Supplementary Information for " Ineffectiveness of Formamidine in Suppressing Ultralow Thermal Conductivity in Cubic Hybrid Perovskite $FAPbI_3$"

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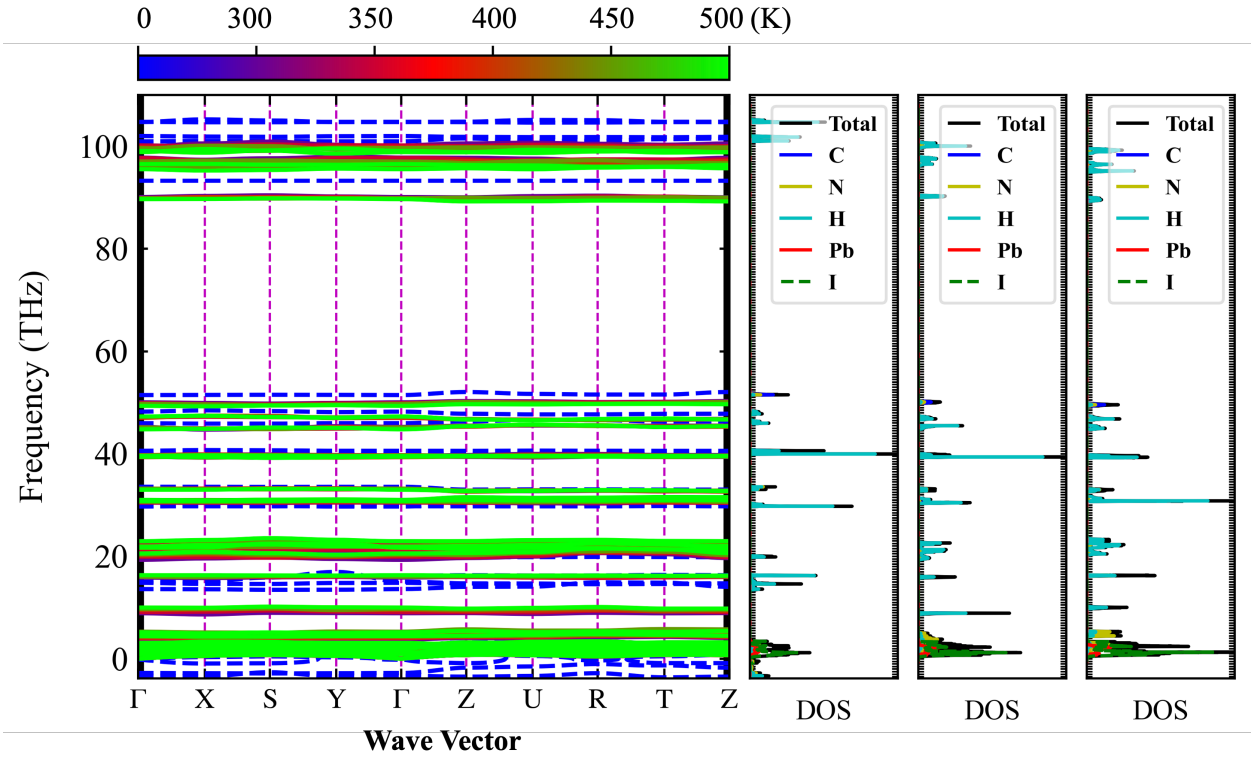
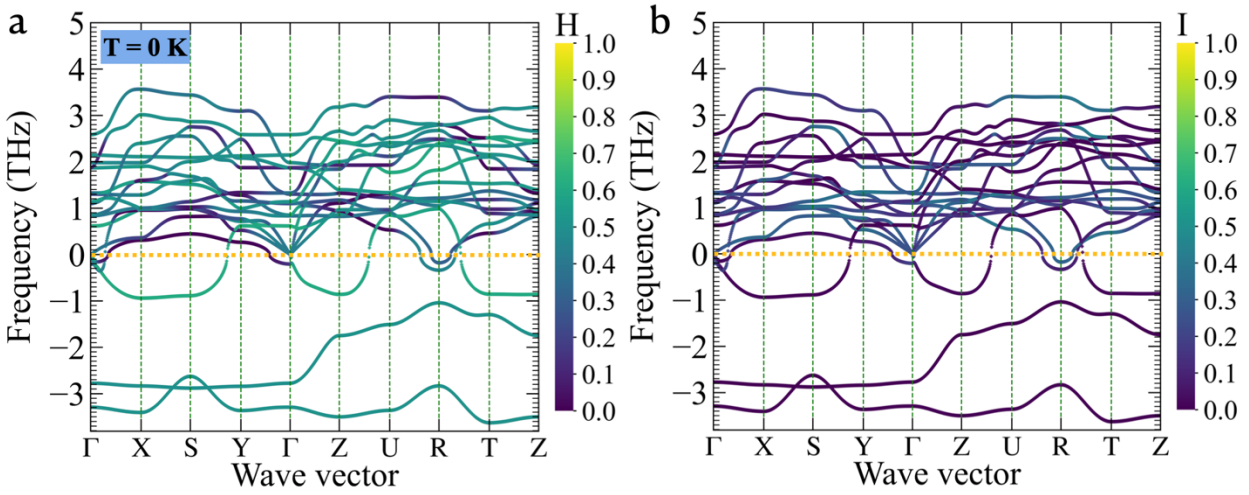
Supplementary Figures

I. Full phonon dispersions and DOS



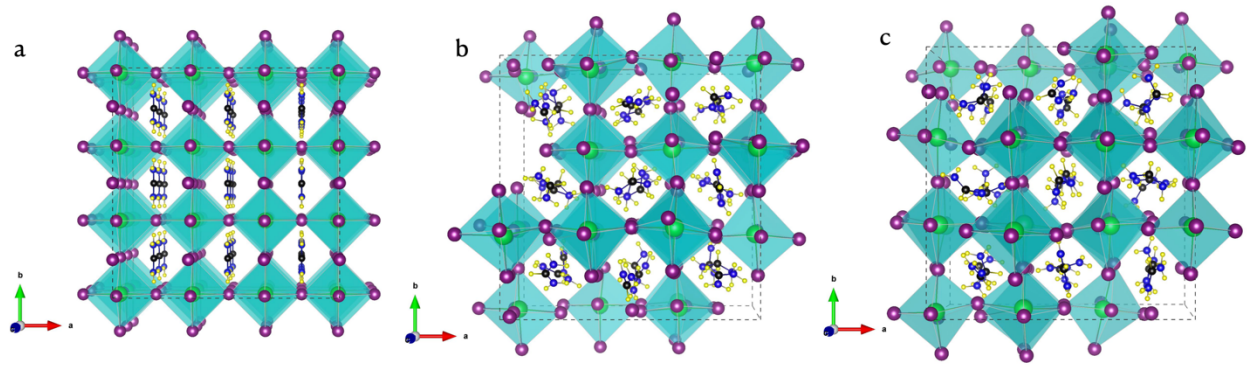
Supplementary Figure 1. Left panel: Comparison of finite-temperature phonon dispersions calculated from 300 to 500 K with those obtained from the harmonic approximation treatment at 0 K. right panel: Atom-decomposed partial and total phonon density of states (DOS) calculated at 0 K, 300 K, and 500 K, respectively.

II. Atomic Participation Ratio



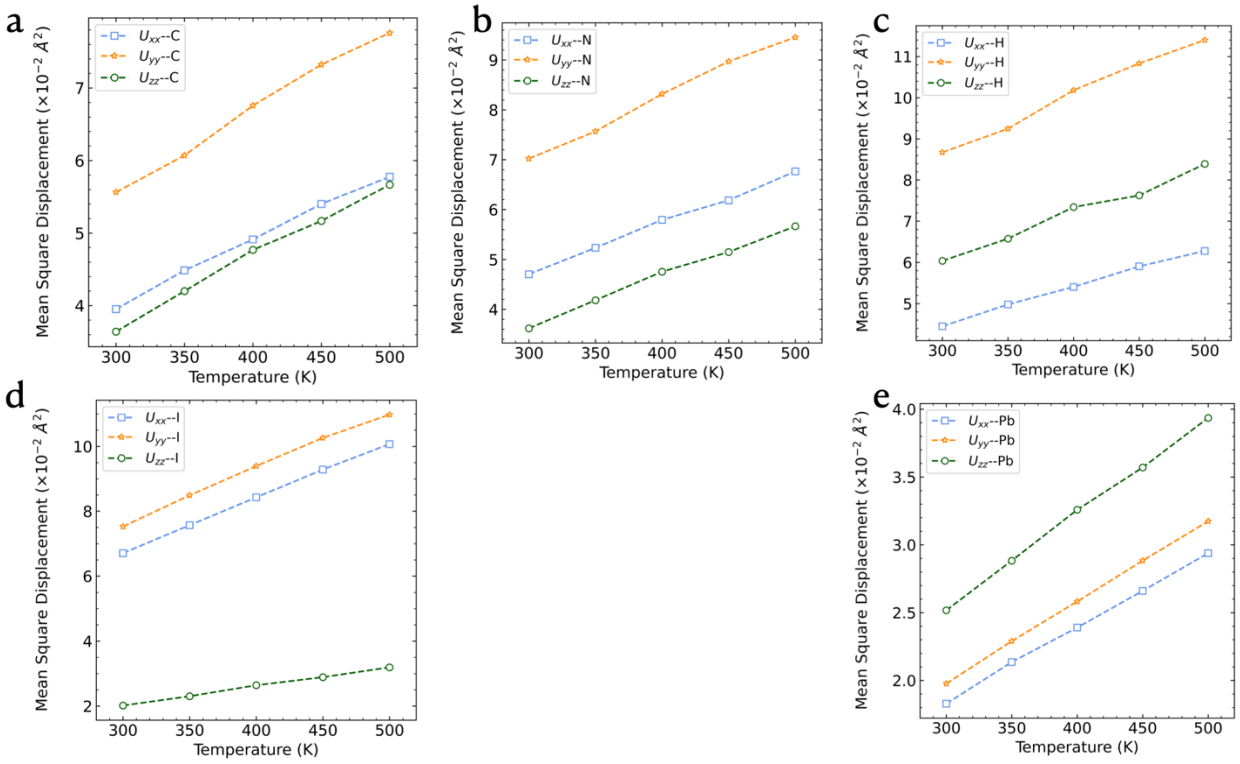
Supplementary Figure 2. (a) The color-coded atomic participation ratio (APR) of cubic crystalline $FAPbI_3$, projected onto the phonon dispersions along the high-symmetry paths at 0 K. The fraction displayed in the color bar indicates the atomic participation ratio of Hydrogen (H) atom on specific phonons. (b) The same as (a), but for iodine (I).

III. AIMD trajectories at 300 K



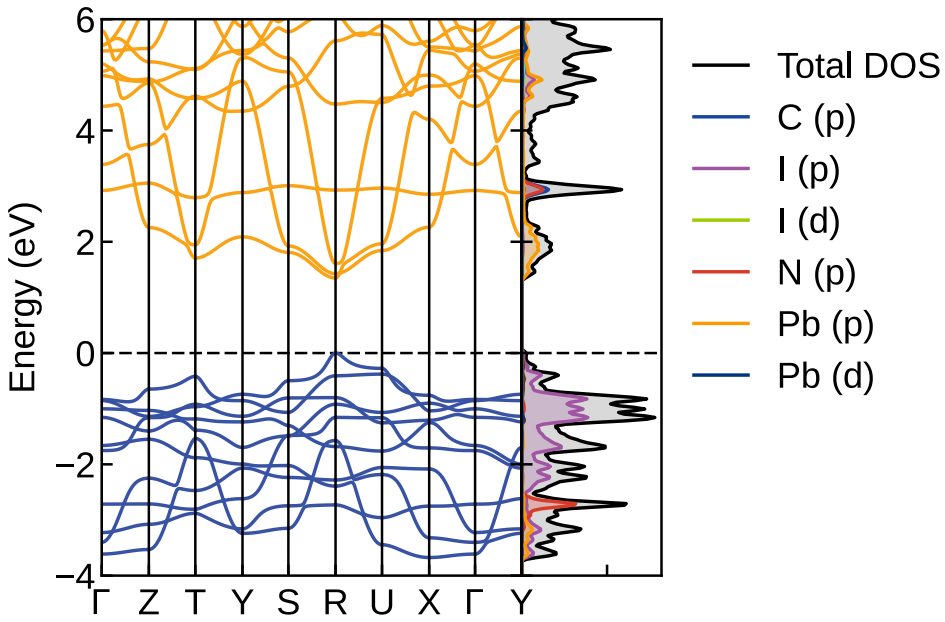
Supplementary Figure 3. (a) The equilibrium supercell of cubic $FAPbI_3$. (b) Calculated Snapshot of cubic FAPbI3 at 300 K, taken at step 2,500 of the AIMD simulation using the NVT ensemble. (c) Calculated Snapshot of cubic FAPbI3 at 300 K, taken at step 5,000 of the AIMD simulation using the NVT ensemble.

IV. Temperature-dependent mean-squared displacement



Supplementary Figure 4. (a) Calculated temperature-dependent atomic mean-squared displacements along different axis for C atom within the temperature range of 300 to 500 K. (b) The same as (a), but for N atom. (c) The same as (a), but for H atom. (d) The same as (a), but for I atom. (e) The same as (a), but for Pb atom.

V. Full Electronic Band Structure and DOS



Supplementary Figure 5. (a) Left panel: calculated electronic band structure. Right panel: Calculated atom-decomposed partial and total electronic density of states (DOS).