About MoO3 as buffer layer in organic optoelectronic devices, Technology Letters

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Résumé en anglais	MoO_3 is well known as efficient anode buffer layer in optoelectronic devices. Actually, MoO_3 can be easily deposited under vacuum, by sublimation for instance, and also by wet process. So it is known from a long time that the films deposited by sublimation are amorphous and slightly oxygen deficient, which induces a light blue coloration due to oxygen vacancies. These oxygen vacancies imply the presence of Mo^{4+} and Mo^{5+} in the films. The presence of oxygen vacancies increases the conductivity from 10^{-12} to 10^{-6} $(\Omega cm)^{-1}$, while stoichiometric films are insulating and MoO_2 has a metallic like behaviour with s = 2 10^2 $(\Omega cm)^{-1}$. About the efficiency of MoO_3 as buffer layer, recent studies questioned the MoO_3 band structure generally admitted. Under ultra high vacuum, the measured ionisation energy, IE, and electron affinity are found to be 9.7 eV and 6.7 eV respectively, while the films are strongly n-type. Its means that the very large IE energy of the MoO_3 excludes any hole transport via the valence band, while the energy alignment between the band conduction minimum, CB, of MoO_3 and the Highest Occupied Molecular Orbital (HOMO) of the organic material is favourable for electron transfer between the two materials. In the case of organic photovoltaic cells, the photogenerated hole recombines with an electron at the interface between MoO_3 and the organic layer. Indeed, the work function, WF, of the molybdenum oxide films depends strongly of its composition, WF decreases when the oxygen deficiency increases, and on the exposition, or not, of its surface to air contamination. This makes that WF varies from 6.9 eV for a layer studied under ultra high vacuum to 5.2 eV for a layer exposed to the air a few hours. However, since the initial value of WF is very high, MoO_3 remains effective if the Highest Occupied Molecular Orbital of the organic material is lower than 6 eV. The band structure of MoO_3 and the large possible variations of WF make that, for specific conditions of preparation and conditioning, MoO_3 can also be used as CBL.

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