Interface engineering of stable, efficient polymer solar cells

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Interface modification in polymer solar cells using chemically tailored self-assembled monolayers significantly enhances device performance.

Polymer solar cells are a promising source of low-cost renewable energy because of their potential for large-area solar-energy conversion. Over the past decade, key efforts to improve polymer solar-cell performance focused on understanding the device physics, optimizing the morphology of polymer blends through advanced processing methods, and developing high-performance materials. This led to very encouraging power-conversion efficiencies of 5–6%\(^1,2\). However, for practical applications, both device efficiency and stability need further improvements. Our ongoing research, therefore, focuses on optimization of the electrical contact at different interfaces and, equally important, development of advanced device structures.

We have fabricated polymer solar cells on the basis of two types of device structure. Conventionally, a polymer donor and a fullerene acceptor bulk-heterojunction (BHJ) composite layer is sandwiched between a high-work-function transparent indium tin oxide (ITO) anode and a low-work-function metal cathode. Upon illumination, photo-generated excitons dissociate at the donor-acceptor interface because of the difference in energy offset between both semiconductors. The charges drift under influence of the built-in electric field created by the work-function difference and are subsequently collected at the electrodes. Since low-work-function metal is vulnerable to oxidation in ambient air, electrode degradation is a major concern.\(^3\) To circumvent this problem, one can change the device architecture to an inverted structure in which a hole-blocking layer (such as titanium dioxide, TiO\(_2\), or zinc oxide, ZnO) is inserted between the ITO and the active layer for selective electron collection, while a more air-stable, high-work-function metal is used as the top electrode for hole collection.\(^4\)

In both types of architecture, the nature of the electrical contact at the electrodes is critical for device performance. Ohmic contact is required at both electrodes to optimize open-circuit voltage and contact resistance. We have developed a simple method to improve the performance of both conventional and inverted polymer solar cells by maximizing charge collection through surface modifications with tailored self-assembled monolayers (SAMs).

Figure 1. (a) Architecture of polymer solar cells with self-assembled molecule (mercaptoundecanoic acid)-modified zinc oxide (ZnO) nanoparticle film/metal bilayer cathodes. TiO\(_2\): Titanium dioxide. ITO: Indium tin oxide. PEDOT:PSS: Poly(3,4)thiophene/polystyrenesulfonate acid. C\(_{60}\): C\(_{60}\) fullerene. (b) Schematic illustration of the devices’ energy-level diagram with (i) ZnO/metal cathode and (ii) ZnO/self-assembled monolayer (SAM)/metal cathode. \(E_{\text{vac}}\): Vacuum energy. (c) Current-density-voltage characteristics and power-conversion efficiencies (\(\eta\)) of polymer solar cells made of silver (Ag), gold (Au), and aluminum (Al) with and without SAM-modified ZnO/metal cathodes measured under AM1.5 (airmass 1.5, average solar irradiance at sea level) illumination with a light intensity of 100mW/cm\(^2\).

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The cathode interface can be tuned by inserting a layer of solution-processable ZnO/SAM between the P3HT—poly(3-hexylthiophene)—and PCBM—[6,6]-phenyl C_{61} butyric acid methyl ester—BHJ film and a metal cathode: see Figure 1(a). Device performance was significantly improved, depending on the dipole direction and the SAM/metal chemical bonding: see Figure 1(b). SAMs that form unfavorable dipoles across the ZnO and metal thin films result in Schottky contacts characterized by poor device efficiencies. However, SAMs with appropriate dipoles generate Ohmic contacts and dramatically improved device efficiency and stability. High-work-function metals such as silver (Ag, 4.6eV) and gold (5.1eV) could be used as the cathode to reach high power-conversion efficiencies comparable to those of state-of-the-art polymer solar cells: see Figure 1(c).

Inverted-structure polymer solar cells using ITO modified with SAM-functionalized ZnO or TiO_{2} layers as the electron-collecting cathode and poly(3,4)ethylenedioxythiophene/poly(styrenesulfone acid (PEDOT:PSS)/Ag as the hole-collecting anode represent another effective technique to improve device performance. In general, charge recombination loss at the organic/inorganic interface significantly limits the performance of inverted-structure devices because of unfavorable energetics and a poor chemical interface. This loss can be prevented using a fullerene-based SAM: see Figure 2(a). Such a functional monolayer can serve multiple purposes, including enhancing interfacial exciton-dissociation efficiency, enabling passivation of inorganic-surface trap states, and optimizing upper organic-layer morphology. This approach can increase the performance of inverted devices by \sim 30% with power-conversion efficiencies as high as 5%: see Figure 2(b). Moreover, this new inverted device architecture enables the use of stable and printable materials as the top electrode (PEDOT:PSS/Ag), which improves device stability: see Figure 2(c). Under ambient testing conditions, unencapsulated flexible devices retain over 85% of their initial efficiency after 40 days, while conventional devices show negligible photovoltaic activity after only four days.

In conclusion, we have optimized the interface between metal oxide/metal and metal oxide/organic material in conventional and inverted polymer solar cells, respectively, using chemically tailored SAMs. The latter serve multiple purposes, including alignment of energy levels at interfaces, enhancement of interfacial exciton-dissociation efficiencies, and optimization of upper-organic-layer morphologies. This interface-engineering approach significantly improves the efficiency and stability of polymer solar cells and could enable large-area device manufacturing using low-cost, all-printable processes. Our ongoing research focuses on implementing these interface- and device-engineering strategies in new photovoltaic materials and tandem cells to further improve device performance, with a target efficiency of 10%.

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Hin-Lap Yip received his PhD in materials science and engineering from the University of Washington in 2008. His research focuses on material, device, and interface engineering of inorganic and organic hybrid materials for very-high-mobility transistors and efficient photovoltaic cells. He is currently leader of a team aiming to develop organic photovoltaic technology.
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Alex Jen is the Boeing-Johnson Chair Professor and department chair. He is also the founding director of the Institute of Advanced Materials and Technology. He was elected a fellow of the American Association for the Advancement of Science in 2005, the International Society of Optical Engineering in 2006, the Optical Society of America in 2007, and the Division of Polymeric Materials Science and Engineering of the American Chemical Society in 2008. He has co-authored more than 400 papers and 50 patents and inventions in the interdisciplinary areas of organic functional materials and devices for optoelectronics and photonics, and molecularly or biologically inspired self-assemblies for sensing and electronics.

References