Abstract Submitted
for the APR20 Meeting of
The American Physical Society

Intrinsically Localized Lattice Vibrations in Crystalline Lattices. BENJAMIN AGYARE, Stockton University — We examined the formation of Intrinsically Localized Modes (ILMs) for a pair of harmonic phonons along the direction [111] of the Sodium Iodide (NaI) crystalline lattice. The tendency for ILMs to form at a certain center-of-mass momentum q and corresponding relative momentum vector k is attributed to the van-Hove singularities condition in the non-interaction two-phonon density of states continuum. We observed that, as q converges to the high-symmetry point L=q (π, π, π) of the Brillouin zone, the relative momentum vector k remains invariant at k($\pi/2$, $\pi/2$, $\pi/2$) for a certain threshold value of q, and coalesces at the upper-edge of the two-phonon density of states spectrum with high degeneracy in the two-phonon critical energy. We conclude that the excitation spectra of the pairs of harmonic phonon excitations become energetically degenerate past the threshold q value towards L at the invariant vector k, announcing the strong presence of ILMs. The calculated ILMs were observed at critical energies of 20.0 meV and 25.0 meV for the spring coupling constants ratios 0.598 and 0.202 respectively. Reports of Inelastic Neutron Scattering experiments have identified one-phonon breather excitations energy of 10.2 meV at elevated temperatures of 555 K. The formation of ILMs, or multi-phonon bound states, is expected to arise as a result of the anharmonic interactions that lift these degeneracies to enhance the formation of ILMs.

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Date submitted: 10 Jan 2020 Electronic form version 1.4