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(Research Article)
Phonon transport analysis of $CsCaX_3$ (X=Cl, Br) perovskites using the density functional theory

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Abstract

Phonon transport of CsCaBr3 and CsCaCl3 halide perovskites was investigated to identify their potential applications in various fields including cooling and thermoelectric. Ab-initio studies of these materials were performed in their cubic phase in generalized gradient approximation. Second and third order force constants were calculated with supercell approach and phonopy and phono3py packages. Lattice constant was obtained 5.463 and 5.768 the for CsCaCl3 and CsCaBr3 respectively. From a comparison of electron density and phonon properties, it was found that the halide atom in both compounds plays an important role in phonons' propagation, while calcium atom has a negligible role in phonon scattering and phonon group velocity. Phonon velocities of both materials at intermediate frequencies (between 2 and 4 THz) are 5000 and 3000 m/s, and their phononic lifetime is 0.2 and 0.1 ps, for CsCaCl3 and CsCaBr3, respectively. Due to the higher phonon transport of CsCaCl3 in almost frequency and with a difference of 2000 m/s in the middle frequency range, it is predicted to be more effective in applications requiring higher acoustic and thermal conductivity. However, CsCaBr3 is expected to be useful in thermoelectric applications owning to rattling motion and consequently higher phonon scattering of Cs atom in CaBr6 cages.

Keywords: Perovskite, Phononic transport, Phonon group velocity, Phonon scattering, Phonon lifetime.

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