Foundations of DFT Simulations with VASP

A Two-Day Hands-On Workshop for Beginners

22–23 June 2026
Conference Room, Research Laboratories Building

Organized by
Laboratory of Physics of Experimental Techniques and its Applications (PTEA)
Faculty of Sciences, University of Medea

Instructor: Dr. Ahmed Redha Benrekia

Workshop Overview

VASP (Vienna Ab initio Simulation Package) is one of the most powerful and widely used software packages for quantum mechanical calculations in materials science and chemistry using molecular dynamics, DFT methods within different exchange and correlation approximations. It can be used for bulk crystals(3D) or two dimensions (2D) systems.

Objectives

- Demystify the use of its "black box": Understand Core Concepts.
- Give tips to use VASP by explaining the basic principles of DFT and the purpose of a total energy calculation.
- Give practical examples, by applying to real 3D systems.
- Discuss real problems.
- Overcoming the Input/Output Barrier.

Practical Information

- Schedule: 09:00 – 17:00 (both days)
- Format: Presentations + Hands-on sessions
- Participation is FREE.

Register Now **Venue: Conference Room, Research Laboratories Building**

Program

Day 1: Foundations & The Ground State

Goal: Go from zero to a relaxed bulk crystal structure.

- **09:00 - 09:30 — Welcome and Setup**
  Activity: Workshop introduction. Ensure everyone can log into a provided HPC cluster or a pre-configured virtual machine. Check that VASP binaries and VESTA are accessible.

- **09:30 - 10:45 — Session 1 (Presentation): Theory for Users**
  Title: "From the Schrödinger Equation to a Calculable Quantity"
  Content: Why DFT? The problem of the many-body wavefunction. The Hohenberg-Kohn Theorems and the Kohn-Sham ansatz. Introduction to Exchange-Correlation functionals (LDA, GGA).
  Key Message: DFT maps the real interacting system onto a system of non-interacting electrons in an effective potential. We don't need to be experts, but we must understand the approximations we are making.

- **10:45 - 11:00 — Coffee Break**

- **11:00 - 12:30 — Session 2 (Presentation): The VASP Toolbox**
  Title: "The Fantastic Four: INCAR, POSCAR, POTCAR, KPOINTS"
  Content: Deep dive into the four input files.
  POSCAR: Crystal geometry (lattice vectors, atomic positions). Introduction to VESTA for creating/modifying structures.
  POTCAR: The PAW pseudopotential. How to concatenate them and why the order matters.
  KPOINTS: Sampling the Brillouin zone. The concept of k-points and convergence.
  INCAR: The master control file. Key tags explained: SYSTEM, ISTART, ICHARG, ENCUT (cutoff energy), ISMEAR, SIGMA, NSW, IBRION, ISIF.

- **12:30 - 13:30 — Lunch Break**

- **13:30 - 15:00 — Session 3 (Hands-on): Your First Calculation**
  Exercise: "Relaxing Bulk Silicon"
  Tasks:
  - Use VESTA to generate the POSCAR for diamond Silicon.
  - Setup a POTCAR using the recommended Si potential.
  - Create a KPOINTS file (e.g., 8x8x8 Gamma-centered mesh).
  - Create an INCAR for a full relaxation (NSW=100, IBRION=2, ISIF=3).
  - Submit the job and monitor its progress (OUTCAR, OSZICAR).

- **15:00 - 15:15 — Coffee Break**

- **15:15 - 16:45 — Session 4 (Hands-on): Analyzing Results & Convergence**
  Title: "Is My Answer Right?"
  Tasks:
  - Examine the relaxed CONTCAR and compare it to the initial POSCAR using VESTA.
  - Extract the final energy from the OUTCAR (grep "energy without entropy" OUTCAR).
  - Convergence Exercise 1: Vary ENCUT (200, 300, 400, 500 eV) and plot Total Energy vs. Cutoff Energy. Determine a suitable ENCUT for production runs.

  - Convergence Exercise 2: Vary the KPOINTS mesh and plot Total Energy vs. k-points.

- **16:45 - 17:00 — Q&A and Day 1 Wrap-up**
  Discuss the day's challenges and what to expect tomorrow.

Day 2: Properties of Bulk Crystals

Goal: Extract meaningful physical properties from the ground state.

- **09:00 - 09:15 — Recap of Day 1**
  Quick review of the four input files and the concept of convergence.

- **09:15 - 10:30 — Session 5 (Presentation): From Wavefunctions to Properties**
  Title: "What Can We Calculate?"
  Content:
  - Total Energy: The fundamental output.
  - Electronic Structure: Band structures and Density of States (DOS). What are bands? What is the Fermi level? Direct vs. indirect band gaps.
  - Charge Density: CHGCAR and what it represents.

- **10:30 - 10:45 — Coffee Break**

- **10:45 - 12:30 — Session 6 (Hands-on): Electronic Properties**
  Exercise: "Calculating the Band Gap of Silicon"
  Workflow:
  - Static Calculation: Use the relaxed CONTCAR from Day 1 as the new POSCAR. Setup an INCAR for a static run (NSW=0, IBRION=-1, ICHARG=1 or 2) with the converged ENCUT and k-points. Run VASP to get a accurate charge density.
  - Band Structure Calculation:
    * Generate a high-symmetry k-point path for the Brillouin zone.
    * Create a special KPOINTS file for the band structure (line mode).
    * Run a non-self-consistent calculation (ICHARG=11).
  - DOS Calculation:
    * Use a very dense KPOINTS mesh (e.g., 20x20x20).
    * Run a second static calculation for DOS.

- **12:30 - 13:30 — Lunch Break**

- **13:30 - 15:00 — Session 7 (Hands-on): Data Visualization**
  Title: "Turning Numbers into Figures"
  Tasks:
  - Use py4vasp (recommended) or command-line tools to plot the Band Structure from the output files.
  - Plot the Total and Projected Density of States (DOS/PDOS).
  - Overlay the band structure and DOS plot to identify the band gap.
  - (Optional) Use VESTA to visualize the charge density from CHGCAR.

- **15:00 - 15:15 — Coffee Break**

- **15:15 - 16:30 — Session 8 (Presentation + Q&A): Next Steps & Best Practices**
  Title: "Beyond Bulk Crystals and Common Pitfalls"
  Content:
  - Brief overview of other properties: Elastic constants, phonons (with caution that this is advanced), optical properties.
  - Best Practices: Always cite VASP correctly. Organize your directories (e.g., 01_relax, 02_static, 03_bands). The importance of keeping a laboratory notebook.
  - Common beginner mistakes and how to debug them.
  - Resources for help: VASP Wiki, VASP Forum, mailing lists.
- **16:30 - 17:00 — Final Q&A, Feedback, and Close**