

Controlling recombination kinetics of hybrid poly-3-hexylthiophene (P3HT)/titanium dioxide solar cells by self-assembled monolayers

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Abstract

Self-assembled monolayers (SAMs) of benzoic acid based molecules are used to modify the metal oxide–polymer interface in a hybrid poly-3-hexylthiophene (P3HT)/TiO₂ photovoltaic device structure. The effect of SAMs on current density is in accordance with expectation from the driving force for charge separation of metal oxide–polymer interface in a hybrid poly-3-hexylthiophene (P3HT)/TiO₂ photovoltaic device. However, the effect of monolayers on open circuit voltage is quite unexpected from the interfacial energetics as all the monolayers improve the open circuit voltage in spite of different sign of the interfacial dipole for different SAMs. This suggests that the monolayers have additional functions. Overall device performance is enhanced by more than a factor of two using a SAM with permanent dipole pointing towards the TiO₂ surface or pointing towards polymer when compared to a control device with no interface modifiers. This study concludes that the SAM layer has two functions that are to shift the position of the conduction band of the porous TiO₂ relative to the polymer HOMO level so as to influence interfacial charge separation and to act as a barrier layer, insulating back electron transfer from the TiO₂ to the polymer. Both effects can benefit the performance of hybrid polymer metal oxide solar cells. © 2016, Springer Science+Business Media New York