

First determination of the valence band dispersion of $\text{CH}_3\text{NH}_3\text{PbI}_3$ hybrid organic-inorganic perovskite

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Organic-inorganic hybrid perovskites are promising absorber materials for low-cost photovoltaic solar cells or optoelectronic devices [1-5]. Among these perovskites, methylammonium triiodideplumbate ($\text{CH}_3\text{NH}_3\text{PbI}_3$, MAPbI_3 or MAPI) exhibits currently the highest efficiency. Here we have analyzed the structural transition in MAPI by X-ray diffraction at the β phase and we have correlated it to its electronic properties. Despite all the extensive work on hybrid organic-inorganic halide perovskites, their experimental band structure measured with k-resolution has remained elusive. Such an experimental determination is a necessary requirement for an accurate theoretical description and understanding of the system. The impact of the structural phase transitions on the band structure in the operation temperature range of solar cells needed also to be elucidated. Herein, we present the experimental determination of the band structure of MAPI with k resolution by angle-resolved photoemission at 170 K [6]. Our results show that the spectral weight is strongly affected by the cubic symmetry although traces of the tetragonal band structure are appreciated. Some deviations with respect to theoretical calculations are observed, which may help to reach a more precise description of this paradigmatic system of the hybrid perovskite family. The project leading to this application has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 687008 (GOTSolar).

References

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