**First-Principles Study of Phonon Anharmonicity in CsPbBr3**

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Halide perovskites ABX3 (A=CH3NH3,Cs; B=Pb,Sn; X=Cl,Br,I) have attracted significant attention in recent years for their excellent optoelectronic properties. Both organic-inorganic (A=CH3NH3) and all-inorganic (A=Cs) halides perovskites have been investigated for potential applications in light- and energy-harvesting devices such as photovoltaics and thermoelectrics. Recent experimental studies have shown that the lattice thermal conductivity of CH3NH3PbI3 is unusually low (~ 0.5 W/mK), which was attributed to the rotational motion of the guest molecule. However, a similar value of has also been reported in CsPbX3, which is free from the rotational degree of freedom of the guest molecule. While several theoretical studies on CsBX3 have been reported so far, the origin of the ultralow is still an open question.



Figure: Calculated phonon dispersion curves of three phases of CsPbBr3.

To elucidate the microscopic origin of the ultralow of halide perovskites, we have investigated phonon anharmonicity and thermal conductivity of CsPbBr3 by using accurate first-principles methods. To see the effect of the structural phase transition on phonon anharmonicity, we have compared thermal conductivities of three different phases of CsPbBr3: cubic, tetragonal, and orthorhombic (see Fig.). For the high-temperature phases, we have conducted the self-consistent phonon (SCP) calculations [1,2] to obtain the well-defined stable phonons at finite temperature. We will show the temperature dependence of phonon frequencies and lattice thermal conductivity of CsPbBr3 and discuss the origin of the ultralow .

References:

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