Electronic Supplementary information (ESI)

A New Organic Compound of 2-(2,2-diphenylethenyl) anthracene (DPEA) Showing Simultaneous Electrical Charge Transport Property and AIE Optical Characteristics

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Experimental Section

All solvents and materials were used as received from commercial sources without further purification. ^{1}H-NMR spectra was recorded on Bruker 400 MHz spectrometer using $CDCl_3$ as the solvent and chemical shifts were reported as δ values (ppm) relative to an internal tetramethylsilane (TMS) standard. UV-Vis absorption spectra were recorded by a Jasco V-570 UV-Vis spectrometer and Photoluminescence (PL) spectra were recorded on a Jasco FP-6600 spectrofluorometer. Electrochemical measurements (CV) was performed with a CHI660C electrochemistry station in acetonitrile solution with sample concentration of 10^{-3} M using Bu_4NPF_6 as electrolyte, and using Pt as working electrode, platinum wire as auxiliary electrode, and a porous glass wick Ag/AgCl as pseudo-reference electrode. UPS measurements were recorded on a KRATOS Axis Ultra DLD spectrometer. The sample for UPS measurement was

prepared by depositing a thin film (15nm) of DPEA on a small plate of Si (size:1cm×1cm). Thermal gravimetric analysis (TGA) was performed on a STA 409 PC thermogravimeter under an N_2 flow at a heating rate of 10 $^oC\ min^{-1}$, Differential scanning calorimetry was carried on a Q2000, (TA Instruments, USA) under nitrogen atmosphere. Absolute quantum yield measurement (LabSphere®, FluoroMax-4, HORIBA JobinYvon, PLQY software package) was used for powder sample and crystalline sample. In this experimental setup, it is possible to measure the PLQY by 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. Time-resolved peak fluorescence of DPEA in DCM and crystals were determined by FSL980. SEM images were taken by using Scanning Electron Microscope (Hitachi S-4800). For the preparation of the SEM sample, first of all, we should configure solutions with a certain content of water, and dipped it on the cleaned SiO_2/Si substrate. Then, in order to avoid further aggregation caused by the evaporation of the solution, the solvent should be absorbed away by filtrate paper. Atomic force micrographs image of crystal was taken on a Digital Instruments Nanoscope III atomic force microscope in tapping mode.

Single crystals of DPEA were germinate from saturated DCM:PE= 1:2 solution at room temperature for the X-Ray diffraction and its XRD data was collected on a Rigaku Saturn 724 CCD diffract meter with graphite monochromated Mo Ka radiation. In addition, high-quality Single crystals for OFETs were prepared by physical vapor transport (PVT), The powder of DPEA was heated to 120 ℃ and then the crystals were deposited on the OTS-modified SiO_2/Si substrate. And top-contacted OFETs based on the DPEA crystals are constructed on OTS-modified SiO_2/Si substrates, OFET characteristics were recorded by a Keithley 4200 SCS and Micromanipulator 6150 probe station in a clean and shielded box, All the device fabrication and characterization steps were carried out at room temperature under ambient laboratory conditions.

Synthetic details

1-(anthracen-2-yl)-2,2-diphenylethanol（ADPE）: A schlenk tube (100 mL) was oven-dried, and its fitted with magnetic bar was added 2-bromoanthracene(1 g, 3.8 mmol), then protected under argon, anhydrous THF (20 mL), TMEDA (0.63 mL, 4.2 mmol) were injected into the system. After cooling down to -78℃, n-BuLi (2.7 mL, 4.2 mmol, 1.6M) was added slowly and this mixture was stirred for 90 min at -78℃. Then diphenylacetaldehyde (0.824 g, 4.2 mmol) was slowly added dropwise via syringe. The mixture warmed up to room temperature and was stirred for 12 h. The resultant precipitate was washed successively with H_2O and evaporated under reduced pressure, the crude product was purified by flash column chromatography over silica gel eluting with PE/DCM (1:1 v/v) to obtain ADPE (1.103 g, 78% yield) as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 8.35 (s, H), 8.26 (s, H), 7.98 – 7.90 (m,3H), 7.76 (s, H), 7.47 – 7.28 (m, 10H), 7.19 - 7.04 (m, 6H). MS (EI): m/z: 374 (M^+).

2-(2,2-diphenylethenyl)anthracene (DPEA): p-Toluenesulfonic acid monohydrate (24.7mg, 0.13mmol) was added to a stirred solution of ADPE (500 mg, 1.3 mmol) in toluene (20 mL) under argon at room temperature. and the resulting mixture was heated under reflux for 12 h. the reaction was then cooled to room temperature and filtered through the filter paper. The solvent was removed under reduced pressure to give a residue, which was purified by flash column chromatography over silica gel eluting with PE/DCM (5:1 v/v) to obtain DPEA (0.379 g, 79.8% yield) as a light yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 8.24 (d, 2H), 7.94 (m, 2H), 7.77 (s, H), 7.67 (d, H), 7.43 - 7.27 (m, 12H), 7.18 (s, H), 7.01 (d, H). MS (MALDI-TOF): cacld for M^-, 356; found, 356. MS (EI): m/z: 356 (M^+). Anal.calcd for $C_{28}H_{20}$ (%): C:94.34, H: 5.66. Found: C: 94.16%, H: 5.74%.

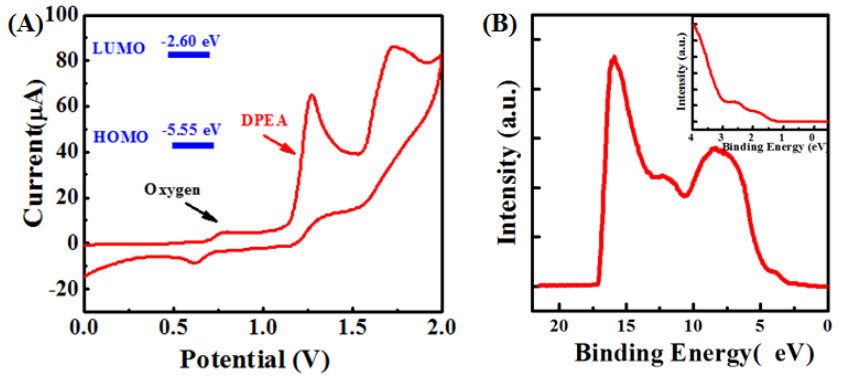

Figure S1. (A) Cyclic voltammetry measurement of DPEA in the acetonitrile solution. (B) UPS Energy distribution curve of DPEA thin films. HOMO = hv + Ecutoff - E_F, hv = 21.22 eV.

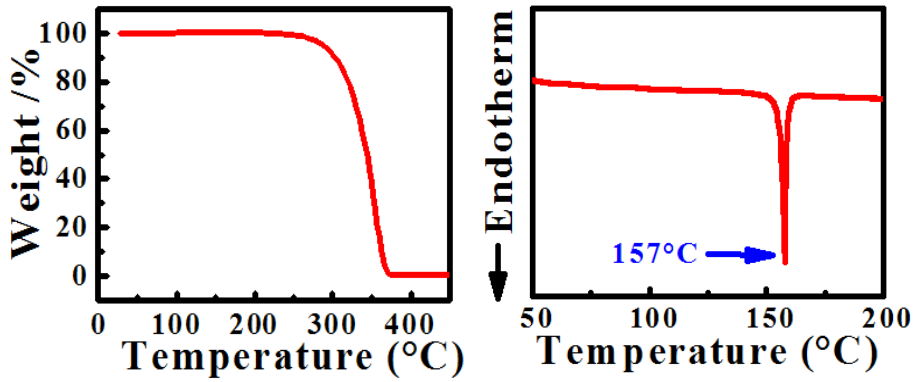

Figure S2. Thermal gravimetric analysis and differential scanning calorimetry of DPEA.

Table S1. Crystal Data and Structure Refinement for DPEA. (CCDC: 1574336)

Empirical formula	C28 H20	
Formula weight	356.44	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P b c a	
Unit cell dimensions	a = 11.0823(6) Å	α= 90°.
	b = 8.2233(4) Å	β= 90°.
	c = 42.789(2) Å	γ = 90°.
Volume	3899.5(3) $Å^3$	
Z	8	
Density (calculated)	1.214 Mg/m^3	
Absorption coefficient	0.069 mm^{-1}	
F(000)	1504	

Crystal size	0.347 x 0.324 x 0.098 mm^3
Theta range for data collection	1.904 to 27.424°.
Index ranges	-14<=h<=10, -9<=k<=10, -38<=l<=55
Reflections collected	17298
Independent reflections	4364 [R(int) = 0.0489]
Completeness to theta = 25.242°	98.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.0000 and 0.81795
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4364 / 0 / 253
Goodness-of-fit on F^2	1.186
Final R indices [I>2sigma(I)]	R1 = 0.0752, wR2 = 0.1717
R indices (all data)	R1 = 0.0901, wR2 = 0.1817
Extinction coefficient	n/a
Largest diff. peak and hole	0.200 and -0.182 $e.Å^{-3}$

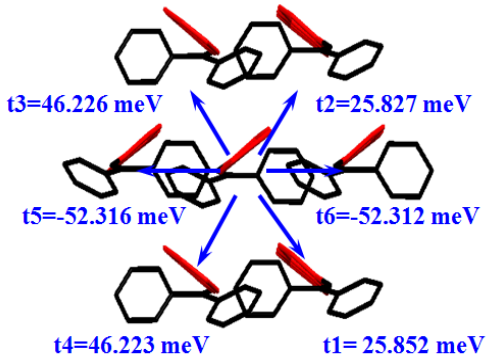

Figure S3. Illustrations of transfer integrals for the nearest neighboring molecular pairs considered in the calculations for the DPEA crystal based on the direct integration with site-energy correction.

Table S2. Time-resolved PL measurements of DPEA in dilute dichloromethane solution (A) and single crystals (B).

(A) In solution τ = 3.71 ns	**(B) Crystals τ = 1.98 ns**
τ_1 = 0.25 ns (57.08 %)	**τ_1 = 0.19 ns (74.92 %)**
τ_2 = 8.33 ns (42.92 %)	**τ_2 = 4.48 ns (10.84 %)**
	τ_3 = 9.49 ns (14.24 %)

The lifetime was calculated using the approximation formula $\tau \approx \tau_1 \times$percentage of τ_1 (%) + $\tau_2 \times$percentage of τ_2 (%) + $\tau_3 \times$percentage of τ_3 (%) + ⋯⋯.

Table S3. The best-Fit parameters of fluorescence of DPEA and the deactivation rates.

	Φ_F	τ_{FL}（ns）	kr(s^{-1})	knr(s^{-1})
in solution	**0.01**	**3.71**	**2.69×10^{6}**	**2.67×10^{8}**
Crystals	**0.30**	**1.98**	**1.52×10^{8}**	**3.54×10^{8}**

Fluorescence quantum yield of DPEA in dichloromethane was measured by referring to quinine sulfate and the crystals were measured by a calibrated sphere.

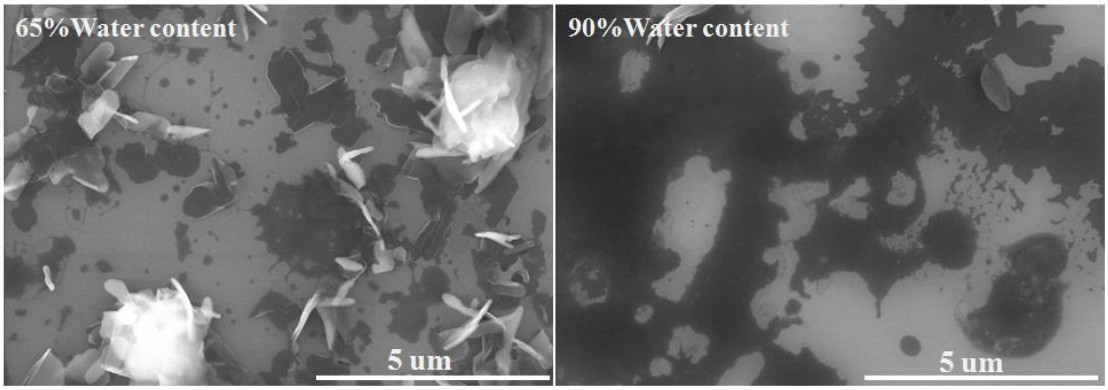

Figure S4. SEM images of DPEA aggregations in the mixture solutions with water contents of 65% and 90%, respectively.

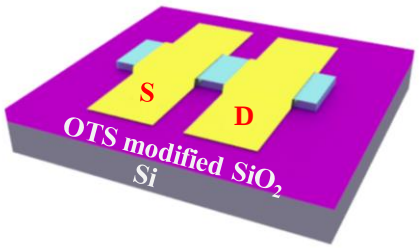

Figure S5. Schematic of the DPEA single-crystal-based transistor with bottom-gate top-contact configuration.

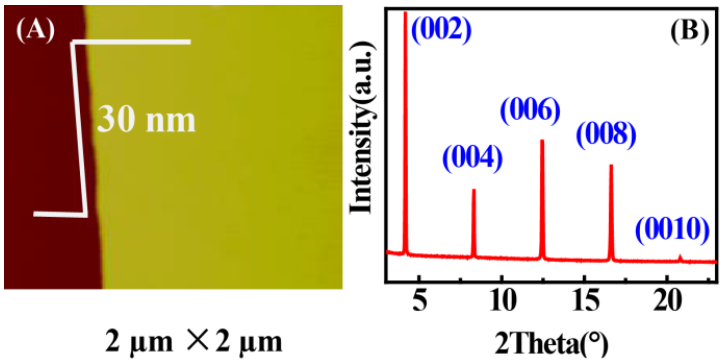

Figure S6. (A) AFM image of DPEA crystal prepared by physical vapor transport. (B) XRD diffractions of DPEA crystals on OTS-modified Si/SiO_2 substrate.