

# Polymer Based Nanocomposites for Solar Energy Conversion

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## ABSTRACT

Organic semiconductor-based photovoltaic devices offer the promise of low cost photovoltaic technology that can be manufactured via large-scale, roll-to-roll printing techniques. Existing organic photovoltaic devices are currently limited to solar power conversion efficiencies of 3–5%. This is because of poor overlap between the absorption spectrum of the organic chromophores and the solar spectrum, non-ideal band alignment between the donor and acceptor species, and low charge carrier mobilities. To address these issues, we are investigating the development of dendrimeric organic semiconductors that are readily synthesized with high purity. They also benefit from optoelectronic properties, such as band gap and band positions, which can be easily tuned by substituting different chemical groups into the molecule. Additionally, we are developing nanostructured oxide/conjugated polymer composite photovoltaics. These composites take advantage of the high electron mobilities attainable in oxide semiconductors and can be fabricated using low-temperature solution-based growth techniques. Here, we discuss the synthesis and preliminary device results of these novel materials and composites.

## 1. Objectives

The long-term goal of this research is to realize the potential that organic photovoltaics (OPV) have as a low-cost alternative to conventional photovoltaics. These devices can be fabricated using solution-based printing techniques for high throughput production of solar modules. State-of-the-art devices, as demonstrated recently by Siemens [1] and others, have a power conversion efficiency of ~5%. Our goal is to develop materials and devices architectures that are capable of making large improvements in efficiency.

## 2. Technical Approach

We are developing materials to address several hurdles to higher efficiencies in OPV devices. To achieve better overlap of the organic chromophore with the sun's spectrum, we are developing dendrimeric organic semiconductors that can be made with high purity. These materials can exhibit strong self-ordering phenomena, leading to more optimal morphologies and high carrier transport. The importance of the morphology in organic solar cells has already been established [2].

Additionally, we are developing composite materials consisting of nanofibers of ZnO intercalated with an organic semiconductor [3]. These structures are fabricated by first

growing ZnO fibers directly onto a transparent conducting oxide substrate using a chemical solution growth technique. The fibers are then intercalated with a hole-conducting organic semiconductor into the pores of the oxide. When used as the active layer in a solar cell, these composites can take advantage of the light-absorbing and hole-transporting properties of the organic material and the high electron mobility of the oxide nanofibers. In the case of ZnO, the mobility of such fibers has been measured as high as  $100 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ , which is several orders of magnitude higher than is typically found in organic semiconductors.

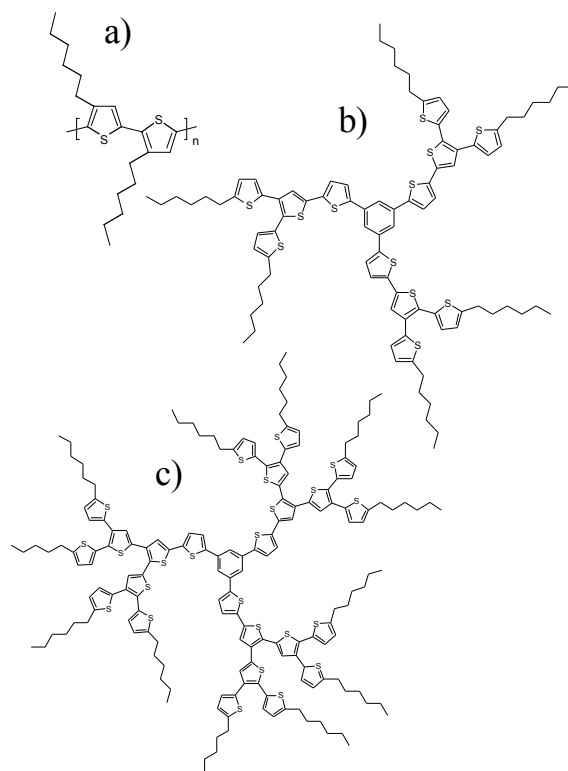


Figure 1. Molecular structures of a) poly(3-hexylthiophene) and b) 1<sup>st</sup>-generation and c) 2<sup>nd</sup>-generation thiophene dendrimers.

## 3. Results and Accomplishments

### Dendrimeric Organic Semiconductors

We have chosen thiophenes as a base unit for the synthesis of dendrimeric hole conductors. Polymers based on thiophene, such as poly(3-hexylthiophene) (P3HT) have yielded the highest efficiencies in bulk heterojunction organic solar cells to date [4]. The dendrimers are prepared by a convergent synthesis method. Initially, the surface

groups are prepared by alkylation of thiophene. A Grignard reaction of these surface groups with a further thiophene moiety gives the 1<sup>st</sup>-generation dendron. Subsequent generations of dendron are prepared by Stille coupling. These dendrons are then coupled with a benzene core again via a Stille couple to give the desired dendrimer. Figure 1 depicts P3HT, as well as 1<sup>st</sup>- and 2<sup>nd</sup>-generation thiophene dendrimers. Fabrication and characterization of preliminary OPV devices based in these materials is underway.

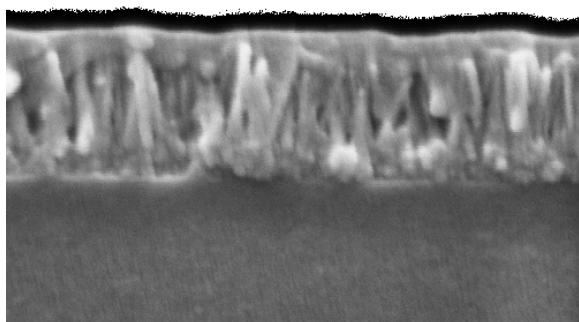
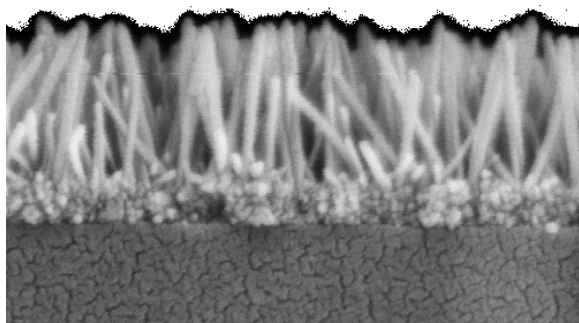
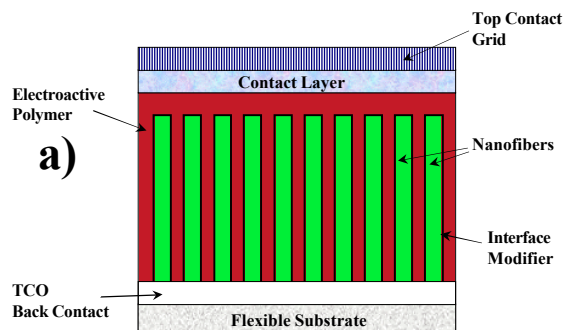


Figure 2. a) Idealized structure of a ZnO nanofiber/polymer composite solar cell, b) SEM image of ZnO nanofibers grown on glass, and c) SEM image of a polymer intercalated in ZnO nanofibers.

## ZnO Nanofiber/P3HT Composite PV Devices

Figure 2.a depicts the idealized structure of a nanostructured oxide/polymer composite photovoltaic device. We have fabricated devices that closely resemble this geometry. In the fabrication of such structures, a nucleation layer of nanocrystalline ZnO is deposited onto the substrate using an aqueous solution of zinc acetate. Fibers with diameters ~20 nm and lengths of between 100 nm and 1000 nm are then grown onto this nucleation layer from an aqueous solution of zinc nitrate. A polymer film is then deposited by solution casting onto the fibers, and thermal annealing is used to induce intercalation of the polymer into the pores of the ZnO fibers. Finally, a metallic top electrode is deposited through vacuum deposition. Figures 2.b and 2.c show images of the ZnO fibers before and after filling with polymer, respectively. Preliminary devices consisted of the structure ITO/ZnO/P3HT/Ag exhibit a power conversion efficiency of 0.5% under AM1.5 illumination.

## 4. Conclusions

OPV is a promising long-term technology for low-cost production of solar cells. Novel dendrimeric semiconductors and nanostructured oxide/polymer composite structures have been developed that will potentially enable gains in the efficiency of these devices.

## ACKNOWLEDGEMENTS

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