Vienna Ab initio Simulation Package (VASP)

The Vienna Ab initio Simulation Package (VASP) is a package for performing quantum mechanical molecular dynamics (MD) using quasi-potentials and a smooth wave cut. The approach implemented in VASP is based on a finite-temperature local density approximation (with free energy as the amount of change) and a detailed evaluation of the instantaneous electronic ground state in each MD step using effective matrix designs and Pulay mixing scheme. . These techniques avoid all the problems encountered in the original Car-Parrinello method based on the simultaneous integration of electrons and ionic equations of motion. Interactions between ions and electrons are described using Vanderbilt ultrasoft (US-PP) quasi-potentials or the Advanced Projector Wave Method (PAW). Both techniques allow for a significant reduction in the number of waves per atom for transition metals and first-order elements. The forces and stress can be easily calculated with VASP and used to relax the atoms in their instantaneous pitches.

Vienna Ab initio Simulation Package Features:

- Dynamics and relaxation: Oppenheimer molecular dynamics, conjugate gradient relaxation, coated molecular dynamics, dimeric climbing (transition state search)
- Linear response to electric fields: Static dielectric properties, piezoelectric tensors (including ionic)
- Optical properties: Frequency-dependent dielectric degradation in independent particle approximation, Frequency-dependent tensor in RPA and TD-DFT, Cassida equation for TD-DFT and TD-Hartree-Fock
- Magnetism: The approach of limited magnetic moments

- Linear response to ionic displacement: elastic constants (including ionic), internal stress tensors
- Steps: Macroscopic polarization and finite electric fields

System Requirements

System requirements : GNU / Linux x86_64