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Energy level alignment regimes at P3HT and modified ITO interfaces: The influence of the substrate work function

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In organic based electronics the device performance and life time depend critically on the properties of both the active materials and their interfaces. In this work Photoelectron Spectroscopies have been utilized to characterize and determine the energy level alignment at interfaces of a hole-transporting organic semiconductor (P3HT) and ITO/polyoxometalate substrates. Polyoxometalates of Mo and W were deposited on ITO in order to tune the WF_{sub} from 4.4 eV up to 5.9 eV. Depending on the work function of the substrate, WF_{sub}, a transition between two different energy level alignment regimes has been observed: namely vacuum level alignment and Fermi level pinning (figure 1). The transition denotes the integer charge transfer state energy, E_{ICT+}, which represents the energy required to oxidize the organic polymer at the interface. Above this specific threshold value of 4.5 eV for P3HT, a spontaneous positive charge transfer across the interface to the organic semiconductor occurs. The charge transfer results in an interfacial dipole formation of a magnitude that scales with WF_{sub}. Within the Fermi level pinning regime, the barrier for hole injection remains constant and independent of the substrate work function, while within the vacuum level alignment regime, the barrier follows the Schottky- Mott limit behaviour, i.e., it scales linearly with the work function of the substrate. Thus, the charge-injection barriers can be reduced by modification of the electrode work function only within the limits established by the E_{ICT+} level.

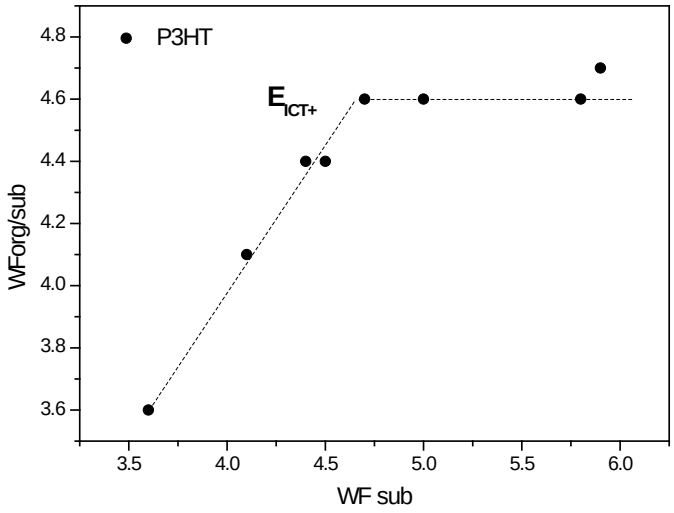

Figure 1. Evolution of work function of P3HT/sub ($WF_{org/sub}$) with respect to the work function of the substrate (WF_{sub}).