Problem 1: Structural, electronic, and dynamical properties of HgSe

In this exercise we study the ab-initio structural, electronic and dynamical properties of HgSe. HgSe is an fcc crystal with the zincblend structure. Taking the origin in an atom, the coordinates of the second atom are $\mathbf{d}_2 = a(1/4, 1/4, 1/4)$. The experimental cubic lattice constant is $a_0 = 6.19$ Å.

1. Study the convergence of the total energy of HgSe with respect to the cut-off energy for the wavefunctions and for the charge density. Choose a cut-off for which the total energy is converged at least within 1 mRy. You can use the pseudopotential `Hg.pz-n-kjpaw_psl.1.0.0.UPF` and `Se.pz-n-kjpaw_psl.1.0.0.UPF` from `pslibrary` for the LDA functional.

2. Study the convergence of the total energy with respect to the mesh of $\mathbf{k}$ points used to sample the Brillouin zone.

3. With the parameters found at previous points, compute the total energy of the system for several volumes about the experimental value. Fit the energy with a Murnaghan equation and determine the theoretical lattice constant and bulk modulus at the minimum energy. Plot the pressure as function of the volume. Study how these values depends on the mesh of volumes chosen for the fit. Check also how they depend on the cut-off energy and on the $\mathbf{k}$-point sampling.

4. At the equilibrium volume compute the band structure of the solid along a few high symmetry lines of the Brillouin zone. Find if it is a metal, a semiconductor, or an insulator. In the latter two cases determine the band gap.

5. At the equilibrium volume compute the phonon dispersions along a few high symmetry lines of the Brillouin zone. Compare with the experimental phonon dispersions that you find in the literature.

6. Interpolating the dynamical matrices on a thick grid, compute the vibrational energy, free energy, entropy, and constant volume heat capacity.

7. Using the pressure versus volume curve determined at point 3, find the lattice constant that is needed to have pressures of 50 kbar, 100 kbar, and 150 kbar.

8. Recompute the phonon dispersions for these three volumes. Evaluate the effect of pressure on the vibrational energy, free energy, entropy, and constant volume heat capacity.