Poster Presentation

MS088.P05

Assessment of alternative space groups for $MAPbI_3$ at room temperature.

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Methyl ammonium lead iodide (MAPbI3) is one of the most prominent and most promising solar absorber materials for non-silicon solar cells. As part of the research efforts in the group of Prof. Schorr, [1] we were most intrigued by the different space groups reported for MAPbI3 at room temperature. While I4/mcm is most commonly given as space group for MAPbI3 at room temperature, [2] other space groups, however, such as I4/m, I4cm and I422 are also found in the literature. We believe that it is more than necessary to give a conclusive overview as to why we believe I4/mcm is the correct space group assignment.

The correct space group attribution is of great importance for a greater audience, due to the tremendous research efforts in the field and the importance of this space group assignment for the desired application. One might think, at first sight, that this discussion is of purely academic importance, but the correct space group assignment for MAPbI3 is in fact crucially important: The alternative space group assignments are made in non-centrosymmetric space groups (e.g. I4cm) or even chiral space groups (I422) and a correct attribution is therefore key to the possibility of phenomena such as piezoelectricity or second-harmonics generation. [3]

This discussion will be of twofold nature: first, we are presenting the crystallographic basis and relationship between the space groups in question to establish a better understanding of the matter as such and secondly, we will present alternatives for the explanation of those effects that have led to the attribution of lower space group symmetries (e.g. the Renninger effect). For this, we are combining a critical assessment of crystallographic studies given in lower space group symmetries from published data with our own experiments specifically targeted at identifying the symmetries in this compound, for instance neutron Laue diffraction and ψ-scans on symmetry breaking reflections to evaluate the possibility of Umweganregung. Further, we will emphasise on the assessment of refined crystal structures, for instance through the use of tools such as Checkcif.

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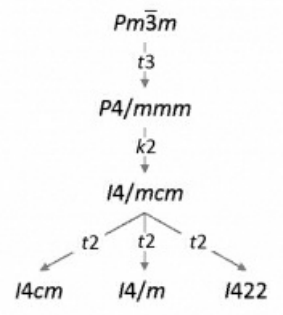
[2] Poglitsch, A., Weber, D. (1987). J. Chem. Phys. 87, 6373–6378.
[3] G, S. et al. (2016). J. Phys. Chem. Lett. 7, 2412–2419.



Keywords: Hybrid Perovskite, Crystallographic Symmetry, Data Analysis