MedeA MD Phonon

Vibrational Properties from Molecular Dynamics Simulations

At-a-Glance

MedeA®[1] *MD Phonon* calculates vibrational properties from velocity auto-correlation functions obtained during molecular dynamics simulations and can be efficiently applied to low symmetry structures such as crystalline structures with defects, amorphous materials and fluids. Based on the vibrational density of states, obtained from the velocity auto-correlation functions, thermodynamic properties such as entropy or Helmholtz free energy can be calculated accurately and efficiently.

Key Benefits

- Study systems with low symmetry. For example, temperature stabilized structures (*i.e.*, perovskites), amorphous materials, or crystalline structures with defects.
- Automated plot creation facilitates analysis of results.
- View the plots for velocity auto-correlation functions of each element in each subset.
- Study the vibrational density of states, its partial contributions of all elements, and all subsets by automatically generated plots on the JobServer and within *MedeA*'s analysis tool.
- Evaluate thermodynamic properties at the chosen temperature such as internal energy, entropy, Helmholtz free energy, and heat capacity.

The vibrational density of states is calculated from velocity auto-correlation functions[2] obtained on-the-fly during LAMMPS microcanonical NVE molecular dynamic simulations thereby making use of the LAMMPS engine for efficient performance on computers from scalar workstations to massively parallel supercomputers. Based on the density of states thermodynamical properties such as internal energy, entropy, Helmholtz free energy, and heat capacity are calculated. This approach can be applied to crystalline systems, amorphous materials and fluids facilitating the vibrational study of complex materials.

The calculated density of states is viewed directly on the *JobServer* or within the *MedeA* graphical-user interface. Thermodynamical properties are reported in the *Job.out* file and are available as variables in the *Flowchart* environment.

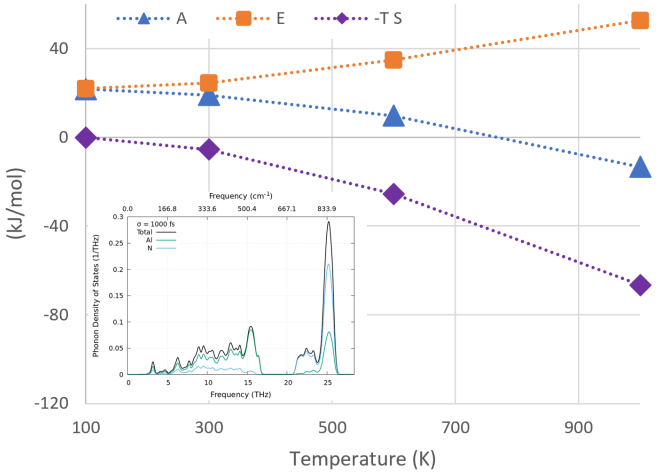

Figure 1: Thermodynamic functions Helmholtz free energy A*, potential energy* E *and entropy times temperature* - T S *are shown for wurtzite aluminum nitride.*

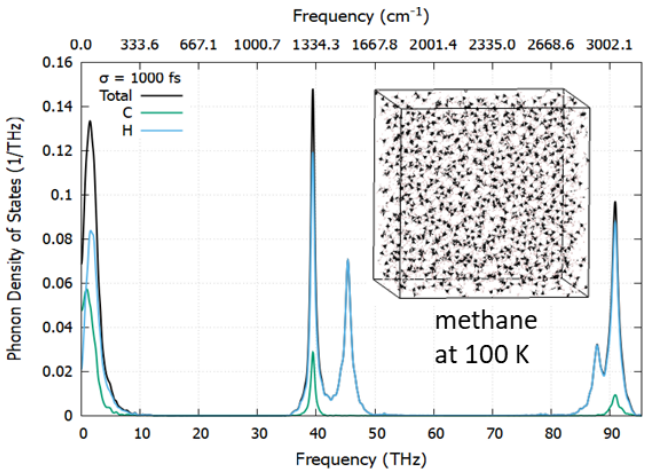

Figure 2: Vibrational density of states for a methane fluid at a temperature of 100 K.

[1] MedeA and Materials Design are registered trademarks of Materials Design, Inc.

[2] Shiang-Tai Lin, Mario Blanco, and William A. Goddard III, J. Chem. Phys. 119, 11792 (2003)

Properties from *MD Phonon*

- Total and partial vibrational density of states
- Zero-point energy
- Thermodynamic properties at a given temperature:
  - Vibrational part of heat capacity
  - Enthalpy
  - Entropy
  - Helmholtz free energy

Characteristics

- Apply *MedeA MD Phonon* to amorphous materials, fluids, and crystalline structures such as metals, and ceramics. Accuracy depends on the quality of the employed forcefield.
- Define subsets (e.g., interface layers, surface layers, nanoparticles, etc.) for which to calculate the partial contributions.
- Plug the *MedeA MD Phonon* module into any LAMMPS simulation workflow and the vibrational density of states, as well as thermodynamic properties, are calculated.

Required Modules

- *MedeA Environment*
- *MedeA Forcefield*
- *MedeA JobServer and TaskServer*

Recommended Modules

- *MedeA Phonon*

12121 Scripps Summit Drive, Suite 160 San Diego CA 92131, USA
P: +1 760 495-4924 - F: +1 760 897-2179 - E: info@materialsdesign.com