Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Suppulementary Information for:

Synthesis and property of wide bandgap polymers based on tetraphenylsilane and their applications as hosts in electrophosphorescent devices

Xiaoxiao Li,[a] Qing Bai,[a] Jinyu Li,[a] Fang Lu,[b] Xiaoyi Sun[a] and Ping Lu[a]

[a]*State Key Laboratory of Supramolecular Structure and Materials, Jilin University, Changchun 130012, People's Republic of China. E-mail address: lup@jlu.edu.cn (P. Lu)*

[b]*Pharmacy Department, Changchun Medical College, People's Republic of China*

Contents

1. Instrumentation

The ^1H NMR and ^{13}C NMR spectra were recorded by a Bruker AVANCE III 500 spectrometer at 500 MHz and 126 MHz, respectively, at 298 K using DMSO-d_6 and $CDCl_3$ as the solvent and tetramethylsilane (TMS) as the internal standard. The elemental analysis was performed on a Vario micro cube, CHNS elemental analysis instrument. The MALDI-TOF-MS mass spectra were recorded by an AXIMA-CFRTM plus instrument. Thermal gravity analysis (TGA) was performed on a Perkin-Elmer thermal analysis system at a heating rate of 10 K•min^{-1} at a nitrogen flow rate of 80 mL•min^{-1}. Differential scanning calorimeter (DSC) analysis was carried out by a NETZSCH (DSC-204) instrument at 10 K•min^{-1} under a nitrogen flow. UV-vis and fluorescence spectra were recorded by a Shimadzu UV-3100 spectrophotometer and a Shimadzu RF-5301PC spectrophotometer, respectively, using a 1 cm path-length cuvette. Electrochemical measurements were performed by CHI660C electrochemical workstation using three-electrode system: a glassy carbon disc electrode as the working electrode, a Pt wire as the counter electrode, Ag/$AgNO_3$ (0.1 M) electrode as the reference electrode and 0.1 Mtetrabutylammoniumhexafluorophosphate (TBAPF6) in dry CH_2Cl_2 or N,N-dimethylformamide (DMF) as the electrolytes at a scan rate of 100 mV•s^{-1}. The devices were fabricated by vacuum evaporation. The ITO coated glass substrates were sequentially cleaned in an ultrasonic bath with toluene, acetone, ethanol and deionized water. They were then dried with nitrogen and finally irradiated in a UV-ozone chamber. The organic materials were sequentially deposited onto cleaned ITO glass substrates by thermal evaporation. The layer thickness of the deposited material was monitored in situ using an oscillating-quartz thickness monitor. Finally, a LiF buffer layer and an Al cathode were deposited onto the organic films. The background pressure of the chamber was less than 10^{-6} Torr during the deposition process. The luminance-current characteristics of devices were measured by a PR650 spectroscan spectrometer. The current-voltage characteristics were studied by a

Keithley 2400 sourcemeter. All of the device measurements were carried out at room temperature under ambient conditions.

2. Synthesis and characterization of M2

Tris(4-bromophenyl)(phenyl)silane (M2): The mixture of 1,4-dibromobenzene (5.23 g, 25 mmol) and ether (100 mL) was put in a round flask, and n-BuLi (2.4 mol/L, 9.5 mL) was then added. The reaction mixture was stirred at 0 °C for 3 h under N_2 atmosphere. After that, $PhSiCl_3$ (1.25 mL) was put into the mixture and the reaction continued for further 12 h. Then, water was added to quench the reaction, the organic layer was extracted, concentrated, and M2 was purified by column chromatography in 82% yield. ^{1}H NMR (500 MHz, $CDCl_3$): (ppm) 7.532-7.511 (d, 6H), 7.486-7.451 (m, 3H), 7.411-7.389 (d, 2H), 7.369-7.349 (d, 6H).

3. Synthesis and characterization of M3

(4-(Bis(4-bromophenyl)(phenyl)silyl)phenyl)diphenylphosphine oxide (M3): M2 (2.73 g, 4.76 mmol) and THF (90 mL) were placed in a round flask, and then n-BuLi (2 mL, 2.4 mol/L) was added. The mixture was kept at 0 °C for 3 h under protection of N_2 atmosphere. Ph_2PCl (1.00 mL) was then added. After 48 h, water was added to quench the reaction. The organic layer was extracted, concentrated. M3 was purified by column chromatography in 54% yield. ^{1}H NMR ($CDCl_3$, 500 MHz): (ppm) 7.711-7.699 (m, 8H), 7.568-7.437 (m, 13H), 7.411-7.358 (m, 6H). Elemental Anal. Calcd. for $C_{36}H_{27}Br_2OPSi$: C, 62.26; H, 3.92. Found: C, 62.34; H, 4.01.

4. Theoretical calculations of corresponding oligomers