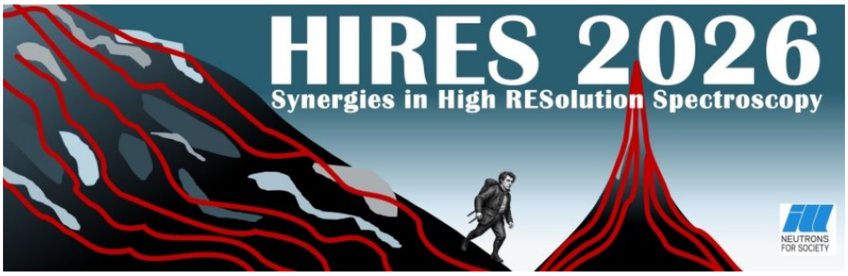

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Atom-scale dynamics in germanium-based hybrid metal halide perovskites

Metal halide perovskites (MHPs) are currently receiving great attention because of their photophysical properties and concomitant promise for use in both solar cells and light emitting diodes, however, fundamental properties surrounding the atomic-scale dynamics remain unclear for these materials. In this contribution, we report on results from inelastic and quasielastic neutron scattering (INS and QENS) studies of the dynamics in the Ge-based hybrid MHPs MASn1-xGexI3, (x = 0, 0.25, 0.5, 0.75, 1; MA = methylammonium) and FAGeX3 (FA = formamidinium; X = I, Br). Of specific interest here, the Ge ions exhibit a polar off-centering distortion and it is of great interest to understand how this affects the materials' dynamical and photophysical properties.

For MASn1-xGexI3, the results show two modes of MA reorientations, with different geometry and time-scale, and that the pace of reorientations increases with increasing Sn concentration. The vibrational frequencies trend in the opposite direction and are related to the space group rather than directly to the Sn concentration, highlighting the importance of the structure. For FAGeX3, several vibrational modes related to the inorganic framework at 20 meV and below of FAGeI3 are blue-shifted compared to FAGeBr3, while several modes above the phonon gap at 65 meV and above are red-shifted, indicating that the type of halide ion influences the external (librational) and internal (vibrational) modes of the organic cation differently. Given the strong correlation between dynamics and electronic and optical properties of hybrid MHPs, such as charge carrier dynamics and photoluminescence etc., this new insight is important for the rational design of hybrid MHPs with specific functions.

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