Covalent Synthesis of Perylenediimide-Bridged Silsesquioxane Nanostructures and Their Electronic Properties

Lan Xu^a, Manda Venkata Ramana^a, Louis E. McNamara^b, Muhammad P. Jahan^c, Hemali Rathnayake^{a*}, Nathan I Hammer^{b*}

^a Department of Chemistry, Western Kentucky University, Bowling Green, KY 42101; ^b Department of Chemistry & Biochemistry, University of Mississippi, MS 38677; ° Department of Architectural & manufacturing Sciences, Western Kentucky University, Bowling Green, KY 42101.

KEYWORDS. Perylenediimide, Polysilsesquioxanes, Nanoribbons, Nanorods, Nanochains, organicbased solar cells



Trial (III)

Trial (IV)



Table S1. Experimental conditions of the trial reactions for the formation of PDIB-nanostructures and their dimensions

Reaction #	Trails	Concentration of NH ₄ OH (mol/L)	EtOH: CHCl ₃ : H ₂ O (mL)	Dimensions of nanostructures (TEM image #)
1	Ι	1.56	150:15: 0	Nanoribbons - width up to 600 nm and average length of untangled ones are in the range of 10-15 µm
	II	1.56	150: 15:0	Nanoribbons - width up to 700 nm and length about 11 µm
	III	1.56	37.5: 3.75:0	Nanoribbons - width 50 to 300 nm and length 6 to 10 µm
2	IV	1.40	37.5: 3.75:5.0	Mostly nanoparticles (average size 30- 50 nm) with few nanorods.
	V	1.47	37.5:4:2.5	Nanorods - width 80-100 nm and length from 2 to 9 µm
				Nanoparticles – Average size range 15- 30 nm
	VI	1.48	37.5:3.75:2.5	Nanorods - width 200-300 nm and length up to 5 µm
				Nanoparticles – Average size range 15- 30 nm
3	VII	2.50	37.5:3.75:0	Nanochains with length up to 2 μ m. The average size of nanoparticles in the nanochains are ~ 50 nm
				Nanorods with spherical nanoparticles on nanorod's surface. Width-50 -150 nm and length 2 to 3 µm
				Nanoparticles – Average size range 15- 30 nm
	VII	2.09	37.5: 4:0	Nanorods with spherical nanoparticles on nanorod's surface. Width- 200 -400 nm and length up to 9 µm
				Nanochains and hydrolyzed polymer fibers
The amount of PDIB silane (1) used for each reaction is 7×10^{-2} mmol.				



Figure S2: TEM images of PDIB- nanostructures formed at high base concentration (2.58 mol/L of base) at different time intervals.



Figure S3: FTIR spectrum of PDIB-Nanoribbons



Figure S4: FTIR spectrum of PDIB-silane



Figure S6: 1H-NMR spectrum of PDIB-silane



Figure S7: Additional AFM images taken from thin films containing PDIB-nanostructures over a scan area of 40 µm x 40 µm: 2D image (left) and 3D image (right).





Figure S8a: Bright field and fluorescence images of the same nanoribbons using the inverted microscope/CCD camera setup.



Fluorescence





Figure S8b: Bright field and fluorescence images of the same nanoribbons using the inverted microscope/CCD camera setup.



Figure S9: Conductivity graphs of nanoribbons and PDI-dimethylethoxysilane precursor