Local structure of lead halide perovskites for photovoltaic applications

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Fabricating high-efficiency, low-cost and long-term stability solar cells is of significant importance to solve energy problems. Recently, hybrid inorganic−organic lead halide perovskites, with the general formula of ABX3 (A = CH3NH3+, ; B = Pb2+; X = I—, Br—), have become promising for easy fabrication and high power conversion efficiency. The high symmetry of the parent perovskite structure ABX3 can be reduced by orientational disorder of methyl ammonium (MA) cations, rotation and distortion of BX6 octahedra. Since this disorder appears to be fundamental to the improved properties of these devices, understanding the crystal structures and phase transitions of perovskite materials can aid in enhancing performance of perovskite materials. Herein, we combine neutron total scattering with Reverse Monte Carlo (RMC) modelling to investigate the rotational disorder of the MA cations. For comparison, we have also studied the inorganic analogue CsPbI3 to give information on the effect of different cations within the perovskite structure, and hence to understand this family's structural flexibility.