Modeling C-V and J-V characteristics of HTM-free perovskite solar cells

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In pace with the enhancement of stability[1], the influence of defects in perovskite based solar cells (PSCs) can be weakened down to an acceptable level, while the band offsets at hetero-junction remain to be one of the major factors impeding high Incident Photon-to-electron Conversion Efficiency (IPCE)[2]. In our work, drift-diffusion and small signal models[3] are used to study PSCs without hole transport material (HTM)[4]. The aim is to better understand the device operation and the effect of the band offset at the hole collector side. As shown in Figure 1, the theoretical static band alignment is calculated for a lightly n-doped[5] $CH_3NH_3PbI_3$ layer sandwiched between heavily n-type doped TiO_2 and hole collector Au layers. The basic current-voltage (J-V) characteristic is reproduced as shown in Figure 2. The bimolecular recombination and trap-assisted recombination models are employed. In Figure 3, capacitance-voltage (C-V) characteristic is presented in comparison with experimental data. An interfacial layer is introduced into the architecture to fit the C-V experimental curve. The C-V characteristic is discussed in detail following a Mott-Schottky analysis. The influence of the work-function (WF) of hole collector metal (HCM) on the performance of HTM-free PSCs is considered. A high efficiency of 14% is expected when the WF of HCM is larger than 5.5 eV.

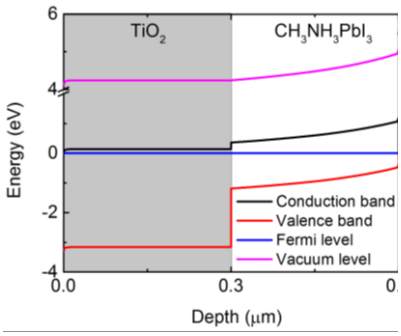

Fig. 1. Static band alignment

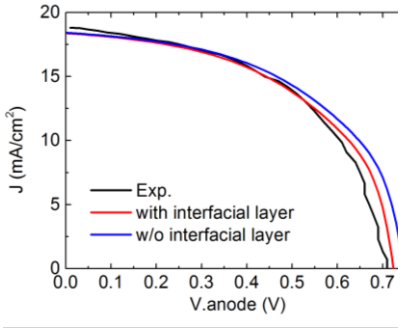

Fig. 2. J-V characteristics under 1 sun illumination of HTM-free PSCs

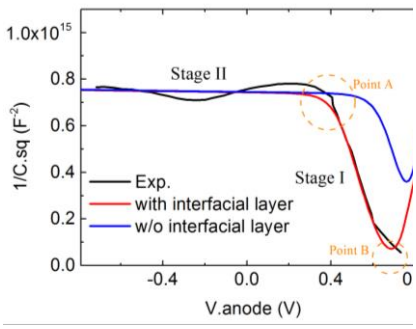

Fig. 3. C-V characteristics in dark of HTM-free PSCs

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