SUPPORTING INFORMATION

The Effect of bulky electron-donating thioether substituents on the performances of Phthalocyanine based Dye Sensitized Solar Cells

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Experimental Section

All chemicals were purchased from Aldrich and used without further purification. All reactions were followed by TLC employing aluminium sheets coated with silica gel 60 F254 (Merck). Column chromatography was carried out on silica gel Merck-60 (230-400 mesh, 60 Å). ¹H-NMR spectra were obtained using a Bruker Avance 400 (400 MHz) spectrometer. UV/Vis spectra were recorded with a Analytic JENA S 600 UV-Vis spectrophotometer. The IR spectra were performed with Perkin-Elmer, FT-IR/MIR-FIR (ATR, Attenuated total reflectance) spectrophotometer. Mass spectrometry analysis was performed on an autoflex III MALDI TOF/TOF MS system (Bruker Daltonics, Bremen, Germany). Ditranol was used as matrix. DFT and TD-DFT calculations were performed using the Coulomb-attenuating B3LYP (CAM-B3LYP) and 6-31G* basis set as implemented in the Gaussian 16 software suit.

Fabrication of DSSCs: Double layered nanoporous TiO₂ electrodes were prepared by applying pastes of TiO₂ nanoparticles having two different diameters of 15-20 and 400 nm onto the transparent conducting glass substrates (SnO₂:F, on 1.8 mm thick glass substrate, Asahi Glass) with the screen printing technique, and the electrodes were sintered at 550 °C for 30 min in air. TiCl₄ treatment was applied to obtain high efficiency. The apparent surface area of the TiO₂ electrode was 0.25 cm² (0.5 x 0.5 cm). The attachment of ZnPc dyes to nanocrystalline TiO₂ films was achieved by immersion of the performed metal oxide electrodes in 0.05 mM toluene or THF solutions of the dyes for 48 hr at 25 °C. The dye-adsorbed TiO₂ electrodes were washed with toluene or THF to remove the physically adsorbed dye completely before measurements. The TiO₂ and Pt counter electrodes were separated by a 50 μ m thick hot melt ring (Surlyn, DuPont) and sealed by heating. Redox electrolytes (0.1 M LiI, 0.6 M 1,2-dimethyl-3-propylimidazolium iodide, 0.5 M 4-*tert*-butylpyridine, and 0.05 M I₂ in acetonitrile) were introduced into the space between the dye-adsorbed TiO₂ electrode and the counter electrode.

Measurements: A black mask (0.16 cm²) was applied on the cell to reduce diffusive light. Photovoltaic performance was under one sun condition (AM 1.5, 100 mW/cm²)

by a solar simulator (Otento-Sun 3SD, Bunko Keiki). Incident photon-to-current efficiency spectra were measured by a monochromator (SM-25A, Bunko Keiki). Electron lifetime was measured by a stepped laser intensity induced photo-voltage transient (S. Nakade, et. al, Langmuir, 21 (2005) 10803-10807). Electron density was measured by charge extraction method (W. Duffy et. al, Electrochemistry Communications, 2 (2000) 658-662). For these measurements, solar cells were prepared with different thickness TiO₂ electrode (around 4 μ m).

Transient absorption of oxidized dyes was measured by a pulsed laser (EKSPLA SL312, 150 ps, 532 nm, 1 Hz), and a probe laser (Coherent, OBIS, 980 nm). To avoid the hole hopping effect on the transient absorption, two polarizers were placed between the pulsed laser and a solar cell and different two polarizers were set between the probe laser and the solar cell. The probe intensity was measured by a nanosecond detector and a voltage amplifier (FEMTO, DHPVA-100), and monitored by a oscilloscope.

The redox potentials were measured by cyclic voltammetry using a Ag/Ag^+ reference electrode and a platinum counter electrode. Electrolyte was TBAP in AN. Ferrocene was used as reference redox material. Working electrodes were prepared by dropping dye solution on porous TiO₂ electrode and dried the solvent. The same preparation method was also applied on MK2 dye and the measured value was the same as the published one.

The adsorption density of ZnPc dye was determined by measuring the absorbance of ZnPc dye released from the TiO₂ electrode by immersing into THF containing tetrabutylammonium hydroxide methanoic solution. The absorbance at the Q band of released dye was converted into the concentration of dye in the TiO₂ electrode. The adsorption density of dye was calculated from the concentration in the TiO₂ electrode, the surface area of mesoporous TiO₂ (61 m²/g determined by BET surface area analyzer), and the weight of TiO₂ electrode on FTO substrate.

Synthesis of ZnPc-1-2



Scheme S1. Synthesis of ZnPc 1 and 2.

General procedure for the synthesis of ZnPc 11 and 12.

To a solution of 4-iodophthalonitrile (27 mg, 0.1 mmol) and corresponding phthalonitrile [4,5-bis(2',5'-diphenylthiophenoxy)phthalonitrile for ZnPc **11** and 4,5-bis(2',5'-diisopropyl thiophenoxy)phthalonitrile for ZnPc **12**] (0.5 mmol) in DMAE (4 mL) was added Zn(OAc)₂ (0.17 mmol, 32 mg). The mixture was heated to 140 °C for overnight. The solvent was evaporated in *vacuo* and the crude mixture was washed with the mixture of MeOH-H₂O (4:1). Purification by column chromatography (Toluene/hexane, 2:1) afforded the desired phthalocyanine in 33% yield.

Zinc (II) 2-iodo-9,10,16,17,23,24-hexakis(2',6'-diphenylthiophenoxy)phthalocyaninato(2-)-N²⁹, N³⁰, N³¹, N³² (ZnPc 11)

¹H NMR (400 MHz, CDCI₃): δ (ppm) 7.73-7.69 (m, ArH, 1H), 7.55-7.51 (m, ArH, 1H), 7.48 (s, ArH, 1H), 7.46 (s, ArH, 2H), 7.44 (s, ArH, 2H), 7.38 (s, ArH, 2H), 7.30 (s, ArH, 6H), 7.28 (s, ArH, 6H), 7.18-7.06 (m, ArH, 66H). IR (ATR): v (cm⁻¹) = 3053, 3025, 1596, 1569, 1494, 1453, 1402, 755, 695. UV/Vis (THF): λ max (log ϵ) = 717 (5.47), 645 (4.82), 347 (5.07).

Zinc (II) 2-iodo-9,10,16,17,23,24-hexakis(2',6'-diisopropythiophenoxy)phthalocyaninato(2-)-N²⁹, N³⁰, N³¹, N³² (ZnPc 12)

¹H NMR (400 MHz, CDCI₃): δ(ppm) 8.53-8.43 (m, ArH, 3H), 8.4-8.32 (m, ArH, 2H), 8.29-8.20 (m, ArH, 2H), 8.08-7.95 (m, ArH, 2H), 7.80-7.63 (m, ArH, 6H), 7.57-7.40 (m, ArH, 12H), 4.12-3.87 (m, 12H), 1.35- 1.21 (m, 72H). UV/Vis (THF): λ max (log ε) = 703 (5.32), 674 (4.46), 633 (4.52), 364 (4.70), 340 (4.70). IR (ATR): v (cm⁻¹) = 3054, 2958, 1592, 1575, 1484, 1459, 1398, 798, 743.

General procedure for the synthesis of ZnPc 9 and 10.

To a mixture of corresponding iodo-ZnPc (ZnPc **11** for ZnPc **9** and ZnPc **12** for ZnPc **10**) (0.02 mmol) in dry THF (6 mL), $PdCl_2(PPh_3)_2$ (0.9 µmol, 0.62 mg), CuI (0,0028 mmol, 0.53 mg) and Et₃N (0.4 mL) were added. The mixture was deoxygenated by bubbling argon and propargyl alcohol (0.044 mmol, 2.56 µL) was added and the mixture was stirred at 70 °C for 18 h. The solvent was then removed under reduced pressure, and the green solid was extracted with CHCl₃, washed with water and HCl 10%. The crude product was purified by column chromatography on silica gel (CHCl₃/Metanol, 10:0.1). ZnPc **9-10** was obtained in 90% yield as a green solid.

ZnPc 9:

2-(3'-Hydroxypropyn-1-yl)-9,10,16,17,23,24-hexakis(2',6'-diphenylthiophenoxy)phthalocyaninato(2-)-N²⁹, N³⁰, N³¹, N³² (ZnPc 9) ¹H NMR (400 MHz, CDCI₃): δ(ppm) 9.43-9.35 (m, Ar, 1H), 9.26-9.13 (m, Ar, 1H), 9.02-8.88 (m, Ar, 1H), 8.3-8.1 (m, Ar, 6H), 7.41-7.38 (m, Ar, 18H), 7.13-7.00 (m, Ar, 60H), 4.6-4.5 (m, CH₂, 2H). IR (ATR): v (cm⁻¹) = 3055, 3027, 1730, 1598, 1491, 1459, 756, 697.

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2-(3'-Hydroxypropyn-1-yl)-9,10,16,17,23,24-hexakis(2',6'-diisopropythiophenoxy)-
phthalocyaninato(2-)-N<sup>29</sup>, N<sup>30</sup>, N<sup>31</sup>, N<sup>32</sup> (ZnPc 10)
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¹H NMR (400 MHz, CDCI₃): δ (ppm) 8.94-8.86 (m, Ar, 1H), 8.52-8.54 (m, Ar, 2H), 8.49-8.37 (m, ArH, 6H), 7.78-7.64 (m, Ar, 6H), 7.56-7.45 (m, Ar, 12H), 4.13-3.90 (m, 14H), 1.43-1.19 (m, 72H). IR (ATR): v (cm⁻¹) = 3261, 3058, 2961, 1723, 1645, 1592, 1483, 1451, 1332, 801, 746.

General procedure for the synthesis of ZnPc 7 and 8.

To a solution of 1-hydroxy-1,2-benziodoxole-3(1H)-one-1-oxide (IBX) (0.1 mmol, 28 mg) in DMSO (3 mL), was added a solution of corresponding ZnPc (ZnPc **9** for ZnPc **7** or ZnPc **10** for ZnPc **8**) (0.05 mmol) in THF/DMSO 1:3 and the reaction mixture was stirred overnight at room temperature. The crude solution was poured into brine and extracted with Et₂O. The solvents were evaporated and the solid was purified by column chromatography on silica gel (CHCl₃/MeOH, 10:0.1) to give desired ZnPc **7** or **8** in 92% yield as a green solid.

2-Formylethynyl-9,10,16,17,23,24-hexakis(2',6'-diphenylthiophenoxy)-

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phthalocyaninato(2-)-N<sup>29</sup>, N<sup>30</sup>, N<sup>31</sup>, N<sup>32</sup> (ZnPc 7)
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¹H NMR (400 MHz, CDCI₃): δ(ppm) 9.74-9.63 (m, Ar, 1H), 9.60-9.48 (m, Ar, 1H), 9.35-9.20 (m, Ar, 2H), 8.22-8.13 (m, Ar, 6H), 7.30-7.28 (m, Ar, 18H), 7.15-7.06 (m, Ar, 60H). IR (ATR): v (cm⁻¹) = 3380, 3052, 3020, 1722, 1594, 1492, 1453, 1438, 755, 695.

2-Formylethynyl-9,10,16,17,23,24-hexakis(2',6'-diisopropylthiophenoxy)-

phthalocyaninato(2-)-N²⁹, N³⁰, N³¹, N³² (ZnPc 8)

¹H NMR (400 MHz, CDCI₃): δ (ppm) 9.7-9.6 (m, ArH, 1H), 9.36-9.24 (m, ArH, 1H), 9.03 (d, J = 8 Hz, ArH, 1H), 8.56 (s, ArH, 2H), 8.41 (d, J = 8 Hz, ArH, 4H), 8.20 (d, J = 8 Hz, ArH, 1H), 7.74-7.68 (m, Ar, 6H), 7.55-7.46 (m, Ar, 12H), 4.09-3.96 (m, 12H), 1.35-1.26 (m, 72H). IR (ATR): v (cm⁻¹) = 3057, 2960, 2168, 1725, 1658, 1591, 1483, 1461, 1400, 1371, 801, 746.

General procedure for the synthesis of ZnPc 1 and 2.

To a solution of corresponding ZnPc derivative (ZnPc 7 or 8) (0.045) mmol in THF at 0 °C was added a solution of H_3NO_3S (0.11 mmol, 11 mg) in water (1 mL) followed by a solution of NaClO₂ (0.11 mmol, 10 mg) in water (1 mL). The reaction mixture was stirred for 2 h at room temperature. The mixture was extracted with THF (2×50 ml). The combined organic layers were washed with brine (20 ml), dried over Na₂SO₄ and evaporated in *vacuo*. The solid was purified by column chromatography on silica gel (CH₂Cl₂/MeOH, 10:1) to give desired ZnPc 1 or 2 in 70% yield as a green solid.

ZnPc 1

2-Carboxyethynyl-9,10,16,17,23,24-hexakis(2',6'-diphenylthiophenoxy)phthalocyaninato(2-)-N²⁹, N³⁰, N³¹, N³² (ZnPc 1)

¹H NMR (400 MHz, CDCl₃): δ(ppm) 9.70 (s, Ar, 1H), 9.50 (s, Ar, 1H), 9.24 (d, J = 7.7 Hz, Ar, 1H), 8.29 (d, J = 8.1 Hz, Ar, 1H), 8.19 (d, J = 7.4 Hz, Ar, 2H), 8.13 (s, Ar, 3H), 7.44-7.38 (m, Ar, 12H), 7.35-7.31 (m, Ar, 18H), 7.15- 7.08 (m, Ar, 48H). IR (ATR): ν (cm⁻¹) = 3051, 3026, 1715, 1583, 1491, 1453, 1438, 756, 695. UV/Vis (CHCl₃): λmax (log ε) = 715 (4.99), 643 (4.27), 356 (4.60). MS (MALDI, ditranol): m/z = 2208 [M⁺].



ZnPc-1_DIT



Figure S1: ¹H NMR (CDCl₃) and MALDI spectra of ZnPc-1.

2-Carboxyethynyl-9,10,16,17,23,24-hexakis(2',6'-diisopropylthiophenoxy)-

phthalocyaninato(2-)-N²⁹, N³⁰, N³¹, N³² (ZnPc 2)

¹H NMR (400 MHz, CDCI₃): δ (ppm) 9.14 (s, Ar, 1H), 8.98 (d, *J* = 8 Hz, Ar, 1H), 8.58 (s, Ar, 2H), 8.44 (s, Ar, 2H), 8.40 (d, *J* = 8 Hz, Ar, 2H), 8.18 (d, *J* = 8 Hz, Ar, 1H), 7.7-7.6 (m, Ar, 6H), 7.5-7.4 (m, Ar, 12H), 4.1-3.9 (m, 12H), 1.4-1.2 (m, 72H). UV/Vis (CHCl₃): λ max (log ε) = 711 (5.00), 639 (4.28), 345 (4.53). IR (ATR): v (cm-1) = 3383, 3054, 2959, 1725, 1653, 1591, 1516, 1451, 1398, 1368, 1018, 800, 747. MS (MALDI, ditranol): m/z= 1799 [M⁺].







Synthesis of Zn(II)Pc-3-4



General procedure for the synthesis of ZnPc 3 and 4.

To a solution of corresponding ZnPc **11** or **12** (0.03 mmol) in CHCl₃ (20 ml) was added $PdCl_2(PPh_3)_2$ (0.003 mmol, 2.1 mg) and a solution of KOH (40% in H₂O, 6 mL). The reaction mixture was stirred overnight at room temperature. The mixture was extracted

with CHCl₃, dried over Na₂SO₄ and the solvent evaporated in *vacuo*. The solid was purified by column chromatography on silica gel (CH₂Cl₂/MeOH, 10:0.2) to give final compound ZnPc **1 or 2** in 52% yield as a green solid.

2-Carboxy-9,10,16,17,23,24-hexakis(2',6'-diphenylthiophenoxy)-phthalocyaninato (2-) -N²⁹, N³⁰, N³¹, N³² (ZnPc 3)

¹HNMR (400 MHz, CDCI₃): δ(ppm) 10.1 (s, Ar, 1H), 9.3 (d, *J*= 8 Hz, Ar, 1H), 8.9-8.8 (m, Ar, 1H), 8.24 (d, *J*= 8 Hz, 2H, Ar), 8.16 (s, 4H, Ar), 7.4-7.3 (m, Ar, 18H), 7.3-7.27 (m, Ar, 12H), 7.1-6.9 (m, Ar, 48H). IR (ATR): v (cm-1) = 3055, 3024, 1703, 1597, 1494, 1453, 1436, 756, 696. UV/Vis (CHCl₃): λ max (log ε) = 713 (4.93), 641 (4.24), 351 (4.54). MS (MALDI, ditranol):m/z= 2184 [M⁺].

Figure S3: ¹H NMR (CDCl₃) and MALDI spectra of ZnPc-3.





2-Carboxy-9,10,16,17,23,24-hexakis(2',6'-diisopropylthiophenoxy)-

phthalocyaninato(2-)-N²⁹, N³⁰, N³¹, N³² (ZnPc 4)

¹H NMR (400 MHz, CDCI₃): δ (ppm) 9.8 (s, Ar, 1H), 9.06 (d, *J* = 8 Hz, Ar, 1H), 8.83 (d, *J* = 8 Hz, Ar, 1H), 8.63 (s, Ar, 1H), 8.58 (s, Ar, 1H), 8.4-8.38 (m, Ar, 3H), 8.3 (s, Ar, 1H), 7.8-7.69 (m, Ar, 6H), 7.64-7.4 (m, Ar, 12H), 4.2-3.9 (m, 12H), 1.4-1.2 (m, 72H). UV/Vis (CHCl₃): λ max (log ε) = 710 (5.11), 636 (4.40), 343 (4.66). IR (ATR): v (cm⁻¹) = 3055, 2958, 1706, 1575, 1484, 1457, 1397, 1052, 744, 721. MS (MALDI, ditranol): m/z= 1775 [M⁺].

Figure S4: ¹H NMR (CDCl₃) and MALDI spectra of ZnPc-4.



ZnPc-4_DHB



Synthesis of ZnPc 5 and 6.



General procedure for the synthesis of ZnPc 13 and 14.

A solution of corresponding ZnPc **11** or **12** (0.13 mmol), 4-formylphenylboronic acid (30 mg, 0.2 mmol), $[Pd(PPh_3)_4]$ (15.3 mg, 0.013 mmol) and a solution of Na₂CO₃ (105 mg, in H₂O (1 ml)) in dimethoxyethane (5 ml) was stirred at 95 °C overnight under argon atmosphere. The suspension was then cooled to room temperature and poured onto a 1M NH₄Cl solution. The mixture was extracted with ethyl acetate and the combined organic extracts were washed with brine, dried over MgSO₄ and evaporated in *vacuo*. The crude product was purified by column chromatography on silica gel (CH₂Cl₂ for ZnPc **13**, Hexane/EtOAc 9:1 for ZnPc **14**) to give desired ZnPc **13** or **14** in 84% yield.

2-formylphenyl-9,10,16,17,23,24-hexakis(2',6'-diphenylthiophenoxy)-

phthalocyaninato (2-) -N²⁹, N³⁰, N³¹, N³² (ZnPc 13)

¹H NMR (400 MHz, CDCI₃): δ (ppm) 10.17 (s, -OCH, 1H), 9.56 (s, Ar, 1H), 9.33 (d, *J* = 7.9 Hz, Ar, 1H), 8.44 (d, *J* = 7.9 Hz, Ar, 1H), 8.32 (d, *J* = 8.2 Hz, Ar, 2H), 8.22-8.14 (m, Ar, 8H), 7.42-7.33 (m, Ar, 18H), 7.28-7.26 (m, Ar, 12H), 7.07-6.92 (m, Ar, 48H). FT-IR (ATR): v (cm⁻¹) = 3050, 3022, 1659, 1598, 1493, 1485, 1450, 754, 694.

2-formylphenyl-9,10,16,17,23,24-hexakis(2',6'-diisopropylthiophenoxy)-

phthalocyaninato (2-) -N²⁹, N³⁰, N³¹, N³² (ZnPc 14)

¹H NMR (400 MHz, CDCI₃): δ (ppm) 10.15 (s, -OCH, 1H), 9.30 (s, Ar, 1H), 9.03 (d, J = 7.9 Hz, Ar, 1H), 8.54 (d, J = 7.9 Hz, Ar, 2H), 8.37-8.14 (m, Ar, 9H), 7.70-7.58 (m, Ar, 6H), 7.49-7.39 (m, Ar, 12H), 4.09-3.90 (m, 12H), 1.27 (dd, J = 14.5, 5.3 Hz, 72H). FT-IR (ATR): v (cm⁻¹) = 3055, 2958, 1704, 1602, 1484, 1460, 1399, 1258, 800, 747.

General procedure for the synthesis of ZnPc 5 and 6.

To a solution of corresponding Pc derivative (ZnPc **13** or **14**) (0,01 mmol) mmol in THF at 0 °C was added a solution of H₃NO₃S (0,25 mmol, 24 mg) in water (1 mL) followed by a solution of NaClO₂ (0,25 mmol, 23 mg) in water (1 mL). The reaction mixture was stirred for 2 h at room temperature. The mixture was extracted with THF (2×50 ml). The combined organic layers were washed with brine (20 ml), dried over Na₂SO₄ and evaporated in *vacuo*. The solid was purified by column chromatography on silica gel (CH₂Cl₂/MeOH, 100:1) to give desired ZnPc **5** or **6** (80%) as a green solid.

2-carboxyphenyl-9,10,16,17,23,24-hexakis(2',6'-diphenylthiophenoxy)-

phthalocyaninato (2-) -N²⁹, N³⁰, N³¹, N³² (ZnPc 5)

¹H NMR (400 MHz, CDCI₃): δ (ppm) 9.63 (s, Ar, 1H), 9.40 (d, *J*= 8 Hz, Ar, 1H), 8.51-8.45 (m, Ar, 3H), 8.29-8.25 (m, Ar, 4H), 8.20 (s, Ar, 4H), 7.40-7.34 (m, Ar, 18H), 7.31-7.28 (m, Ar, 12H), 7.09-6.93 (m, Ar, 48H). FT-IR (ATR): v (cm⁻¹) = 3052, 3022, 1723, 1667, 1595, 1488, 1453, 1437, 756, 695. UV/Vis (CHCl₃): λ max (log ε) = 716 (5.06), 643 (4.31), 355 (4.64). MS (MALDI, ditranol): m/z= 2260.14 [M⁺].



Figure S5: ¹H NMR (CDCl₃) and MALDI spectra of ZnPc-5.



2-carboxyphenyl-9,10,16,17,23,24-hexakis(2',6'-diisopropylthiophenoxy)-

phthalocyaninato (2-) -N²⁹, N³⁰, N³¹, N³² (ZnPc 6)

¹H NMR (400 MHz, CDCI₃): δ (ppm) 9.36 (s, Ar, 1H), 9.10 (d, J = 8.7 Hz, Ar, 1H), 8.63 (d, J = 18.4 Hz, Ar, 2H), 8.43-8.34 (m, Ar, 7H), 8.14 (d, J = 7.9 Hz, Ar, 2H), 7.77-7.67 (m, Ar, 6H), 7.56-7.46 (m, Ar, 12H), 4.17-3.96 (m, 12H), 1.29 (m, 72H). FT-IR (ATR): v (cm⁻¹) = 3054, 2958, 1724, 1591, 1483, 1459, 1398, 1351, 799, 746. UV/Vis (CHCl₃): λ max (log ε) = 711 (5.09), 638 (4.48), 342 (4.73). MS (MALDI, ditranol): m/z= 1851.48. [M⁺].

Figure S6: ¹H NMR (CDCl₃) and MALDI spectra of ZnPc-6





Fig. S7 Photos of TiO_2 electrode stained with ZnPc4 (left) and PcS18 (right).



Fig. S9 Absorption and fluorescence spectra of ZnPc4 (a) and PcS18 (b) in toluene.



Fig. S10 Absorption spectra of ZnPc4 (solid line) and PcS18 (dashed line) adsorbed onto TiO_2 thin film deposited on FTO electrodes.



Fig. S11 Cyclic voltammograms of ZnPc4 (a) and PcS18 (b) adsorbed onto TiO₂ electrode and filled in the pore of TiO₂ electrode in 0.1 M TBAClO₄ in acetonitrile. Working electrode: TiO₂ porous electrode on FTO; counter electrode: Pt wire; reference electrode: Ag/AgNO₃. $E_{1/2}$ of ferrocene was observed at 0.078 V vs. Ag/Ag⁺ under the same measurement condition.

Energy / eV (nm)	f	Configuration (Main percentage contribution)
ZnPc4		
1.92 (645.53)	0.5274	H→L (92%)
1.97 (629.79)	0.6370	H→L+1 (91%)
3.50 (354.64)	0.2955	H-1→L (55%), H-2→L (17%)
PcS18		
1.99 (622.67)	0.5331	H→L (93%)
2.04 (608.69)	0.6005	H→L+1 (92%)
3.68 (337.03)	0.6256	H-1→L (67%), H-2→L (10%)

Table S1. Calculated Transition Energies, Oscillator Strength f, and Configuration of ZnPc4 \Box and PcS18