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Using van Hove singularities of the two-phonon density of states to investigate the intrinsically localized vibrations of NaI crystal. BENJAMIN AGYARE, Physics Program, Stockton University, Galloway NJ Department of Physics, Temple University, Philadelphia PA, PETER RISEBOROUGH, Department of Physics, Temple University, Philadelphia PA — Intrinsically Localized Modes (ILMs) have purportedly been observed in NaI but only for wave-vectors, q 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 frequency producing a large peak in the two-phonon density of state and giving rise to ILMs with these q values. We fit the experimentally determined acoustic and the optic phonon modes using a nearest neighbor and a next-nearest neighbor force constant. We find that the two-phonon density of states, for fixed q exhibits non-divergent van Hove singularities. The frequencies of these features are found to vary as q is varied. We intend to search for q values at which the two-phonon density of states is enhanced and then examine whether the anharmonic interactions can bind the two-phonon excitations to produce a quantized ILM.

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