

Transition Metal Oxides as Hole Selective Interlayers in Organic Photovoltaics

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Organic photovoltaic (OPV) cells based on organic semiconductors (OSCs) can display the remarkable combination of low-cost fabrication, flexibility and performance characteristics tunability [1]. Interfacial layers are critical components of these devices as they are usually incorporated in one or both contacts to control the energy barriers for charge extraction, and consequently, the device performance. Transition metal oxides (TMOs) have been recognized as one of the most advantageous classes of materials used as anode and/or as cathode interfacial layers to enhance charge extraction between electrodes and organic molecules [2]. Especially molybdenum (MoO_x) and tungsten (WO_x) oxides have drawn enormous attention, due to the considerably ameliorated performance of OPVs, when they are employed as a hole extraction layers (HELs) [3]. Recently, under-stoichiometric molybdenum oxides MoO_x ($x < 3$), obtained by thermal evaporation or after annealing of stoichiometric MoO_3 films, were used to enhance hole injection and improve device stability in bulk heterojunction polymer solar cells [2]. The device improvement was attributed to increased n-type conductivity exhibited by these oxides, originated from oxygen vacancies, which give rise to band gap electronic states.

Herein, we demonstrate the beneficial incorporation in OPV cells of molybdenum and tungsten oxides, deposited in hydrogen environment using a simple and cost-effective hot-wire deposition method. These oxides were found to be under-stoichiometric with precise stoichiometry, electronic properties and increased n-type conductivity [2]. Indeed, deposition of Mo oxides in hydrogen environment significantly reduces the electrical resistivity of the films, as it can be deduced from Figure 1. At room temperature the resistivity values for stoichiometric MoO_3 and under-stoichiometric MoO_{3-x} 10 nm thick films, deposited in oxygen and hydrogen environment respectively, were found 400 Ohm·cm and 6.0 Ohm·cm, respectively, which are about two orders of magnitude different. Moreover, resistivity of under-stoichiometric Mo oxides increases with temperature, which is an evidence for metallic-like behaviour, while for MoO_3 the opposite trend was observed. To take advantage of the increased conductivity of under-stoichiometric Mo oxides, next polymer solar cells based on poly(3-hexylthiophene) and [6,6]-phenyl-C71-butyric acid methyl ester blended active layer (P3HT:PC71BM) and incorporating Mo oxides as hole selective interlayers were fabricated and characterized. The device structure is shown in Figure 2. These devices presented large improvement in their short-circuit current (J_{sc}), open-circuit voltage (V_{oc}), fill factor (FF) and external quantum efficiency (PCE) when embedding the under-stoichiometric MoO_{3-x} compared to the devices with MoO_3 HELs (from 6.4 mA cm⁻², 0.52 V, 0.35, 1.05 % to 10.4 mA cm⁻², 0.65 V, 0.50, 3.4 % as it is obtained from J-V curves presented in Figure 3). Similarly, large improvement in OPVs embedding under-stoichiometric WO_{3-x} for hole extraction was observed, as presented in Figure 4, where photocurrent and dark J-V characteristics of devices with tungsten oxide layers of different stoichiometry, are presented. This work demonstrates the unique potentials of hydrogen deposited Mo and W oxides as an advanced class of metal oxide based functional materials with tailored electronic and physical properties for use as highly efficient charge exchange layers in optoelectronic devices.

Acknowledgments

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Figures

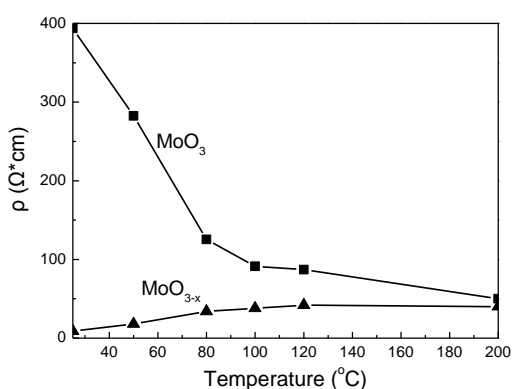


Figure 1 Resistivity measurements vs temperature of stoichiometric and under-stoichiometric MoO_3 .

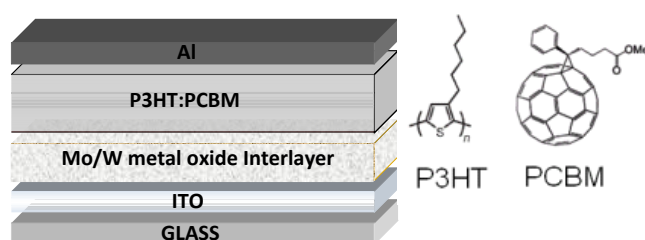


Figure 2 Organic photovoltaic device architecture and materials chemical structures

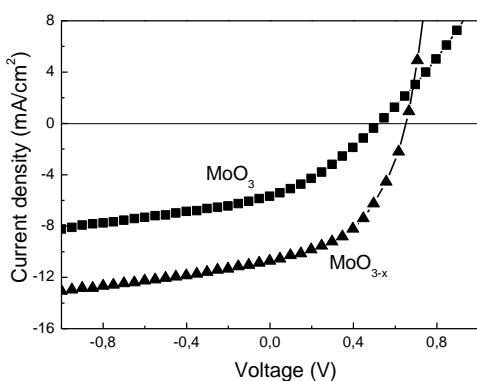


Figure 3 Current density versus voltage characteristics for P3HT:PCBM BHJ devices embedding 10 nm Mo oxide hole extracting layers.

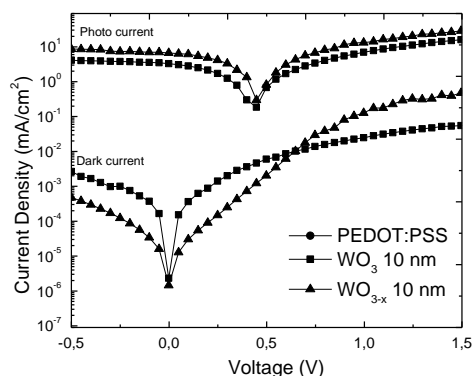


Figure 4 Photocurrent and dark current J-V curves of OPV cells based on P3HT:PC₇₁BM photoactive layer and with a 10 nm thick tungsten oxide layer of different stoichiometry.