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First-principles prediction of a stable hexagonal phase of $CH_3NH_3PbI_3$ ARASHDEEP THIND, XING HUANG, ROHAN MISHRA, Washington Univ — Methylammonium lead iodide ($CH_3NH_3PbI_3$ or $MAPbI_3$) is a promising photovoltaic material with high power conversion efficiency. However, its experimental perovskite phases show poor thermodynamic stability. Using first-principles density functional theory, we predict a hexagonal (*2H*) phase with $P63mc$ space-group symmetry to be the thermodynamically most stable phase. The *2H*-phase consists of infinite chains of face-shared PbI_6 octahedra with organic MA cations taking up the space between the chains, which is in contrast to the corner-connected octahedra observed in the experimental orthorhombic, tetragonal, and cubic phases. It has a negative formation enthalpy, independent of the choice of exchange correlation functional used in the calculations. The absence of soft-phonon modes in the *2H*-phase demonstrates its dynamical stability. The *2H*-phase has an indirect band gap of 2.6 eV, which is ˜1 eV larger than the direct band gap of orthorhombic phase. The change in octahedral connectivity favors strongly anisotropic charge transport. Overall, the *2H*-phase presents a new route to overcome the stability issues in $MAPbI_3$.

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