

Supporting Information

Oligo- and Poly-thiophene/ZnO Hybrid Nanowire Solar Cells

Alejandro L. Briseno, Thomas W. Holcombe, Akram I. Boukai, Erik C. Garnett, Steve W. Shelton, Jean J. M. Fréchet*, Peidong Yang*

Department of Chemistry, University of California, Berkeley, California 94720, and Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, California 94720

Experimental

Structural Characterization. Scanning electron microscopy was done on a JEOL JSM-6340F operating at 5 kV. Transmission electron microscopy was performed on a Philips CM200 FEG operating at 200 kV.

End-Functionalization of P3HT. In a 100 mL 3-neck round-bottom flask, 41 mg of P3HT was dissolved in 50 mL of anhydrous toluene. This required heating at 90 °C for 2 hours. The solution was then cooled to room-temperature and then further cooled to 0 °C. The bright orange solution turns dark orange and opaque at this point. 0.2 mL of 2.5M nBuLi was then added dropwise and stirred at 0 °C for 5 minutes and at room temperature for 1 hour before the reaction was cooled back down to 0 °C and 0.3 mL of diethylchlorophosphate was added dropwise. After 2 hours, the reaction was precipitated into methanol (200 mL) and filtered, with extensive methanol and acetone washing.

QT-ester. In a 100 mL 3-neck round bottom flask, 5,5'-bis(3-dodecyl-2-thienyl)-2,2'-bithiophene (Aldrich, 0.50 g, 0.749 mmol) was dissolved in 40 mL of anhydrous THF. The reaction was cooled to -78 °C (solution became a slurry) and n-butyllithium (Aldrich, 0.315 mL 2.5M in hexanes, 1.15 eq) was added dropwise. The reaction was stirred at -78 °C for 2.5 hours and then diethylchlorophosphate was added dropwise (Aldrich, 0.155 g, 0.898 mmol, 1.2 eq). The reaction becomes an orange color at -78 °C and then turns red over the course of 6 hours as the reactions warms to room-temperature. The crude reaction was quenched with a few drops of water and then diluted with diethylether and washed with 1M HCl. The ether was evaporated to yield crude product that was purified by column chromatography (40% EtOAc in Hexanes). 130 mg, 22% yield. ¹H NMR (400 MHz, Acetone-d₆) ppm 7.49 (d, J = 8.53 Hz, 1H), 7.38 (d, J = 5.21 Hz, 1H), 7.32 (dd, J = 3.77, 1.46 Hz, 2H), 7.25 (d, J = 3.83 Hz, 1H), 7.12 (d, J = 3.80 Hz, 1H), 7.03 (d, J = 5.21 Hz, 1H), 4.15-4.06 (m, 4H), 2.86-2.78 (m, 6H), 1.71-1.61 (m, 4H), 1.40-1.15 (m, 44H), 0.84 (t, J = 6.76, 6.76 Hz, 6H) ³¹P (9.86)

End Functionalization of QT-Acid. In a 1-neck 25 mL round-bottom flask 130 mg of DD-QTPO-Ester was dissolved in 7 mL of dichloromethane. 0.2 mL of bromotrimethylsilane (8 eqs) and 0.21 mL of triethylamine (8 eqs) were stirred overnight. 1 mL of water was added and stirred for an hour as an emulsion with dichloromethane. ~50 mL of dichloromethane was added and the organic phase washed with 1M HCl. The

dichloromethane was removed under reduced pressure to yield a yellow solid (90 mg, 75% yield). ^1H NMR (400 MHz, CD_2Cl_2) δ ppm 7.70-7.30 (m, 2H), 7.21-6.81 (m, 7H), 2.78-2.65 (m, 4H), 1.69-1.52 (m, 4H), 1.38-1.13 (m, 38H), 0.88-0.76 (m, 6H).