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Interfacial Electronic Structures of Graphene
and Its Application in Organic Photovoltaic
Devices

石墨烯介面電子結構的研究及其在有機光
電器件中的應用

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Abstract

Organic photovoltaic (OPV) devices have attracted great interest due to their merits of low-cost, lightweight, ease of fabrication. While recent developments focused on pursuing high power conversion efficiency (PCE), the poor operational/storage stabilities of OPV devices comparing to Si-based solar cells hinder their wide application and commercialization. Therefore, further improvement of OPV stability is of importance. Under normal device operation, the OPV cells are expected to expose to sunlight and atmospheric conditions where oxygen and water can diffuse into the organic photoactive materials through the electrode/buffer layers. It can degrade the organic active materials and lead to device deterioration. While some reports have been devoted on the degradation of OPV devices, detailed degradation mechanisms are still not fully understood. It is due to the fact that the degradation processes can be taken place through many complicated pathways involving various interplaying factors. On the other hand, it is well recognized that performances of OPV devices depend strongly on the electronic structures of all involving organic interfaces. Therefore, considerable efforts have been made to improve the stability of the electronic interface via surface engineering.

One typical example of interfacial electronic engineering is the introduction of

bathocuproine (BCP) as an exciton-blocking layer (EBL) in between the photoactive layer and the cathode. However, the effects of ambient gases such as water and oxygen on the chemical or electronic structures and thus the charge transportation properties at the interface of BCP/C₆₀ are still unclear.

Here, we investigated the electronic structure of EBL/acceptor interface using ultraviolet photoelectron spectroscopy (UPS) and x-ray photoelectron spectroscopy (XPS). It was demonstrated that the interface is highly sensitive to oxygen and water moisture. After exposing the interface to ambient gases, the significant band bending in electronic levels of organic materials suggests (I) the formation of electron traps at the interface and (II) the decrease in electron barrier for reverse leakage current. From our results, we concluded that one effective way to improve the OPV device stability is to choose an EBL that can act as a gaseous diffusion barrier to surrounding oxygen and water moisture.

Another approach to improve the OPV device stability is to insert a modifying layer between the anode and the photoactive layer. Graphene, a hexagonal arrangement of carbon atoms forming a one-atom thick planar sheet, possesses unique and outstanding electrical, mechanical, optical, and chemical properties. It attracts widespread attention since its first report in 2004. Recent reports on large-area graphene fabrication by chemical vapor deposition (CVD) again raised the

growing interest of applying it in different optoelectronic devices. With its merits of its high transparency, good electrical conductivity, and mechanical robustness, it can be used as a transparent conductive electrode that replaces indium tin oxide (ITO). Upon oxidation, graphene can become soluble in water, and allow thin film formation using spin-coating method.

While most reports focused on the performance of graphene oxide (GO) in organic device, little attention have been made on its electronic energy levels, and electronic structures of the graphene (oxide)/organic semiconductor interfaces. In this work, we carried out comprehensive studies on the electronic structures of graphenes before and after oxidation process. The interfacial energy level alignments of graphene (oxide)/ organic semiconductor interfaces and charge-transfer processes were also examined.

We then fabricated OPV devices with graphene oxide (GO) used as anode buffer layers. Both the PCE and storage/operation stability of the OPV device can be dramatically enhanced by introducing the spin-coated buffer layer on ITO without any further treatment. We confirmed that the observed stability enhancement is attributed to the formation of diffusion barrier at buffer layer/anode interface which slows down degradation rates of the organic photoactive layers.

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