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Crystal Structures of a Photovoltaic Two-Dimensional Perovskite

DEPEI ZHANG, TIANRAN CHEN, Department of Physics, University of Virginia, ALEXANDER CHEN, Department of Chemical Engineering, University of Virginia, CRAIG BROWN, LELAND HARRIGER, NIST Center for Neutron Research, National Institute of Standards and Technology, MINA YOON, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, JOSHUA CHOI, Department of Chemical Engineering, University of Virginia, SEUNG-HUN LEE, Department of Physics, University of Virginia — Arguably the biggest challenge of the high-efficiency perovskite solar cells, such as $CH_3NH_3PbI_3$ and $CH(NH_2)_2PbI_3$, is their device instability. A recent study[1] of two dimensional (2D) perovskite compounds, $(CH_3(CH_2)_3NH_3)_2(CH_3NH_3)_{n-1}Pb_nI_{3n+1}$, proposed a solution to this problem. This class of materials shows a maximum photovoltaic efficiency of 12.52%, without any degradation over 2250 hrs of standard light illumination, or 650 hrs of 65% relative humidity test. In this talk, we present our neutron scattering experiments to study the crystal structure of the 2D 3-layer perovskite (n = 3) as a function of temperature. We have observed two phase transitions between 12 K and 370 K. Rietveld refinements as well as the first principle calculations were used to determine the structures of all three phases.

[1]Tsai, Hsinhan, et al. "High-efficiency two-dimensional RuddlesdenPopper perovskite solar cells." *Nature* 536.7616 (2016): 312-316.

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