Contribution ID: **131** Type: **Invited Talk**

Understanding static and dynamic local structure in Hybrid Metal Halide Perovskites

Local atomic structure often differs from the global average structure as measured with diffraction and yet the local structure has a profound impact on materials functionalities. This structure-function relationship applies in many materials classes, ranging from organics to Li-ion battery cathodes to oxide and halide perovskites. Accurately characterizing this local structure has proven challenging but recent advances in neutron and X-ray diffuse scattering ("between"Bragg peaks) has enabled local structure determination.

In this talk, I will discuss the importance of local structure and how this can be quantified and will demonstrate this for organic-inorganic hybrid halide perovskites [1,2]. These materials are a recently re-invigorated class of semiconductors that have demonstrated very high efficiencies for solar cells after just over a decade of research. While the importance of lattice dynamics and dynamical (dis)order have been recognized in these materials, their nature is only poorly known and understood. We used X-ray and neutron diffuse scattering coupled with molecular dynamics to quantify the nature, size, and time scale associated with dynamical local order in CH3NH3PbI3 and CH3NH3PbBr3 perovskites. We observe that the nominally cubic perovskite consists of dynamical, two-dimensional sheets of lower symmetry tetragonal regions of about 3 nm diameter with several picosecond lifetimes. The implications for halide perovskite optoelectronic properties will be discussed.
[1] NJ Weadock et al., Joule 7, 5, 1051-1066 (2023)
[2] DM Ladd, unpublished.

Topical Area

Hard matter: energy materials

Author: TONEY, Michael (University of Colorado Boulder)

Presenter: TONEY, Michael (University of Colorado Boulder)