Energy Focus

Low bandgap, silole-containing heteroarene polymers developed for solar cells

The advantages of polymer solar cells (PSCs) for renewable energy include low cost, light weight, and ease of processing large surface areas. The highest power conversion efficiencies (PCEs) to date for PSCs have been achieved with bulk heterojunction devices composed of a polymer acting as electron donors and derivatized fullerenes as acceptors. Low-bandgap polymers are typically used to enhance light absorption, for example, benzodithiophene polymers, which achieve PCEs of over 7%. Other polymer requisites are high hole (electron vacancy) mobility and the ability to form good films. Recently, A.K.-Y. Jen and co-researchers at the University of Washington, Seattle, designed and synthesized in high yield new low-bandgap copolymers that contain a thiophene-phenylene-thiophene fused ring where silicon atoms replace the linked carbon atoms, resulting in low highest occupied molecular orbital (HOMO) levels and high hole mobilities.

As reported in the September 7th online edition of *Chemistry of Materials* (DOI:10.1021/cm1020228), Jen and co-researchers used the field-effect transistor (FET) technique to measure hole mobilities of PBSTBT and PBSTDTBT (see figure) to be 2.2×10^{-3} cm^2 V^{-1} s^{-1} and 1.1×10^{-2} cm^2 V^{-1} s^{-1}, respectively. Both polymers show good solubility in common organic solvents, an advantage in their device processing, and high thermal stability, with no transitions between 20°C and 350°C detected by differential scanning calorimetry.

Both polymers show long-wavelength absorption, which the researchers attribute to charge transfer from the benzobis (silolothiophene) donor to the acceptor elsewhere in the polymer chain. PBSTDTBT's absorption is much broader and at longer wavelengths than PBSTBT's, which the researchers said is due to the presence of two thiophene units between the donor and the acceptor compared to PBSTBT.

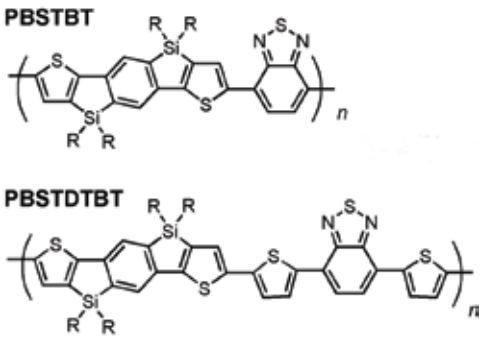
The researchers performed cyclic voltametry (CV) and density functional theory (DFT) calculations to determine HOMO and LUMO (lowest unoccupied molecular orbital) energy levels. Although DFT overestimated the orbital energy levels, it was consistent with the CV trends, for example, that the HOMO for PBSTBT lies lower in energy than PBSTDTBT's HOMO.

In addition, DFT predicts a lower lying HOMO for both polymers relative to their analogues where carbon replaces silicon, which is consistent with the researchers' desire to increase the polymers' open-circuit voltage.

The researchers fabricated PSCs with each polymer and determined good photo conversion efficiency from 400 nm to 700 nm, with external quantum efficiencies about 50% and PCEs about 3.5%.

The researchers said that their work "provides a new method for synthesizing silole-containing heteroarenes, which show great potential in organic electronics applications, such as FETs and PSCs."

Steven Trohalaki



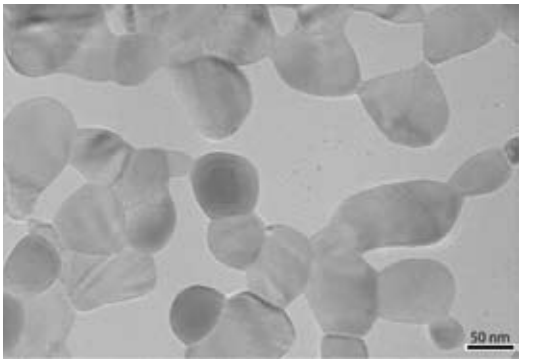
The chemical structure for the two polymers developed by Alex K.-Y. Jen and co-researchers. R = C_8H_{17} for both polymers.

Nano Focus

Low-temperature aqueous synthesis yields large surface area tin oxide nanocrystals

Tin oxide is a critical component of optical devices, lithium batteries, and conducting coatings, and used as a catalyst besides many other applications. Development of tin oxide particles with high surface area is particularly critical for use in chemical sensors and dye-sensitive solar cells. Researchers from the National Institute of Advanced Industrial Science and Technology (AIST) in Japan have prepared tin oxide nanocrystals with unprecedented surface area using novel nanofabrication techniques.

As reported in the August issue of the *Journal of the American Ceramic Society* (DOI: 10.1111/j.15512916.2010.03680.x; p. 2140), Y. Masuda and co-workers prepared nanocrystals by crystallization in the aqueous phase with minimal application of heat. Previous methods for fabricating particles have typically involved high-temperature annealing that causes aggregation and deformation resulting in reduced specific



Transmission electron micrographs of tin oxide nanosheets prepared by precipitation from low-temperature aqueous solution. Reproduced with permission from *J. Am. Ceram. Soc.* **93** (8) (2010) DOI: 10.1111/j.1551-2916.2010.03680.x; p. 2140. © 2010 The American Ceramic Society.

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