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The Surface Electronic Structure of Hybrid Organo Lead Bromide Perovskite Single Crystals

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The electronic structure and band dispersion of methylammonium (MA = $CH_3NH_3^+$) lead bromide, $CH_3NH_3PbBr_3$, has been investigated through a combination of angle-resolved photoemission spectroscopy (ARPES), Fig. 1 and 2, and inverse photoemission spectroscopy (IPES), Fig. 2, as well as theoretical modeling based on density functional theory (DFT). The experimental band structures are consistent with DFT calculations. The results demonstrate the presence of a dispersive valence band in $MAPbBr_3$ that peaks at the $\bar{M}$ point of the surface Brillouin zone (SBZ), Fig. 1. The results also indicate that the surface termination of the $MAPbBr_3$ is the methylammonium bromide (MABr) layer, discussed in our presentation. We find our results support models that predict a heavier hole effective mass in the region of -0.23 to -0.26 m_e, along the $\bar{\Gamma}$ (SBZ center) to $\bar{M}$ point of the SBZ edge. The surface appears to be n-type as a result of an excess of lead in the surface region.

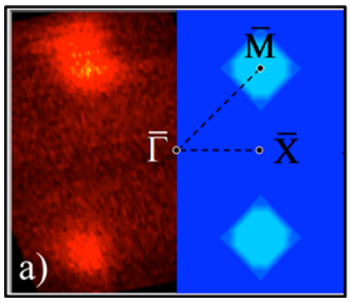

Fig. 1 2-dimensional iso-energy band mapping in k-space, for experimental (left) and bromide terminated theoretical (right) results.

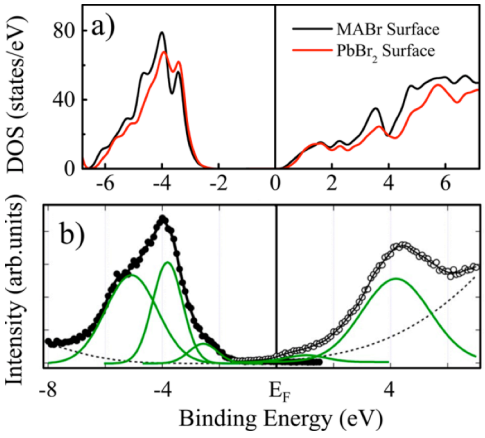

Fig. 2. Combined density of occupied and unoccupied states. (a) The calculated density of states (DOS) for two possible surface terminations of $MAPbBr_3$: MABr (black line) and $PbBr_2$ (red line). (b) The corresponding experimental results from photoemission taken at a photon energy of 23.5 eV (filled circles) and inverse photoemission (open circles). The green lines indicate a possible fit of the experimental data. The calculated DOS in (a) is shifted to match the main experimental peak at binding energy −4 eV and the band gap is adjusted to the experimental bulk band gap. Binding energies are given in terms of E - E_F.