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Structure and Dynamics of hybride perovskites: insights by neutron scattering

Organic (A) metal (B) halide (X) perovskites (ABX_3) are an enchanting class of semiconductor materials giving new possibilities of developing highly efficient, low-cost and stable single and multi-junction solar energy conversion devices. These compounds consist of an organic molecule i.e $CH_3NH_3^+$ (methylammonium abbreviated as MA), Pb on B-position and halides (I, Cl, Br) on X position. Compositional engineering is found to be a fruitful strategy for band gap tuning and obtaining hybride perovskites with enhanced optoelectronic properties.

To understand the origin of their PV performance, it is essential to first understand the crystal structures of the hybrid perovskites, characterized by structural phase transitions, considerable static or dynamic disorder, and unknown concentrations of various defects such as halogen anion or organic cation vacancies. The organic portion makes neutrons particularly useful in such investigations given their sensitivity to hydrogen and ability to distinguish clearly between carbon and nitrogen.

The presentation will show an overview of our studies on MAPI using complementary neutron and synchrotron X-ray powder diffraction as well as our first investigations of the molecule dynamics by quasielastic neutron scattering (QENS)

We are aim to extend our studies to solid solutions obtained by cation and anion mutation to gain understanding of the interrelationship of static and dynamic structure of the material.