

Abstract Submitted  
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**Investigating Intrinsically Localized Vibrations in crystalline lattices using van-Hove singularities.** BENJAMIN AGYARE, Stockton University, PETER RISEBOROUGH, Temple University — Sodium Iodide has a rock salt structure. Intrinsically Localized Modes (ILMs) have supposedly been observed in NaI but only for wave-vectors at the corner of the 3-D Brillouin Zone. It has been suggested that, for high-symmetry  $q$  vectors, several van Hove singularities may converge at one critical energy producing a large peak in the two-phonon density of state spectrum and giving rise to ILMs with these  $q$  values. First, we fit the experimentally determined acoustic and the optic phonon modes using a nearest neighbor and a next-nearest neighbor force constants. We find that the two-phonon density of states, for fixed  $q$  exhibits non-divergent van Hove singularities. The energies of these features vary as  $q$  is varied and we have identified the  $q$  values at which the two-phonon density of states is enhanced. We intend to introduce anharmonic interactions and examine if it can bind the two-phonon excitations to produce a quantized ILM.

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