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First-principles determination of the structural, vibrational, and thermodynamic properties of Methylammonium Lead Iodide Perovskite WISSAM SAIDI, University of Pittsburgh, WISSAM SAIDI TEAM — Intrinsic energy-loss processes in solar cells ultimately increase the operational temperature, which can have profound effect on the power conversion efficiency of solar cells. Here I report investigations on the temperature effects on structural and mechanical properties of $CH_3NH_3PbI_3$ using well-converged first-principles calculations with van der Waals dispersion corrections. The computed lattice parameters for cubic and tetragonal phases *at finite temperature* are found within 1% of experimentally measured values. Furthermore, the finite-temperature potential energy surface shows how the mechanical properties of the cubic and tetragonal phases of $CH_3NH_3PbI_3$ evolve with temperature. Finally, I discuss the implications of these calculations on the nature of the tetragonal-to-cubic phase transition, and show that the underpinnings of this transition can be largely attributed to the phonons associated with methylammonium cations.

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