Synthesis of a Regioregular Amphiphillic Poly (Phenyleneethynylene) for use in Mesoporous Silica/ Semi-Conducting Polymer Nanocomposite Materials.

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Semi-conducting polymers have previously been embedded into the channels of hexagonally oriented mesoporous silica to create nanocomposite organic/inorganic materials. This involved first the creation of mesoporous silica using surfactants which were subsequently removed to form the channels. Into these channels were then incorporated MEH-PPV polymers from solution.[1]

This work focuses on the synthesis of a regioregular amphiphillic poly(phenyleneethynylene) (RAPPE) via a self polymerization reaction from a highly functionalized aromatic monomer. RAPPEs are capable of self-assembly into cylindrical nanostructures under certain solvent conditions, as shown in figure 1. This, in turn, would allow them to be used as scaffolds, similar to the surfactants mentioned above, to generate mesoporous silica. However, in this case the semi-conducting polymer would already be embedded in the mesoporous silica. This eliminates the need to remove the surfactants and then position polymers into the pores of the silica. Also, with this method, the concentration of polymer chains within the channels would be larger than if they had to be inserted, thereby making the process of forming these nanocomposite materials significantly more efficient.

The synthesis of the RAPPE is shown in scheme 1. Beginning with hydroquinone, in a series of steps, the iodo-bromo-alkoxyphenol **3** was synthesized. This intermediate is essential for producing a monomer capable of self-polymerizing to form a regioregular arrangement of the alkyl and amino side chains since subsequent Pd-catalyzed cross coupling would place the alkyne at the iodo position exclusively. With the TIPS protected alkyne in place, alklylation, and deprotection yielded alkyne **4**. Pd catalyzed self-polymerization of **4** generated RAPPE.

The optical and electronic properties of these polymers and nanocomposite materials is currently being determined. Also, their self-assembly is being examined by altering the alkyl chain length, which controls the cylinder's and subsequent pore's diameter.

1. a) Nguyen, T. Q.; Wu, J.; Doan, V.; Schwartz, B.J.; Tolbert, S.H. *Science* **2000**, *288*, 652-656. b) Wu, J.; Gross, A. F.; Tolbert, S. H. *J. Phys. Chem. B.* **1999**, *103*, 2374-2384.

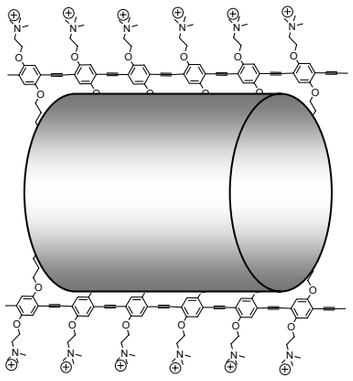
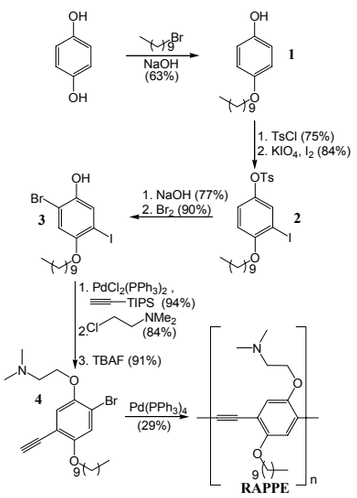


Figure 1



Scheme 1