Supporting Information

Superalkali halide perovskites with suitable direct band gaps for photovoltaic applications

Tingwei Zhou, Anlong Kuang*

Chongqing key Laboratory of Micro&Nano Structure Optoelectronics, School of Physical Science and Technology, Southwest University, Chongqing 400715, China
Corresponding Author *Email: twzhou@swu.edu.cn

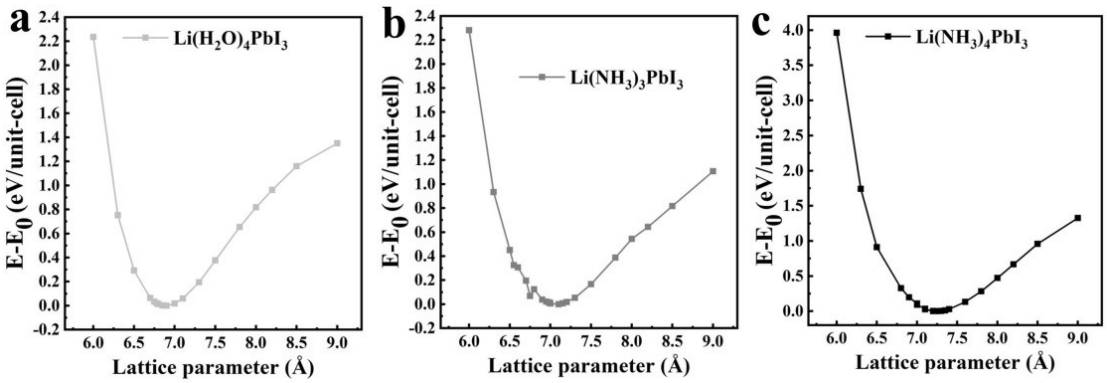

Fig. S1 (a-c) The energies of the cubic $Li(H_2O)_4PbI_3$, $Li(NH_3)_3PbI_3$ and $Li(NH_3)_4PbI_3$ perovskites with different lattice parameters, their lowest energies are set to 0 eV/unit-cell, respectively.

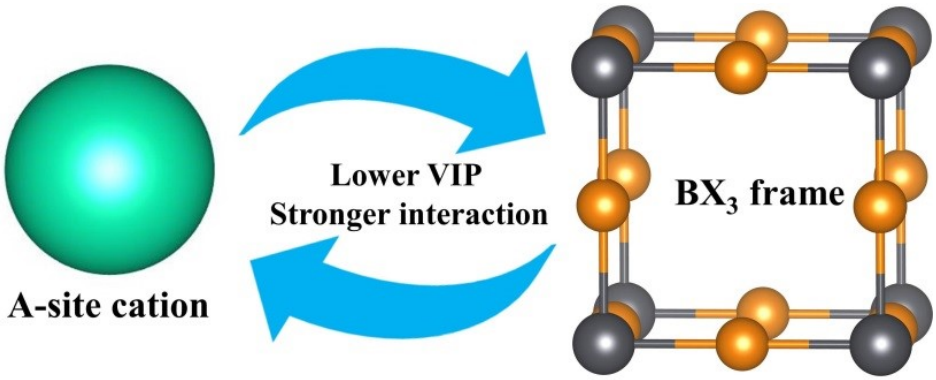

Fig. S2 The diagram of A-site cations and the BX_3 frame for the AMI_3 (A = Cs, $Li(H_2O)_3$, $Li(H_2O)_4$, $Li(NH_3)_3$ and $Li(NH_3)_4$, M = Sn and Pb) perovskites.

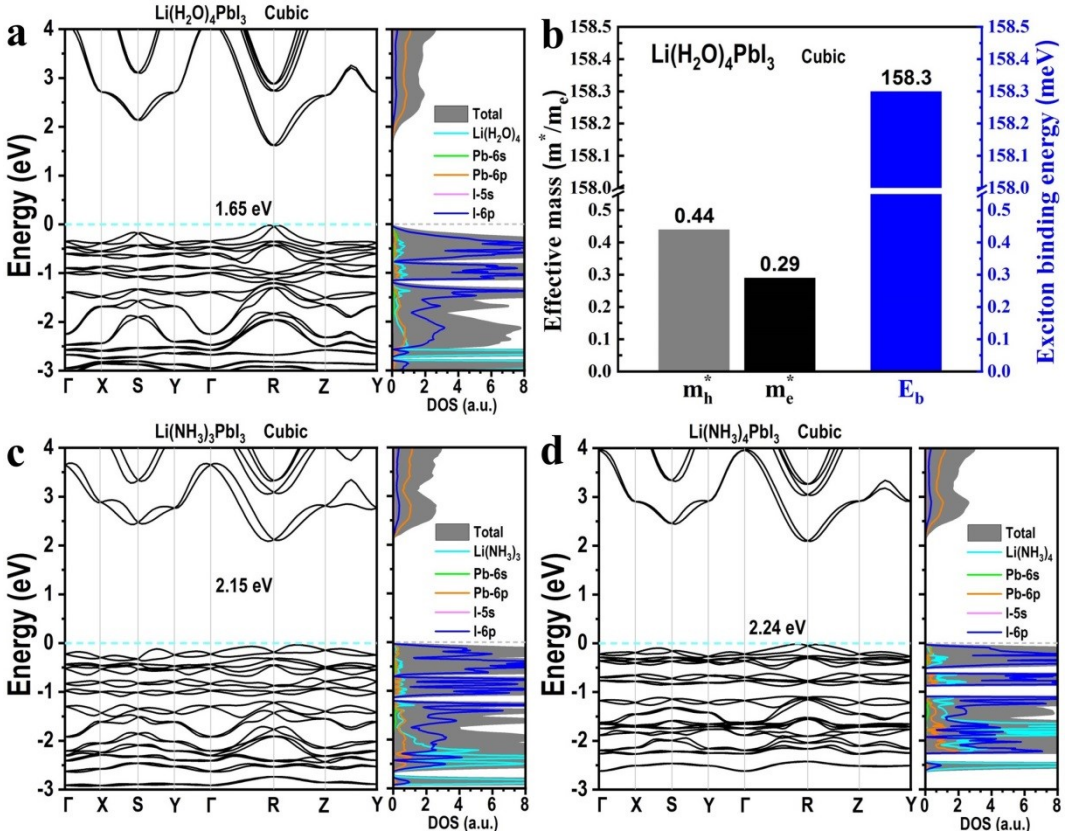

Fig. S3 (a, c, d) The band structures, and total and partial DOSs for the cubic $Li(H_2O)_4PbI_3$, $Li(NH_3)_3PbI_3$ and $Li(NH_3)_4PbI_3$ perovskites, respectively. The dotted line represents Fermi level, which is set to zero. (b) The hole and electron effective masses $\left(m_h^* \; and \; m_e^*\right)$ and exciton binding energy (E_b) of the cubic $Li(H_2O)_4PbI_3$ perovskites, respectively.

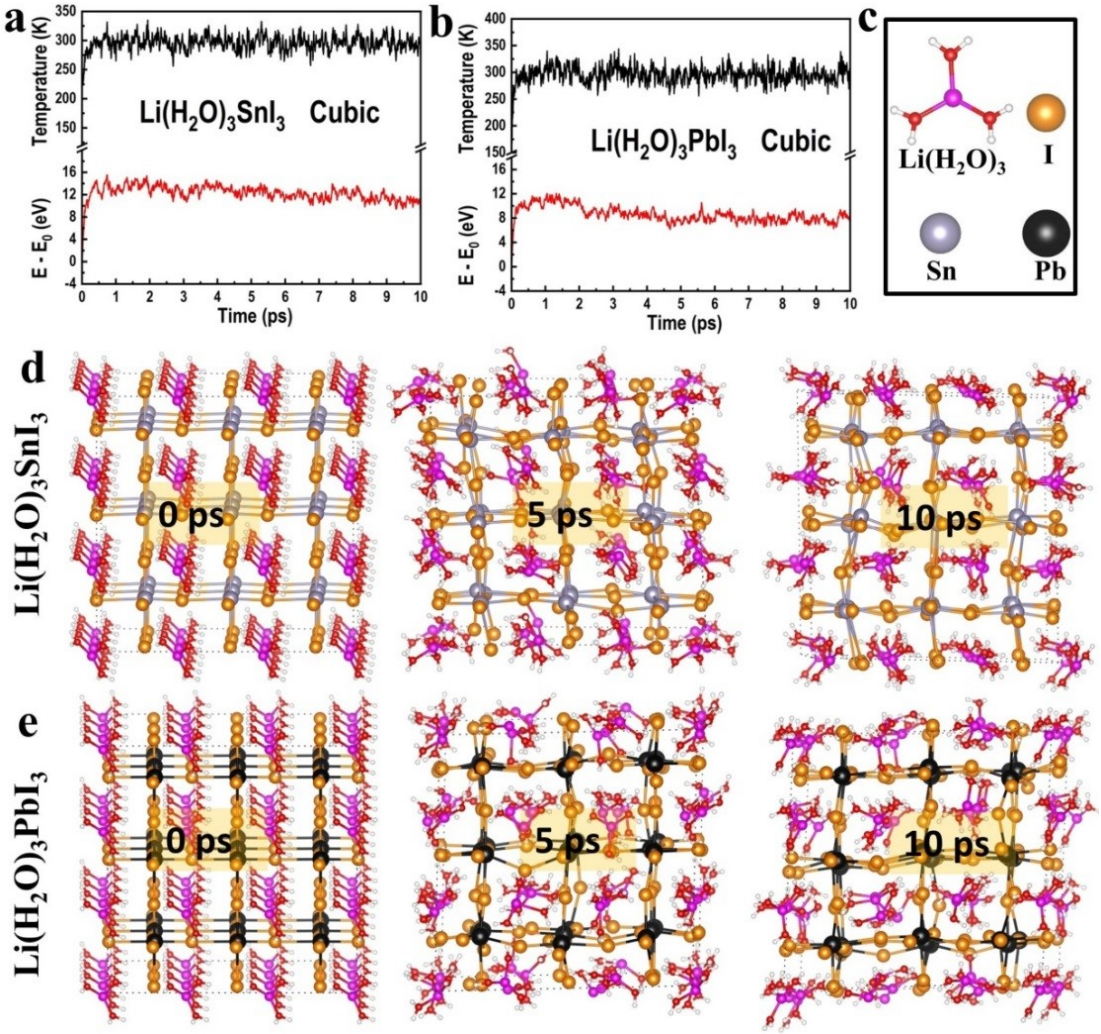

Fig. S4 The AIMD simulated energy and temperature curves (a,b) and structures (d,e), the cubic $Li(H_2O)_3SnI_3$ and $Li(H_2O)_3PbI_3$ perovskites with a 3×3×3 supercell under 300 K and 10^5 Pa, respectively. Here, $Li(H_2O)_3$, I, Sn and Pb is shown in the insert (c). Atomic colors: H (white), Li (purplish red), O (red), I (orange), Sn (silver) and Pb (black).