



MedeA Phonon: Capturing “Relevant Temperatures”

Before scientists and engineers had today’s computing power, it was often a Herculean effort to capture “relevant temperatures” in modeling scenarios. Our Phonon module takes advantage of technology and our computational materials science expertise to compute temperature-dependent vibrational properties of solids, surfaces, interfaces, molecules and clusters. This provides critical insight into temperature dependent effects.

Key Benefits of Phonon:

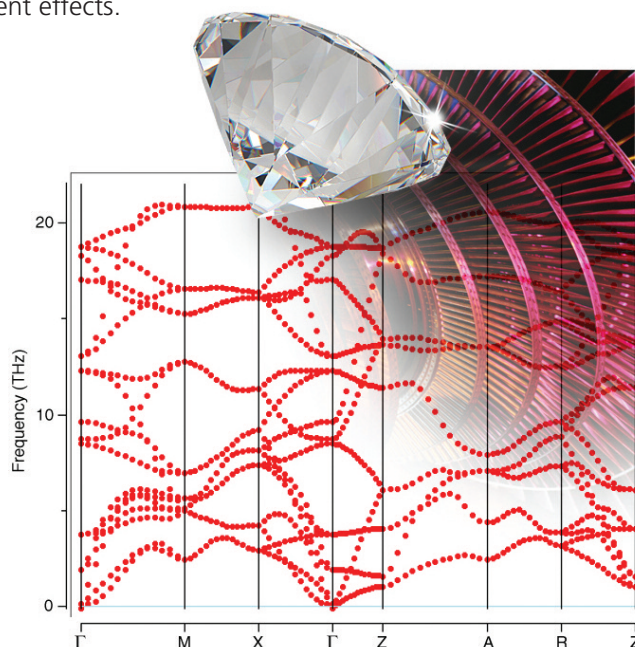
- Ability to describe systems at finite temperatures
- Predicts material behavior over a wide temperature range
- Use Phonon to determine phase stability
- Computes heat capacity, enthalpy, entropy and free energy
- Describes vibrational modes of molecules on surfaces
- Handles hundreds of calculations through JobServer/TaskServer

Properties from Phonon module:

- Phonon dispersions
- Phonon density of states
- Zero point energy
- Vibrational part of heat capacity as a function of temperature
- Vibrational enthalpy, entropy, and free energy as a function of temperature
- Symmetry analysis of vibrational modes at the center of the Brillouin zone with classification in IR active, Raman active and silent modes

Computational characteristics:

- Automatic detection and use of any space-group symmetry
- Fully automatic determination of supercell and all necessary atomic displacements
- Fully automated setup, execution, and processing of VASP jobs
- Uses forces computed with VASP 4.6 or 5.2 with any of the functionals available. This includes the ability to use functionals such as GGA+U and hybrid functionals, and fully relativistic Hamiltonians
- Partial freezing of atoms possible, e.g. to obtain vibrational modes of molecules on surfaces
- Applicable to transition state geometries to obtain vibrational partition functions for the calculation of reaction and diffusion rates within Eyring’s transition state theory
- Restart capabilities in case of hardware or communication failures (larger systems may involve several hundred individual tasks, which are controlled automatically by the JobServer)



Required MedeA modules:

- Core MedeA environment
- MedeA VASP 4.6 or 5.2
- MedeA Phonon
- JobServer and TaskServer

Visit our website www.materialsdesign.com or contact your local Materials Design office for further information.