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Neutron Scattering Studies of Hybrid Perovskites for Photovoltaic Applications MICHAEL CRAWFORD, University of Delaware, PAMELA WHITFIELD, NIINA JALARVO, GEORG EHLERS, Spallation Neutron Source, Oak Ridge National Laboratory, MADHUSUDAN TYAGI, NIST Center for Neutron Research, NORMAN HERRON, DuPont Electronics and Communication Technologies, LYNDA JOHNSON, DuPont Performance Materials, WILLIAM GUISE, Advanced Photon Source, Argonne National Laboratory, IVAN MILAS, DuPont Company, YONGQIANG CHENG, LUKE DAEMEN, ANIBAL RAMIREZ-CUESTA, KATHARINE PAGE, XIAOPING WANG, FENG YE, Spallation Neutron Source, Oak Ridge National Laboratory — Hybrid perovskites (ABX_3) have attracted a great deal of attention as light absorbers for photovoltaics. Here the A site is occupied by organic cations, for example methyl ammonium, $CH_3NH_3^+$; the B site is occupied by metal cations, for example Pb^{2+}; and the X site is occupied by halogen anions: I^-, Br^-, or Cl^-. Typical of perovskites, these materials exhibit structural phase transitions involving rotations or tilts of the BX_6 octahedra, but with the added complexity that the inorganic framework is coupled to order-disorder transitions of the organic cations. We have used neutron scattering techniques to characterize the vibrations and dynamics of several of these compounds as a function of temperature, including samples where the hydrogen atoms are partially or fully substituted by deuterium. Combined with the results of density functional theory calculations, these studies contribute to our understanding of the excellent photovoltaic properties of these materials.

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