

Lattice dynamics in perovskite halides CsSnX$_3$ with X=I,Br,Cl
LING-YI HUANG, WALTER LAMBRECHT, Case Western Reserve Univ — We investigate the origin of the phase transitions between the cubic, tetragonal and orthorhombic phases of CsSnX$_3$, X=I, Br,Cl, in terms of the imaginary phonon frequencies of the higher symmetry phases at the zone boundaries and the associated rotations and tilts of the SnX$_6$ octahedra. We present first-principles calculations of the phonon band-structure and density of states as well as the predicted infrared spectra. The calculations are done using density functional perturbation theory. In the cubic phase, there are three triply degenerate IR active $T_{1u}$ modes and one silent $T_{2u}$ mode. We find that the calculated modes agree with the experiment when we assign the second and third calculated modes to the experimental first and second modes. Our calculated IR spectra show that the third observed mode in IR absorption is actually the highest LO rather than TO mode and the lowest calculated mode is found to overlap in frequency with a peak in density of phonon states. This indicates the possibility of a strong phonon-phonon interaction and hence short phonon-lifetime or strong broadening which could explain why this mode has not been observed.

Ling-Yi Huang
Case Western Reserve Univ

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