

Cation Dynamics as a Probe of Local Structure in 3D Hybrid Perovskites: Insights from High-resolution Inelastic Neutron Scattering

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Organometal Halide Perovskites (OHPs) have emerged as a prospective class of materials holding great promises for efficient conversion of solar energy. While understanding their atomic structure and dynamics is critical to rationalize their exceptional photovoltaic performance and improve their environmental and operational stability, this task remains a formidable challenge for both crystallography and spectroscopy.[1-5] In this contribution, we present a novel, complementary strategy developed to explore the local structure around the organic cations, owing to the superb sensitivity of Inelastic Neutron Scattering (INS) to hydrogen motions.[6,7] We also provide an overview of the application of the developed methodology combining broadband high-resolution INS experiments (TOSCA, ISIS; LAGRANGE, ILL) with state-of-the-art ab initio modelling beyond the harmonic picture (AIMD), to interrogate local structure in the archetypal iodoplumbate-OHP, MAPI, across its pressure-temperature phase diagram and under chemical pressure induced by cation engineering.

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Primary author: Dr DRUZBICKI, Kacper (Materials Physics Center, CSIC-UPV/EHU)

Co-authors: Mr MARIN VILLA, Pelayo (Materials Physics Center, CSIC-UPV/EHU); Dr GABOARDI, Mattia (Elettra–Sincrotrone Trieste S.C.p.A.); Dr ARMSTRONG, Jeff (ISIS Facility, Rutherford Appleton Laboratory); JIMENEZ-RUIZ, Monica (ILL); IVANOV, Alexandre (ILL); Dr ARAUZO, Ana (Instituto de Nanociencia y Materiales de Aragón (INMA), CSIC-Universidad de Zaragoza); Prof. FERNANDEZ-ALONSO, Felix (Materials Physics Center, CSIC-UPV/EHU)

Presenter: Dr DRUZBICKI, Kacper (Materials Physics Center, CSIC-UPV/EHU)

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