Metal Halide Perovskites for Solar Photovoltaic Applications: A Neutron Perspective

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Perovskites and neutron scattering share a long history that dates back more than 50 years. Early neutron inelastic scattering studies provided fundamental insights into the mechanism that drives the structural phase transitions in classic perovskite oxides such as $SrTiO_3$, $BaTiO_3$, and $PbTiO_3$ through measurements of soft phonons. The deceptively simple ABX_3 perovskite structure can host a wide variety of different cations/anions on the A and B/X sites, respectively, which spawn a remarkable range of physical properties including insulating and metallic behavior, magnetism, ferroelectricity, and superconductivity. In 2009, Kojima *et al*. published a study of metal halide perovskites (*J. Am. Chem. Soc.* **131**, 6050) in which an organic cation ($CH_3NH_3^+$) resides on the A site, and these materials showed promise in photoelectrochemical cells. In just over 10 years, this finding has fueled an intense research effort into perovskite solar cells, the efficiencies of which (25.5%) now nearly eclipse the best values measured with single-crystal Si cells (26.1%). In this talk, I will discuss the insights that neutron inelastic scattering has brought to this subject. Measurements on single-crystal $CH_3NH_3PbI_3$ and $CH_3NH_3PbCl_3$ reveal extremely short acoustic phonon lifetimes that are 50 to 500 times shorter than those in conventional semiconductors such as Si, GaAs, and CdTe. Such short lifetimes imply an inability to dissipate heat efficiently and are consistent with the very low thermal conductivity. Given the central importance of electron-phonon coupling to the cooling and transport of photoexcited electrons, these very short phonon lifetimes suggest a plausible explanation for the long carrier lifetimes that have been reported in these materials. Similar neutron measurements on fully inorganic analogues such as $CsPbCl_3$ and $CsPbBr_3$ will also be discussed.