

Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Lattice dynamics in perovskite halides CsSnX_3 with $\text{X}=\text{I,Br,Cl}$
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 , $\text{X}=\text{I, Br,Cl}$, 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

Date submitted: 14 Nov 2013

Electronic form version 1.4