

Abstract Submitted  
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**Calculating the Phonon Dispersion From First Principles** FRANK CEBALLOS, ANDY O'HARA, UT Austin, ALEXANDER SLEPKO, ALEXANDER DEMKOV, UT Austin — The goal of this project was to construct a user-friendly tool that can compute the phonon dispersion for any solid with a periodic crystal structure. The phonon dispersion describes the crystal's vibrational properties and thermodynamic properties of the solid. Using the Vienna Ab-initio Simulation Package (VASP) we compute the forces between the atoms. Assuming harmonic approximation we numerically evaluate force constant matrix. The lattice Fourier transform of the force constants yields the dynamical matrix, whose eigenvalues and eigenvectors represent the allowed phonon frequencies and displacement patterns for specific k-vectors. Our code then plots the frequencies along high symmetry lines in the Brillouin zone. We will present our results for silicon, GaAs and ZrO<sub>2</sub>.

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