Contribution ID: **308** Type: **Talk (17 + 3 min)**

Exploring The Structure of MAPbI3 Across its Phase Diagram Using Neutron Spectroscopy, Thermophysical Properties and First-Principles Simulations –A Closer Look at High Pressures

Tuesday, 21 March 2023 12:10 (20 minutes)

Hybrid Organic-Inorganic Perovskites (HOIPs) have attracted an unprecedented attention as promising candidates for the next-generation of photovoltaic materials due to their exceptional energy conversion rates. Moreover, a better understanding of their remarkably soft atomic structures and their stabilization mechanisms is still necessary [1,2]. In this contribution we present an extensive study on the structure of the prime example of HOIPs methylammonium lead iodide ($MAPbI_3$) using a wide variety of radiation-scattering techniques validated by first-principles simulations across the temperature and pressure axes. We shall first introduce a model-selection protocol using inelastic-neutron scattering, thermophysical properties like the heat capacity, and density-functional theory simulations [3]. This protocol was successfully implemented for $MAPbI_3$, showing that an alternative *P1* structure is statistically sounder than the crystallographic *Pnma* model. Furthermore, we present the first results of high-pressure radiation-scattering experiments performed on $MAPbI_3$ together with a new set of extensive ab initio molecular dynamics simulations. These findings will pave the way towards a better understanding of the fundamental yet scarcely explored role played by pressure in the stability of $MAPbI_3$.

[1] K. Druzbicki et al. J. Phys. Chem. Lett., 7(22), 2016
[2] J. Breternitz et al. Angew. Chem. Int. Ed. 59(1), 2019
[3] P. Marín-Villa et al. J. Phys. Chem. Lett., 13(36), 2022

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Session Classification: Energy Materials

Track Classification: Chemistry of Materials (Structure and Spectroscopy)