Electronic Supplementary Information

High hole mobility of 1,2-bis[4'-(diphenylamino)biphenyl-4-yl]-1,2-diphenylethene in field effect transistor

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Materials and Instrumentations

Tetrahydrofuran (THF) was distilled from sodium benzophenone ketyl under nitrogen immediately prior to use. All the chemicals and other regents were purchased from Aldrich and used as received without further purification. 1H and 13C NMR spectra were measured on a Bruker AV 300 spectrometer in deuterated chloroform using tetramethylsilane (TMS; δ = 0) as internal reference. UV spectra were measured on a Milton Roy Spectronic 3000 Array spectrophotometer. Photoluminescence was recorded on a Perkin-Elmer LS 55 spectrofluorometer. The MALDI-TOF mass spectrum was recorded on a GCT premier CAB048 mass spectrometer. Elemental analysis was performed on an Elementary Vario EL analyzer. Cyclic voltammetric measurement of p-BTPATPE in 0.1 M Bu4NPF6 in dichloromathene solution was carried out in a conventional three-electrode cell using platinum working electrodes, a platinum wire counter electrode, and a Ag/AgCl reference electrode at room temperature. The experiment was calibrated with the ferrocene/ferrocenium (Fc/Fc+) redox system.
TOF Experiment

Poly(styrene) (PS, average MW 200 000 (Typical)) and C₆₀ (99.95%) were purchased from Aldrich and used as received. Thick polymer film (10 µm) of PS doped with the sample molecules was sandwiched between two ITO-coated glass slides. The film had the following compositions: PS/sample/C₆₀ 50/48.5/1.5 wt%. Sample was prepared as follows: firstly, sample molecules and PS were dissolved in THF. Separately, and C₆₀ was also dissolved in toluene. Then the solutions were mixed and then the final solution was filtered through an 11 µm pore size filter paper. The solvent was evaporated under reduced pressure on a rotary evaporator. The mixture was dried for 12 h in an oven at 80 °C. Next, the dried materials were melted and mechanically mixed between two large glass slides to remove trapped air bubbles from the film. This procedure was repeated several times until the mixture was optically clear and uniform. A small piece of this film was melted in a hot plate between two ITO-coated glass slides (previously cleaned by ultrasonic treatments in sequential baths of distilled water and ethanol) at a temperature between 150 and 170 °C. The sample cell was removed from the hot plate and placed on a cool metal surface. Calibrated glass spacers of 10 µm were used to ensure a uniform sample thickness. Finally, samples were sealed with quick setting epoxy adhesive.

Photocurrent generation and charge transport properties in polymer film of PS doped with the sample molecules was determined by using TOF (Time of Flight Technique). Measurements were realized on indium–tin oxide/polymer composites/indium–tin oxide samples (ITO/composite/ITO).

A nitrogen laser (λ = 337 nm) with a 4 ns pulse width and 0.5 Hz of repetition rate was used as irradiation source. The photocurrent generated by irradiation on the sample through one of the ITO electrodes (illuminated area ~ 0.05 cm²) was amplified using a low noise preamplifier and monitored across an external load resistor with a digital oscilloscope. A low noise high voltage power supply was used for applying the bias voltage to samples. Due to the strong absorption in the UV region the excitation pulse is completely absorbed within a distance of less than 500 nm in the sample. The experiments were performed in the single shot regime. All measurements were made in air.
FET fabrication and measurement

For fabrication and characterization of thin films transistors please refer to our previous works\(^1\).

Preparation of Nanoaggregates

Stock THF solutions of the compounds 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 (0–99.5 vol %). The PL measurements of the resultant solutions were then performed immediately.

Synthesis

\(4',4''-(1,2\text{-Diphenylethene-1,2-diyl)bis(N,N-diphenylbiphenyl-4-amine)}\) (\(p\)-BTPATPE): To a solution of 4 (2.1 g, 5 mmol), zinc dust (0.78 g, 12 mmol) in 50 mL dry THF was added dropwise of titanium(IV) chloride (1.15 g, 6 mmol) under nitrogen at \(-78\) °C. After stirring for 20 min, the reaction mixture was warmed to room temperature and then heated to reflux for 12 h. The reaction mixture was then cooled to room temperature and poured into water. The organic layer was extracted with dichloromethane, and the combined organic layers were washed with saturated brine solution and water and dried over anhydrous magnesium sulfate. After filtration and solvent evaporation, the residue was purified by silica-gel column chromatography using \(n\)-hexane/dichloromethane as eluent. Pale yellow solid of \(p\)-BTPATPE was obtained in 84% yield (1.71 g). \(^1\)H NMR (400 MHz, CDCl\(_3\), \(\delta\)): 7.45–7.42 (m, 4H), 7.33–7.31 (m, 4H), 7.28–7.22 (m, 8H), 7.12–6.99 (m, 30H); \(^1\)H NMR (133 MHz, CDCl\(_3\), \(\delta\)): 148.3, 147.7, 144.5, 143.1, 143.0, 141.3, 139.0, 138.9, 135.3, 135.2, 132.5, 132.1, 129.9, 128.5, 128.3, 128.1, 127.2, 127.1, 126.4, 126.3, 125.0, 124.7, 123.5. HRMS: \(m/z\) 818.3692 (M\(^+\), calcld 818.3661). Anal. Calcd for C\(_{62}\)H\(_{46}\)N\(_2\): C, 90.92; H, 5.66; N, 3.42. Found: C, 90.90; H, 5.61; N, 3.44.

Reference