Abstract Submitted
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A Numerical algorithm for finding pressure induced Acoustic phonon instabilities in crystals OSCAR GUERRERO[1], Retired — In this talk, I will present a fast-efficient computational Pseudo code to find acoustic phonon instabilities in crystals [1]. The code use the stress-strain relations to numerical find sound velocities in terms of second-order elastic constants for various wave modes in uniaxial and hydrostatically compressed crystals for a given wave direction k [2,3]. I use Tantalum as the testing material and the results are compared with Molecular dynamics simulations using the EAM potential formalism [4,5], DFT calculations via VASP and via a stability of the lattice as a function of uniaxial compression by determining the phonon-dispersion relation over the entire BZ [6] . All three methods predict that the lattice first goes unstable at 25% of uniaxial compression along the <100>direction. The implementation of the code is discussed using the free open source software OCTAVE and the symbolic program MATHEMATICA

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