Electronic Supplementary Information

Naphthalene-substituted 2,3,4,5-tetraphenylsiloles: synthesis, structure, aggregation-induced emission and efficient electroluminescence

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General Information

THF was distilled from sodium benzophenone ketyl under dry nitrogen immediately prior to use. All other chemicals and reagents were purchased from Aldrich and used as received without further purification. ¹H and ¹³C NMR spectra were measured on a Bruker AV 400 spectrometer in deuterated chloroform using tetramethylsilane (TMS; $\delta = 0$) as internal reference. UV spectra were measured on a Milton Roy Spectronic 3000 Array spectrophotometer. PL spectra were recorded on a Perkin-Elmer LS 55 spectrofluorometer. High resolution mass spectra (HRMS) were recorded on a GCT premier CAB048 mass spectrometer operating in MALDI-TOF mode. Single crystal X-ray diffraction intensity data were collected at 100 K on a Bruker–Nonices Smart Apex CCD diffractometer with graphite monochromated Mo K α radiation. Processing of the intensity data was carried out using the SAINT and SADABS routines, and the structure and refinement were conducted using the SHELTL suite of X-ray programs (version 6.10). TGA analysis was carried on a TA TGA Q5000 under dry nitrogen at a heating rate of 10 °C/min. The ground-state geometries were optimized using the density functional with B3LYP hybrid functional at the

basis set level of 6-31G(d). All the calculations were performed using Gaussian 03 package. Cyclic voltammetry was performed on a CHI660A electrochemical work station at room temperature with use of a standard three-electrode electrochemical cell in dichloromethane containing 0.1 M tetra-*n*-butylammonium hexafluorophosphate. The working and reference electrodes were platinum and Ag/AgCl. The reference electrode was checked versus ferrocene as internal standard as recommended by IUPAC. All the solutions were deaerated by bubbling nitrogen gas for a few minutes prior to the electrochemical measurements.

Device Fabrication

The devices were fabricated on 80 nm-ITO coated glass with a sheet resistance of $25\Omega/\Box$. Prior to load into the pretreatment chamber, the ITO-coated glass was soaked in ultrasonic detergent for 30 min, followed by spraying with de-ionized water for 10 min, soaking in ultrasonic de-ionized water for 30 min, and ovenbaking for 1 h. The cleaned samples were treated by perfluoromethane plasma with a power of 100 W, gas flow of 50 sccm, and pressure of 0.2 Torr for 10 s in the pretreatment chamber. The samples were transferred to the organic chamber with a base pressure of 7×10^{-7} Torr for the deposition of NPB, emitter, and TPBi, which served as hole-transport, light-emitting, and electron-transport layers, respectively. The samples were then transferred to the metal chamber for cathode deposition which composed of lithium fluoride (LiF) capped with aluminum (Al). The light-emitting area was 4 mm². The current density-voltage characteristics of the devices were measured by a HP4145B semiconductor parameter analyzer. The forward direction photons emitted from the devices were detected by a calibrated UDT PIN-25D silicon photodiode. The luminance and external quantum efficiencies of the devices were inferred from the photocurrent of the photodiode. The electroluminescence spectra were obtained by a PR650 spectrophotometer. All measurements were carried out under air at room temperature without device encapsulation.

Preparation of Nanoaggregates

Stock THF solutions of D-1-NpTPS and D-2-NpTPS with a concentration of 10^{-4} M were prepared. Aliquots of the stock solution were transferred to 10 mL volumetric flasks. After appropriate amounts of THF were added, water was added dropwise under vigorous stirring to furnish 10^{-5} M solutions with different water contents (0–90 vol %). The PL measurements of the resultant solutions were then performed immediately.



Fig. S1 ORTEP drawing of 2,5-bis(4-bromophenyl)-1,1-dimethyl-3,4-diphenylsilole (3) (CCDC 888228).



Fig. S2 (A) PL spectra of D-1-NpTPS in THF/water mixtures with different water fractions (f_w). (B) Plot of ($I/I_0 - 1$) values versus water fractions in THF/water mixtures of D-1-NpTPS. I_0 is the PL intensity in pure THF solution.