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Neutron and X-Ray Scattering Studies of Hybrid Perovskites for Photovoltaic Applications MICHAEL CRAWFORD, DuPont Company, PAMELA WHITFIELD, NIINA JALARVO, GEORG EHLERS, SNS, Oak Ridge National Laboratory, MADHUSUDAN TYAGI, NIST Center for Neutron Research, NORMAN HERRON, LYNDA JOHNSON, DuPont Company, WILLIAM GUISE, DuPont Company and APS, Argonne National Laboratory, IVAN MILAS, DuPont Company, YONGQIANG CHENG, LUKE DAEMEN, ANIBAL RAMIREZ-CUESTA, KATHARINE PAGE, XIAOPING WANG, FENG YE, SNS, Oak Ridge National Laboratory — Hybrid perovskites (ABX_3) have attracted a great deal of attention recently as light absorbers for photovoltaics. In these materials the A site is occupied by organic cations, for example methyl ammonium (MA) or formamidinium (FA) cations, the B site is occupied by metals, for example Pb or Sn, and the X anions are halogens (I, Br, or Cl). Typical of perovskites, these materials exhibit a series of 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 structures and dynamics of several of these compounds as a function of temperature. In addition, high resolution synchrotron x-ray diffraction measurements have been performed to investigate the structural phase transitions. These studies yield a detailed picture of the structures, dynamics, and structural phase transitions of these compounds, and provide a firm basis for understanding their excellent photovoltaic properties.

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