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New anthracene derivatives integrating high mobility and strong emission

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Experimental Section

General methods

All reagents and chemicals were obtained from commer-cial sources and used without further purification. 1HNMR spectra were taken in CDCl3 with TMS (δ 0.00 ppm) as internal standard at room temperature and were recorded on Bruker 400 NMR spectrometer. UV-Vis spec-tra were obtained on SHIMADZU UV-3600 UV-Vis-NIR spectrophotometer. Photoluminescence (PL) spectra were recorded on a HITACHI F-7000 spectrofluorometer. Thermal gravimetric analysis (TGA) was carried out on a METTLER TOLEDO TGA2 apparatus with a scanning rate of 10 °C /min. Differential scanning calorimetry was performed on Diamond DSC apparatus under a dry ni-trogen flow at a rate of 10 °C/min. Absolute quantum yield measurement (LabSphereR, FluoroMax-4, HORIBA JobinYvon, PLQY software package) was used for pow-der sample. In this experimental setup, it is possible to measure the Photoluminescence Quantum Yields (PLQY) via using the integrating sphere in combination with a commercial fluorimeter. Emission spectra including the scattering region of excitation light were recorded for both blank and test samples, and these spectra were corrected with instrumental factors to calculate the quantum yield. Cyclic voltammetirc (CV) measurements were conducted using a CHI660C electrochemistry station with tetrabut-lyammonium hexafluorophosphate (Bu4NPF6) as elec-trolyte (0.001 M in dry CH2Cl2). The working, counter and reference electrodes were Glassy carbon, Pt wire and Ag/AgCl, respectively. OFET characteristics were recorded by a Keithley 4200 SCS and Micromanipulator 6150 probe station.

Synthesis of Compound **Ant-Th-Ph**[1]

Anthracen-2-ylboronic acid (1.00 g, 4.5 mmol), 2-bromo-5-phenylthiophene (1.29 g, 5.4 mmol), Na_2CO_3 (3.17 g, 2.0 M) and $Pd(PPh_3)_4$ (0.21 g, 0.18 mmol) was added to a 100 mL flask two-neck bottle under N_2. 30 ml of toluene and 15 mL H_2O were added and then heated to 90 ºC and stirred for 24 hours. The system was then filtered, washed successively with triethylamine, dichloromethane, water, and ethanol and purified by sublimation. Ant-Th-Ph was obtained as a yellow solid, with a yield of 72.6% (1.1 g). ^{1}HNMR (400 MHz, $CDCl_3$): δ [ppm] 8.5 (s, 1H), 8.47

(s, 1H), 8.31 (s, 1H), 8.10 (d, 1H), 8.06 (t, 2H), 7.84 (d, 1H), 7.74 (d, 2H), 7.56 (d, 1H), 7.53 (t, 2H), 7.46 (m, 3H), 7.36 (t, 1H). MS (EI) m/z: 336 [M+]; Anal. calculated for $C_{24}H_{16}$ S (%): C: 85.68, H: 4.79. Experimental: C: 85.58%, H: 4.64%.

Compound **Ant-ThPh**[1]

Anthracen-2-ylboronic acid (1.00 g, 4.5 mmol), 2-bromobenzo[b]thiophene (1.15 g, 5.4 mmol), Na_2CO_3 (3.17 g, 2.0 M) and $Pd(PPh_3)_4$ (0.21 g, 0.18 mmol) was added to a 100 mL flask two-neck bottle under N_2. 30 ml of toluene and 15 mL H_2O were added and then heated to 90 ºC and stirred for 24 hours. The system was then filtered, washed successively with triethylamine, dichloromethane, water, and ethanol and purified by sublimation. Ant-ThPh was obtained as a yellow solid, with a yield of 78.69% (1.1 g). ^{1}HNMR (400 MHz, $CDCl_3$): δ [ppm] 8.43 (s, 1H), 8.38 (s, 1H), 8.26 (s, 1H), 8.02 (d, 1H), 7.96 (m, 2H), 7.82 (m, 2H), 7.71 (d, 1H), 7.70 (s, 1H), 7.43 (m, 2H), 7.29 (m, 2H). MS (EI) m/z: 310 [M+]; Anal. calculated for $C_{24}H_{16}$ S (%): C: 85.13, H: 4.55. Experimental: C: 85.23%, H: 4.41%.

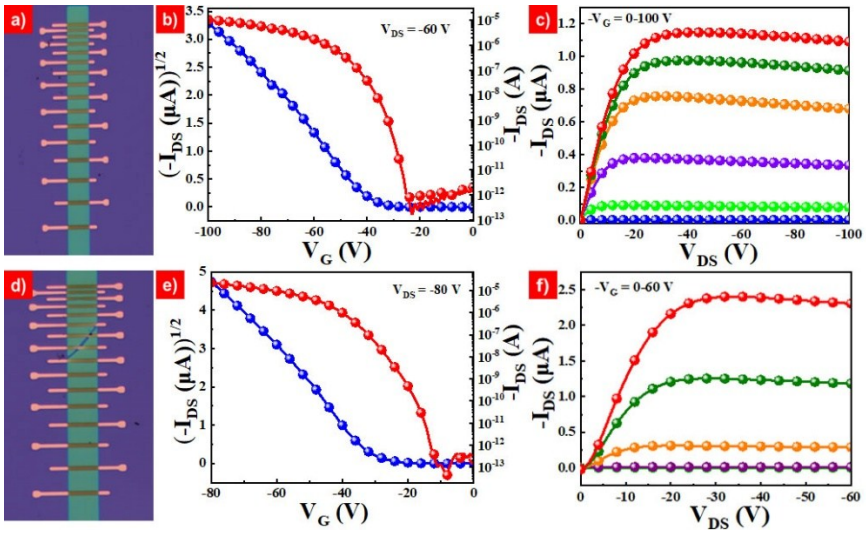

Figure S1 a) and d) Thin film-based transistor of Ant-Th-Ph (the ratio of W/L of best data is 9/1) and Ant-ThPh (the ratio of W/L of best data is 9/1). b) and c) Typical transfer and output curves of thin film-based transistor of Ant-Th-Ph. e) and f) Typical transfer and output curves of thin film-based transistor of Ant-ThPh.

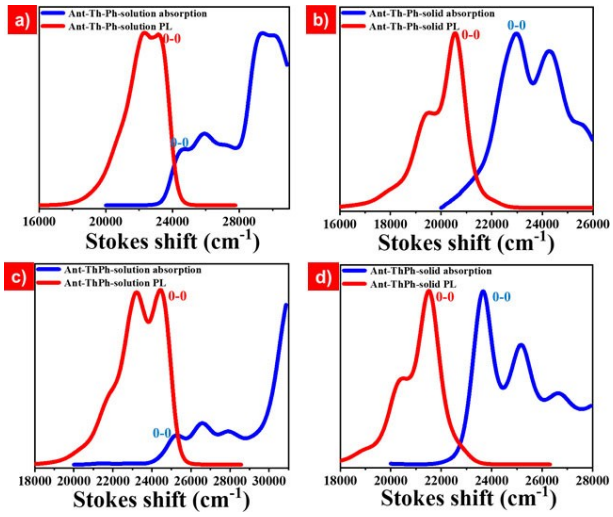

Figure S2 Stokes shift (blue absorption, red PL). a) Ant-Th-Ph solution b) Ant-Th-Ph solid c) Ant-ThPh solution d) Ant-ThPh solid

Reference:

1. T Komori, H Nakanotani, T Yasuda, C Adachi. *J. Mater. Chem. C*, 2014, **2**, 4918-4921