

Supporting Information

Perylenediimide Functionalized Bridged-Siloxane Nanoparticles for Bulk Heterojunction Organic Photovoltaics

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Experimental Part

Materials. 3,4,9,10-tetracarboxyanhydrideperylene, regioregular poly(3-hexylthiophene) (average M_n 30,000 - 60,000 g/mol), tert-butylmagnesiumchloride (1M in THF), and anhydrous tetrahydrofuran were obtained from Aldrich chemicals. Ammonium hydroxide (28%) was obtained from Fischer Scientific. Tetraethoxysilane, and 3-aminopropyltriethoxysilane were purchased from Alfar Aesar and used as received. Unless otherwise specified, all chemicals were used as received.

Characterization. Proton NMR spectra were recorded on a 500 MHz Jeol using $CDCl_3$ as a solvent. FTIR spectra were measured using a Perkin-Elmer Spectrum One FT-IR spectrometer equipped with a universal ATR sampling accessory. Transmission electron microscopy (TEM) observations were performed on a 100CX JEOL at 80 keV. Thermogravimetric analysis was performed at Thermal Analysis Laboratory at Western Kentucky University. The samples were analyzed by a TA Q5000TGA. The samples were held isothermal at room temperature for 30 min and then heated from room temperature to 650 °C at 10 °C/min in nitrogen. The purge gas

was heated at 10 °C/min to 800 °C. The elemental compositions of the silane precursor (**1**) and the PDIB-NPs were analyzed by Micro-Elemental Analysis Lab at Advanced Materials Institute, Western Kentucky University. The photophysical properties in solution were performed on fluorescence spectrometer (Perkin Elemer LS 55) and UV-visible spectrometer (Perkin Elemer, Lambda 35). Thin films were prepared by spin coating the blends onto cleaned glass coverslips. The 457 and 514 laser lines from a Coherent Innova 200 Ar ion laser were used to excite the thin films with a typical excitation power of 100 μ W. A Nikon TE2000U inverted microscope with a 100x 1.4 NA oil immersion objective was employed for laser excitation and also for collection of the emitted light. Spectra were dispersed using a Princeton Instruments 2150 spectrograph (300 grooves/mm grating) and detected using a Princeton Instruments ProEM EMCCD camera (1024 x 1025 pixels). To reduce filter effects on the resulting spectra, a mirror rather than a dichroic filter was employed for excitation of the sample and either a long pass filter (for 457 nm excitation) or 514 nm notch filter was employed in the collection of the emitted light.

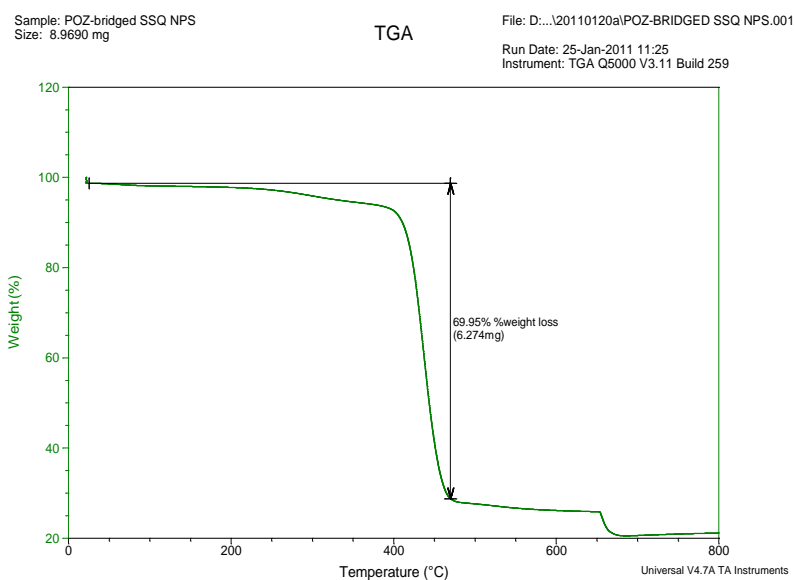


Figure S1: TGA curve of PDIB-1-NPs in Table 1

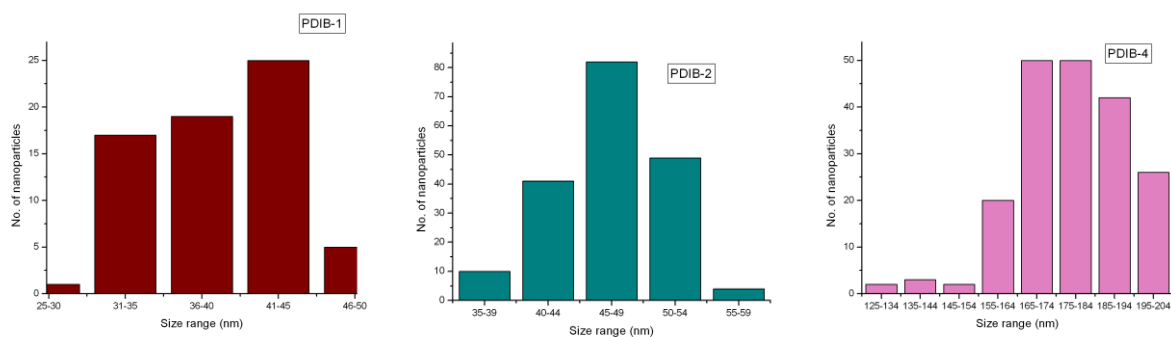


Figure S2: Size-distribution graphs for **PDIB-1**, **PDIB-2** and **PDIB-4**.

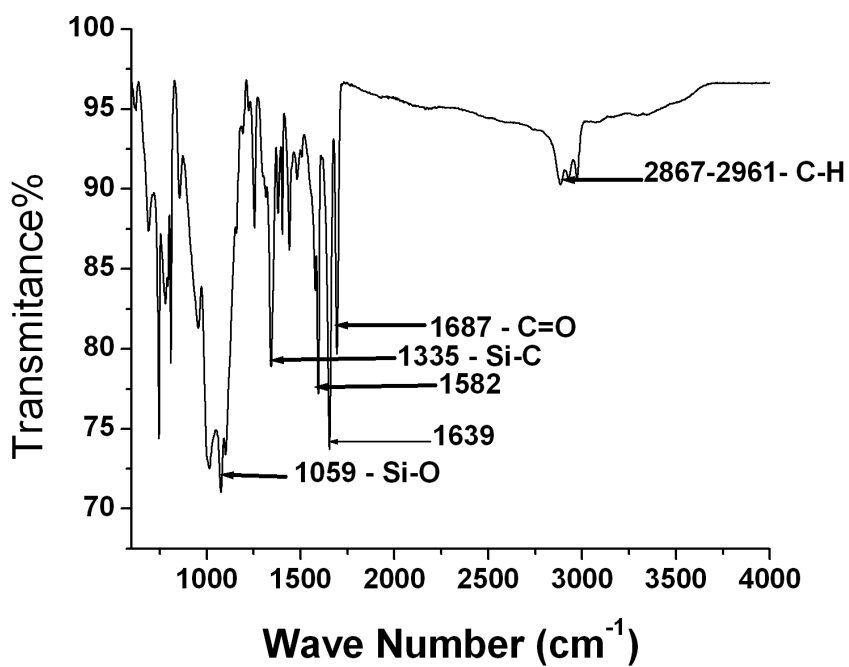


Figure S3: FT-IR spectrum of PDI-bridged-silane precursor.

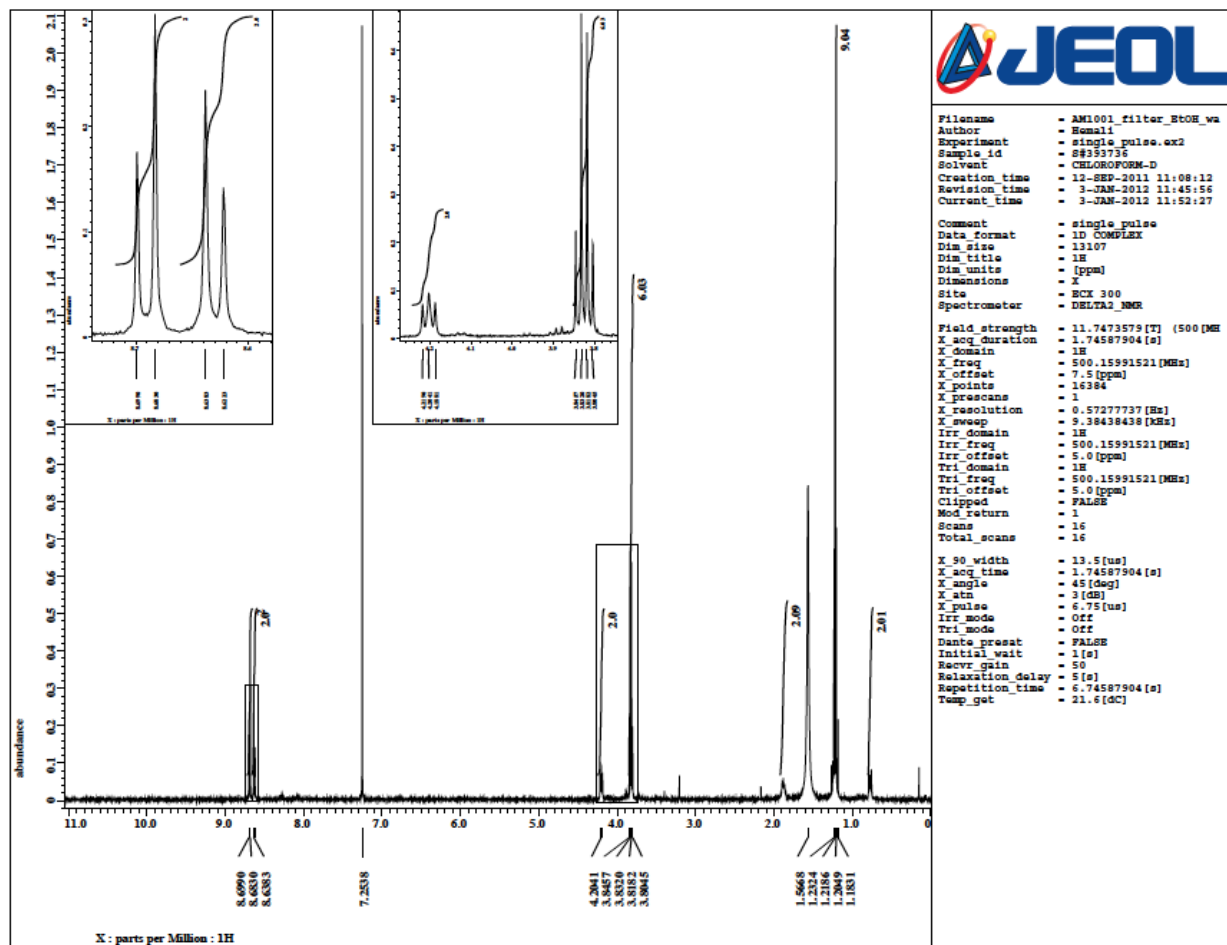


Figure S4: ^1H -NMR spectrum of PDI-bridged-silane precursor.

Photovoltaic properties of PDIB- NPs:

Three sets of model devices with device area of $2 \times 6 \text{ mm}^2$ were prepared by changing the following device parameters;

Set 1: The device configuration used was ITO/PEDOT:PSS/1:1 P3HT-PDIB-NPs/ LiF/Al.

Set 2: Active layer blending ratio of PDIB-NPs: P3HT was 2:1 with the device configuration of ITO/PEDOT:PSS/PDIB-NPs-P3HT/ Ca-Al.

Set 3: Devices with the configuration of ITO/PEDOT:PSS/PDIB-NPs-P3HT/ Ca-Al were annealed at annealation temperatures of 50, 75, 100, and 150 °C.

The Table S1 shows the device parameters and Figure 10 and 11 present the J-V curves for each set.

Table S1.

Test devices	V_{OC} (V)	J_{SC} (mA/cm ²)
Set 1	0.27	2.13
Set 2	0.47	0.50
Set 3	0.53	0.76 at 50 °C, 1.34 at 75 °C, 1.68 at 100 °C