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First-principles based calculation of phonon spectra and related properties in disordered alloys SUBHRADIP GHOSH, BISWANATH DUTTA, Indian Institute of Technology Guwahati — The study of lattice vibrations in the presence of substitutionally disordered alloys is one of the most fascinating areas of condensed matter physics. A huge array of.experimental data is available for over nearly half a century awaiting interpretation of the microscopic understanding of the various kinds of disorder that play a role in the lattice dynamical properties of these alloys. The theoretical calculations, on the other hand, were limited due to the lack of a suitable tool which can address both diagonal(mass) and off-diagonal(force-constant) disorder in these systems. This problem has been alleviated recently with the advent of the 'Itinerant Coherent Potential Approximation'. In this work, we propose a first-principles based methodology to compute the phonon spectra and properties derivable from them. The method is a combination of first-principles density functional perturbation theory, the transferable force constant approach by Van De Walle et al (Rev. Mod. Phys. 74, 11(2002)) and Itinerant Coherent Potential Approximation. We present results for the phonon spectra and elastic constants of disordered FePd alloys. .

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