Siesta: A Complete Guide
Hand-on 4: Phonons and Ab Initio Molecular Dynamics

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14/11/2024

Outline

Phonons

Definition of Phonons

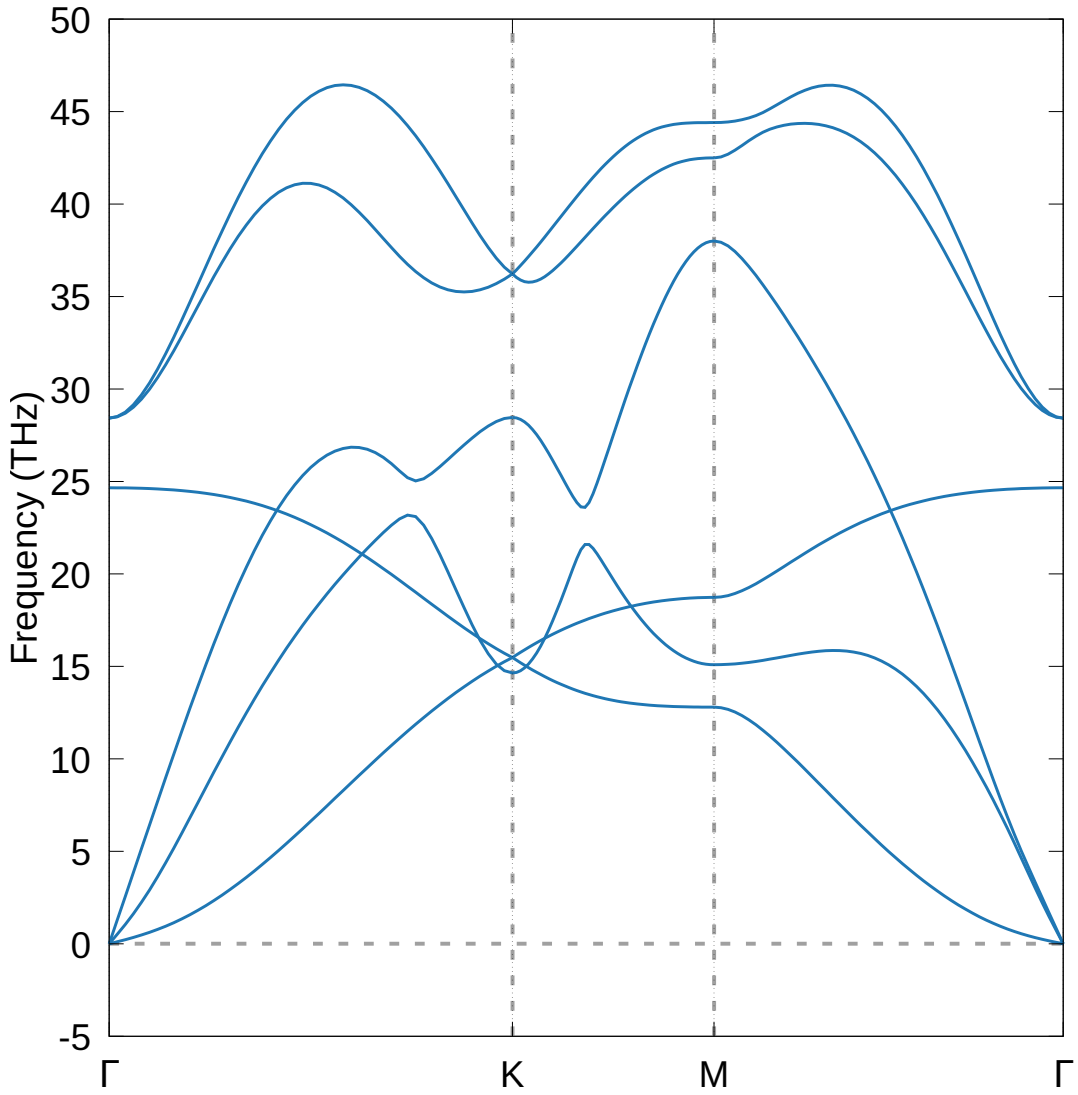
Phonons are quantized normal modes of vibration in a crystal lattice, analogous to photons in electromagnetic waves. They are bosonic quasiparticles and play a crucial role in thermal and electrical transport.

Types of Phonons

Phonons are categorized into two types based on atomic displacements:

- **Acoustic Phonons:** Atoms move in phase, producing sound waves. The frequency approaches zero as $\mathbf{q} \to 0$.
- **Optical Phonons:** Atoms in the unit cell move out of phase, typically have higher frequencies, and interact with electromagnetic radiation (e.g., infrared absorption).

Graphene's phonons dispersion



Phonons

Phonon Dispersion Relation

The dispersion relation connects the frequency ω with the wavevector $\mathbf{q}$.
In a crystal with N atoms, there are $3N$ vibrational modes:

- 3 acoustic modes (1 longitudinal, 2 transverse),
- $3N - 3$ optical modes.

A negative frequency indicates dynamical instability and a possible structural phase transition.

Ab initio molecular dynamics

Introduction

- AIMD combines quantum mechanics and molecular dynamics.
- Based on solving the electronic structure using *ab initio* methods, typically Density Functional Theory (DFT).
- Enables the study of atomic-scale dynamics in solid-state materials without empirical force fields.

Methodology

- The electronic structure is solved at each time step using DFT.
- Forces on atoms are computed from the Hellmann-Feynman theorem.
- Uses algorithms like Born-Oppenheimer MD or Car-Parrinello MD.

Applications in Solid-State Physics

- Study of defect dynamics in semiconductors and insulators.
- Investigation of phase transitions in crystalline materials.
- Simulation of thermal transport properties in nanostructures.
- Understanding electronic and vibrational properties of novel materials.

Your turn!

- Obtain the phonons and a AIMDs to MoS_2 in 2H phase.