MidTerm Project of DFT

Group:

Lecturer: Henry P. Pinto
Date: 11/04/2025

Using GGA-PBE as implemented in VASP, predict the structure of the given fcc crystal:

1) Compute ECUT needed to converge the energy <1 meV/atom. Use energies from 250 to 900 eV (use `en_cut.sh`), the `KPOINTS` for this calculation is a mesh 17x17x17.

2) Compute KPOINTS needed to converge the energy <1 meV/atom. Use a point mesh from 15 to 28 (use `k_points.sh`)

3) Compute the EOS (use `cell.sh` from `part6_silicon4`): for this use the following initial volumes:

Crystal	Ag	Al	Au	Cu	Ir	Pd	Pt
Vol (Å^3)	17.0	16.5	17.0	12.0	14.0	14.8	15.0

and create a range using Mathematica as

```
Range[val - 3, val + 5, 0.5]//Map[(#//ToString) <> " " &, #] &//StringJoin
```

where **val** are the values for the initial volume displayed in the Table.

4) From EOS determine V_{opt}, a_0, B_0 and B'

5) Compute the ground state of the crystal (use V_{opt} and the script bulk.sh): from this get the crystallographic data (use FINDSYMM) and the distance between atoms. This info has to be reported in a table similar to Table II of the manual.

6) Show the plot of the PDOS (what is the composition in terms of s, p and d states?) and the charge density (use VESTA and display using boundary menu with 3x3x3), Is the system metal, semiconductor or insulator? Explain.

8) Compute the band structure of the ground state of the crystal along the following high-symmetry points path: Γ—X—U—W—K—Γ—L, use 45 intersections in the `KPOINTS-bs` file. Is the system metal, semiconductor or insulator? Explain.

9) Compute the cohesion energy (you will need to compute the energy of isolated atom, then use a box of 15 Å in length like POSCAR-atom, and the ENCUT has to be the same as the one used in the bulk calculation). The `KPOINTS` for this calculation has a mesh 1x1x1 (see `KPOINTS-atom`)

10) All the predicted values: V_{opt}, a_0, B_0 have to be compared with experimental values reported in Kittel book on solid state physics; compute the percentage error and comment the results

$$\text{error} = \frac{x_c - x_{expt}}{x_{expt}} \times 100,$$

where x_c (x_{expt}) is the computed (experimental) value.