Improving the Performance of Titanium Dioxide / Polymer Solar Cell by Introducing Monolayers at the Interface

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Abstract: Solar cell comprising conjugated polymer with porous metal oxides that could serve as electron transporter is the theme of several recent researches because of the desirable properties possessed by the metal oxide such as its stability, better electron transport properties, ease of fabrication, low cost and environmental friendly as well as possibilities for controlling surface morphology. Although the hybrid metal oxide / polymer solar cells provide several merits, its photovoltaic power conversion efficiency is still poor compared to polymer / fullerene solar cells due to interfacial charge recombination. Suppressing recombination relative to charge transport is therefore a key issue in improving the device performance. This study focuses on strategies to control charge recombination kinetics by introducing a series of self-assembled monolayers (SAMs) of para-substituted benzoic acids with varying dipoles at the metal oxide-polymer interface in hybrid conjugated polymer / titanium dioxide (TiO_2) photovoltaic devices. The effects of all monolayers on current densities are in accordance with expected effect of the self-assembly monolayers. However, the effect of monolyers on open circuit voltage is quite unexpected from the interfacial energetics as all the monolayers improve the open circuit voltage suggest that the monolayer has an additional function. Overall device performance is enhanced by over 100% using a SAM with permanent dipole pointing towards the TiO_2 surface, compared to a control device with no interface modification. This study concludes that the SAM layer has two functions: (i) to shift the position of the conduction band of the porous TiO_2 relative to the polymer HOMO level so as to influence interfacial charge separation and (ii) to act as a barrier, insulating back electron transfer from the TiO_2 to the polymer. Both effects can benefit the performance of hybrid polymer metal oxide solar cells.

Keywords: Self-assembled-monolayer, Solar cells, Titanium dioxide