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Electronic structures at the interface between Au and $CH_3NH_3PbI_3$[1] CONGCONG WANG, University of Rochester, XIAOLIANG LIU, Central South University, CHENGGONG WANG, University of Rochester, LU LYU, Central South University, ZHENGGUO XIAO, CHENG BI, JINSONG HUANG, University of Nebraska-Lincoln, YONGLI GAO, University of Rochester
— Organometal trihalide perovskite ($CH_3NH_3PbI_3$)-based solar cells have been developed rapidly in decades. The electronic properties of interfaces formed between Au and $CH_3NH_3PbI_3$ are investigated with ultraviolet photoemission spectroscopy (UPS), X-ray photoemission spectroscopy (XPS) and inverse photoemission spectroscopy (IPES). The two-step method prepared $CH_3NH_3PbI_3$ film, coated onto the poly (3,4-ethylenedioxythiophene) poly (styrenesulfonate) (PEDOT:PSS)/indium tin oxide (ITO) substrate, presents n-type semiconductor behavior with a band gap of 1.7 eV and a valence band (VB) edge of 1.0 eV below the Fermi energy (E_F). There is an interface dipole of 0.1 eV at $CH_3NH_3PbI_3$/Au interface. The energy level of $CH_3NH_3PbI_3$ is lifted ca.0.4 eV with Au coverage of 64 Å upon it, resulting in band bending and a built-in field in $CH_3NH_3PbI_3$ that encourages hole transport to the interface. Hole accumulation near the interface facilitates the hole transfer from $CH_3NH_3PbI_3$ to Au. Furthermore, the decreasing offset between the VB maximum of $CH_3NH_3PbI_3$ and the E_F indicates a decrease of energy loss as extracting holes from $CH_3NH_3PbI_3$ to Au coverage.

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