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A Combined Theoretical and Experimental View on Valence and Conduction Band Densities of States of Lead Halide Perovskites LEEOR KRONIK, Weizmann Institute of Science, Israel, JAMES ENDRES, Princeton University, DAVID A. EGGER, MICHAEL KULBAK, Weizmann Institute of Science, Israel, ROSS A. KERNER, LIANFENG ZHAO, SCOTT H. SILVER, Princeton University, GARY HODES, Weizmann Institute of Science, Israel, BARRY P. RAND, Princeton University, DAVID CAHEN, Weizmann Institute of Science, Israel, ANTOINE KAHN, Princeton University — We present results for the valence and conduction band density of states (DOS), measured via ultraviolet and inverse photoemission spectroscopies for three lead halide perovskites. Specifically, the DOS of $MAPbI_3$, $MAPbBr_3$, and $CsPbBr_3$, grown on different substrates, are compared. Theoretical DOS, calculated via hybrid density functional theory and including spin-orbit coupling, are compared to experimental data. The agreement between experiment and theory, obtained after correcting the latter for quantitative discrepancies, leads to the identification of valence and conduction band spectral features. In particular, this comparison allows for precise determination of the energy position of the band edges, namely ionization energies and electron affinities of these materials. We find an unusually low DOS at the valence band maximum (VBM) of these systems, which confirms and generalizes previous findings of strong band dispersion and low DOS at the VBM of $MAPbI_3$. This calls for special attention when using electron spectroscopy to determine the frontier electronic states of lead halide perovskites.
[1] Endres et al., J. Phys. Chem. Lett. 7, 2729 (2016)

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