Light Soaking Effect on Band Bending of the $MAPbI_3$-Based Perovskite Solar Cell with Nano-ZnO as Electron-Transport Material

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Perovskite-based solar cells (PSCs) have attracted a lot attention over the past few years in academy and industry because of its excellent power conversion efficiency (PCE%) and low-cost fabrication. Electron transporting materials (ETMs) used in PSCs play a crucial role in PSCs performance by compensating the difference of diffusion lengths between holes and electrons, and serve as a block layer to prevent holes transported from the perovskite active layer. Compared with TiO_2, ZnO has advantages to act as ETM for PSCs due to its higher electron mobility and low-cost fabrication. In this work, $CH_3NH_3PbI_3$ ($MAPbI_3$) active layers (400nm) were spin-coated on two kinds of ZnO ETMs, ZnO thin film (ZnO_{film}) and ZnO nanoparticles (ZnO_{nano}), with surface roughness of 24.6nm and 12.9nm, respectively. Our preliminary results reveal that the roughness of $MAPbI_3$ is obviously influenced by roughness of its bottom layer ($MAPbI_3/ZnO_{film}$ and $MAPbI_3/ZnO_{nano}$ with surface roughness of 20.1 nm and 8.4 nm, respectively), which further affects the PSCs performance drastically (with PCE% as 7.2% to 15.4%, respectively). To understand the mechanism behind PCE% enhancement and change of electronic structure under light expose, we utilized hard X-ray photoelectron spectroscopy (HAXPES) cooperated with xenon lamp as a solar simulator to investigate the real band bending behaviors on the electronic structure of $MAPbI_3$ under light soaking. In our results, the valence band maximum (VBM) of $MAPbI_3$ on ZnO_{nano} have a downward band bending under light expose. However, we observe that the VBM of $MAPbI_3$ on ZnO_{film} is pinned under light expose. The Pb 4*f* and I 4*d* core-level spectra of $MAPbI_3/ZnO_{film}$ have a lower-binding-energy shift as compared to those of $MAPbI_3/ZnO_{nano}$, which indicates a smaller concentration ratio of PbI_2/MAI and hence a PbI_2-poor surface in $MAPbI_3/ZnO_{film}$. However, the XRD results show a clear reflection of PbI_2 in $MAPbI_3/ZnO_{film}$, which originates from the bulk region in $MAPbI_3$. In summary, PbI_2 is possibly existed at/near the $MAPbI_3/ZnO_{film}$ interface, which causes a higher barrier between $MAPbI_3$ and ZnO_{film}. Insufficient PbI_2 in $MAPbI_3$ would lead to the creation of detects in its crystal matrix, which increases the recombination probability of electron-hole pairs and results in fermi level pinning under light expose. On the other hand, ZnO_{nano} served as ETM can suppress the formation of PbI_2 due to its flat surface roughness, which has a benefit to obtain a better quality of $MAPbI_3$ crystal structure and hence can observe the band bending behavior under light expose.