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Anharmonicity in Hybrid and Inorganic Perovskite Materials used for Photovoltaics Applications

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Hybrid organic-inorganic perovskite materials have emerged over the past five years as absorber layers for new high-efficiency yet low-cost solar cells that combine the advantages of organic and inorganic semiconductors. Despite this sky rocketing evolution, the physics behind the electronic transport in these materials is still poorly understood.

Here, employing the linear response (DFPT) approach of Density Functional Theory (DFT) and frozen phonon calculations, we reveal strong anharmonic effects in the inorganic CsPbI₃ perovskite structure compared to the hybrid CH₃NH₃PbI₃ (MAPbI₃) material, and found a double-well instability at the center of the Brillouin Zone. We show that previously reported¹ soft modes are stabilized at the actual lower symmetry equilibrium structure, which occurs in a very flat energy landscape. These findings highlight the crucial role played by temperature in these materials, showing that this perovskite structure can oscillate between two equilibrium states at room temperature. Taking into account these low energy-highly occupied phonon states into the models used for electron-phonon interactions² and band gap calculations³ could lead to a better understanding of the electrical transport properties of perovskite solar cells.

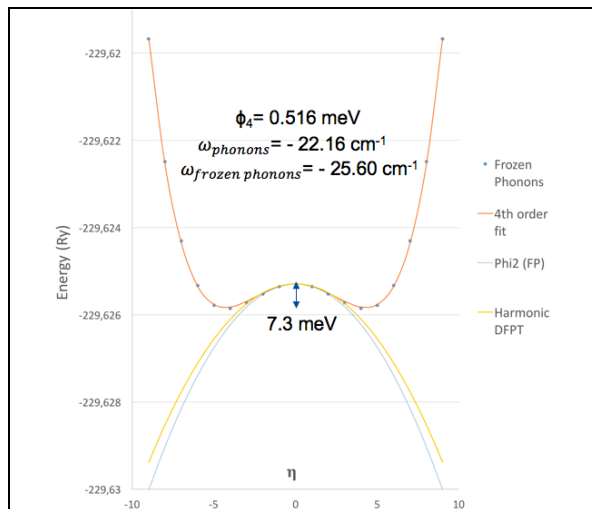


Figure 1: Potential-energy surface from frozen phonon energy calculations of cubic CsPbI₃ for the soft phonon mode at Γ versus the displacement parameter η . The maximum displacement ($\eta = 10$) corresponds to around 0.8 Å.

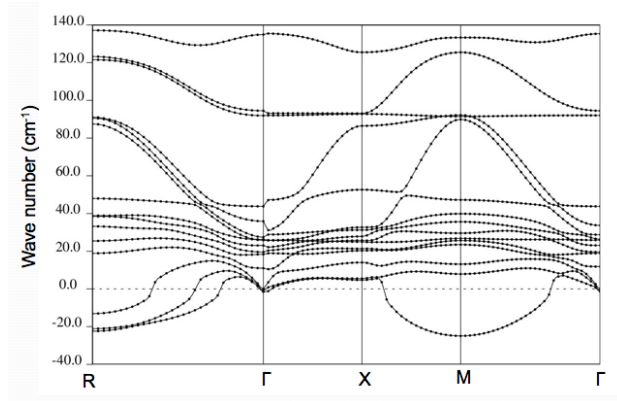


Figure 2: Phonons modes of cubic CsPbI₃ at the new equilibrium position determined in Fig. 1. Using both a tight convergence threshold and the results of our frozen phonon calculations allowed us to remove the soft modes at Γ .

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