.28362800	-0.04819700
O	2.16408600	5.16547500	-0.41303900
C	-1.42313000	7.23354400	0.03007600
O	-2.51324600	5.06951200	-0.26329100
C	-0.21819700	7.93051100	0.09354800
H	1.92860300	7.85127700	0.00430700
C	3.42923300	5.81961700	-0.34036400
H	-2.36087400	7.76302300	0.14467800
C	-3.79640300	5.67718200	-0.12909400
H	-0.23509600	9.00479000	0.25776000
C	4.50647800	4.75948900	-0.52853800
H	3.53832500	6.31752400	0.63444200
H	3.49881400	6.59031600	-1.12224900
C	-4.84511300	4.58306100	-0.27959000
H	-3.92729400	6.45050800	-0.90044800
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C	5.92455700	5.34102200	-0.45775900

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H	4.34729800	4.26665300	-1.49619000
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H	-4.71130600	4.10234200	-1.25710100
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C	8.44069100	4.84691900	-0.56839400
H	-7.22641100	3.55336800	-1.29199500
H	-7.17585000	3.24213700	0.43648000
C	-8.77940100	4.56142600	-0.17192000
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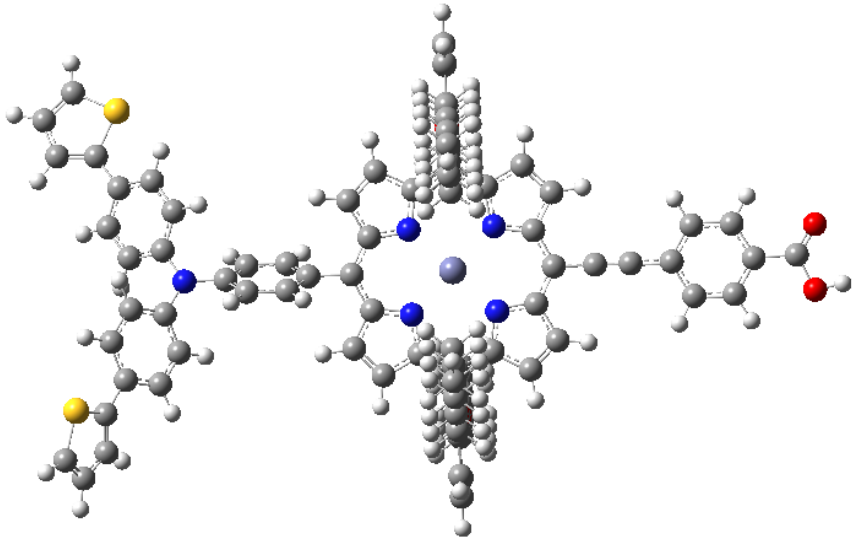
3. ZLD15



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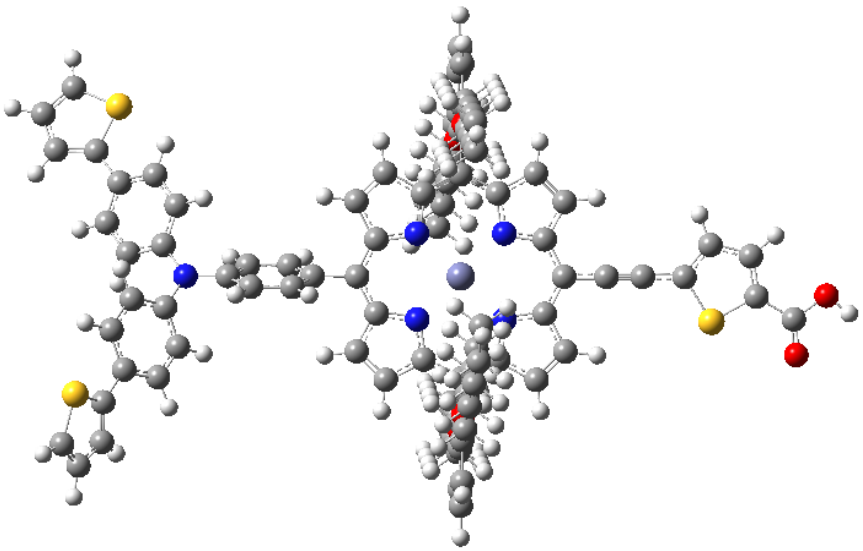
4. ZLD16



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C	-5.21800300	-1.24060500	-0.39221300
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H	-5.73639000	-2.17808400	-0.56672400
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C	-10.46802400	2.97104100	3.46093500
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S	-9.76319700	3.66642200	4.91050600
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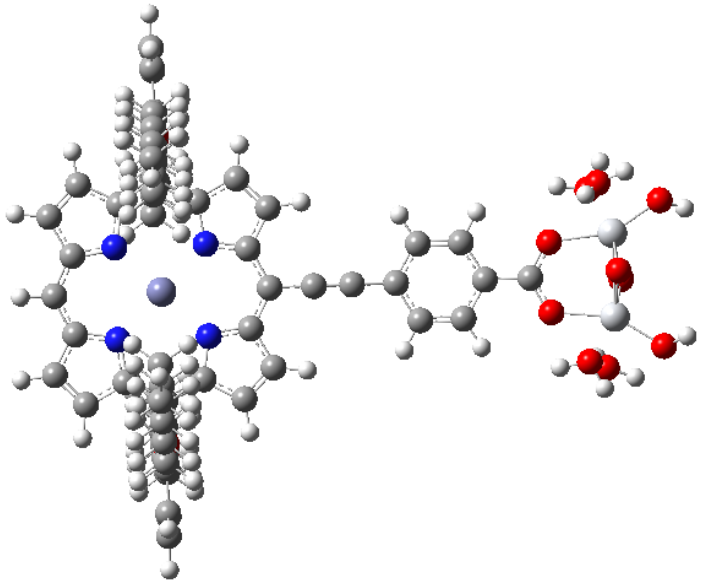
5. ZLD13-Ti



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O	11.00915600	0.03336900	-2.90110700
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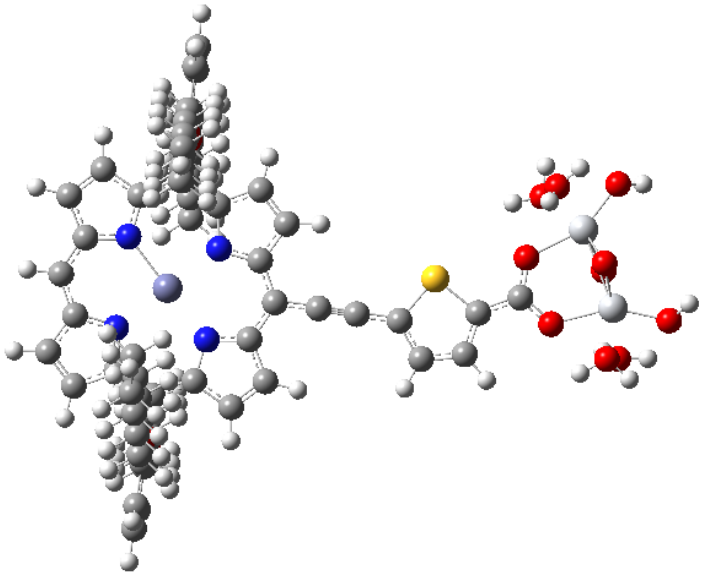
6. ZLD14-Ti



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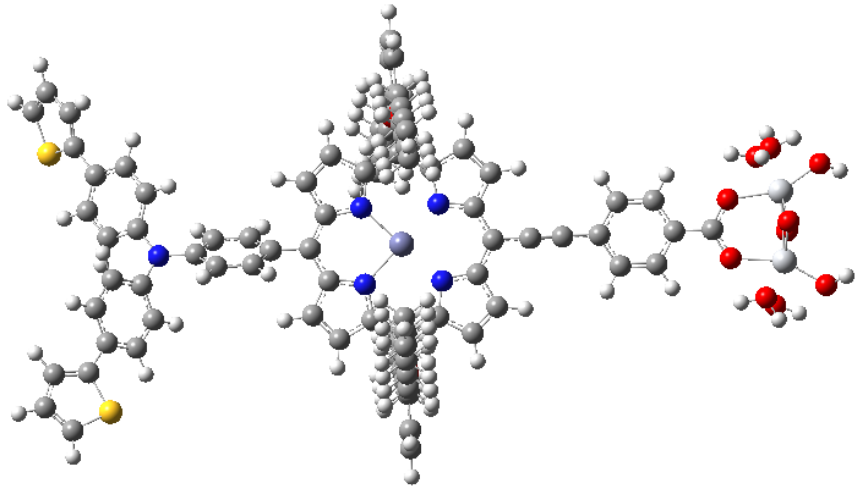
7. ZLD15-Ti



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H	0.90794500	3.36683200	4.85142400
H	-0.85276200	3.36052800	4.86587300
C	0.35293500	-8.03901100	2.06569700
H	1.24169800	-7.48067900	3.95562200
H	-0.51365100	-7.56784200	3.98916000
C	0.02802200	5.90331800	5.66312900
H	-0.83763700	4.53859100	7.09960300
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H	-0.55097900	-7.80105200	1.48580400
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C	0.43419600	-9.55582000	2.28207400
H	0.90242900	5.94115700	4.99715300
H	-0.85474200	5.93659900	5.00770100
C	0.03053600	7.13617900	6.57646400
C	0.44208300	-10.36378800	0.97776400
H	-0.41420500	-9.87913600	2.90368400
H	1.34014600	-9.79131400	2.86005100
C	0.02323600	8.46587200	5.81089800
H	0.91304000	7.10020600	7.23233300
H	-0.84404100	7.09634900	7.24292800
C	0.52338400	-11.88021300	1.19783600
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C	0.02537100	9.69877900	6.72443900
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H	-0.85900800	8.50287200	5.15419500
C	0.52758400	-12.68175000	-0.10816800
H	1.43013700	-12.11385400	1.77364200
H	-0.32321200	-12.20091300	1.82164900
C	0.01806300	11.02275700	5.95294500
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H	0.01983100	11.88218500	6.63297000
H	0.89916300	11.10900500	5.30512000
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C	5.81000700	-1.14453300	0.29596800
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H	5.26925400	2.13497100	-0.37783400
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C	11.16821700	-1.52937500	0.50311400
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C	10.37942400	-1.73719100	3.16264000
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C	10.05331000	0.87254600	-0.84910200
C	9.66491900	0.98629500	-2.19326400
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C	10.37559300	1.79985900	-3.06839600
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H	11.48234400	1.52836800	0.62675500
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H	10.06857900	1.84563800	-4.10977800
H	12.72832400	2.97539600	-0.92221300
C	12.27128700	3.37533700	-3.55961600
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S	11.53071400	4.10522400	-4.97376100
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C	13.67547600	-5.08547500	4.72978700
H	13.35850800	-4.26071100	6.70521900
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O	-12.31569100	-0.44167800	1.02146000
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O	-14.54111400	1.08175100	0.40873300
O	-14.52745700	-1.18258500	-0.49221700
O	-15.86696100	0.94500800	-2.18423800
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H	-16.64111600	1.36669000	-1.77780300
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H	-13.96919200	2.56588600	-3.06295800
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O	-13.98795800	0.44261200	3.14784700
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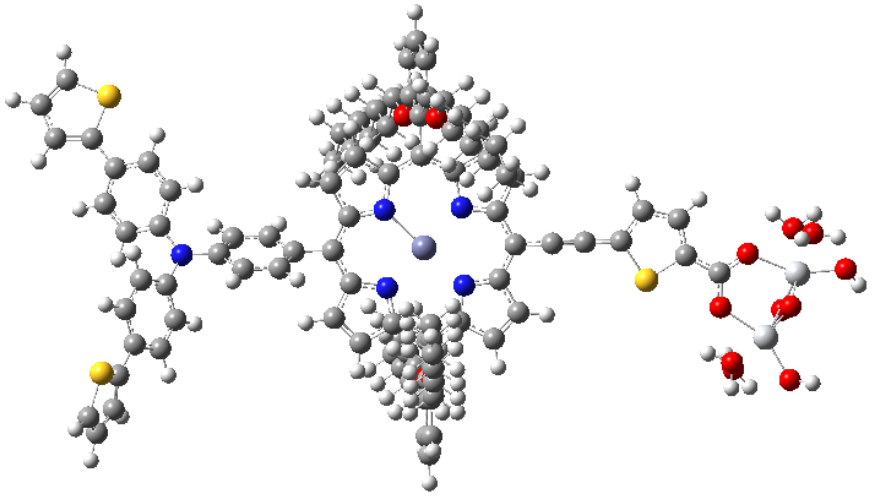
8. ZLD16-Ti



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C	2.90318900	-0.66892100	-2.78128700
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C	-3.45382100	0.02708300	-0.05234600
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C	0.39164200	-7.07898700	6.74811200
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Ti	13.14825300	-0.67886700	-1.87411400
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O	11.75728800	-2.20285500	-2.57208900
H	11.81820500	-2.40478900	-3.52088000
H	10.83993200	-1.94989700	-2.36388100
O	14.40804300	-1.00496000	2.35488800
H	13.89163400	-1.82728900	2.30160900
H	15.34722900	-1.26486100	2.35199300

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