Problem 1: Phonon dispersions and Grüneisen parameters of Sc

In this exercise we study ab-initio the phonon dispersions and the Grüneisen parameters of Scandium. Scandium is an hcp crystal with two atoms in the unit cell. The experimental lattice parameters are $a = 3.309$ Å and $c/a = 1.594$. We compute the total energy of Scandium using density functional theory. You can use the pseudopotential `Sc.pz-spn-kjpaw_psl.1.0.0.UPF` from `pslibrary` for the LDA functional.

1. At the experimental structure, study the convergence of the total energy as a function of the kinetic energy cut-off of the wavefunctions and determine for which value the energy is converged within 1 mRy. Keep the charge density cut-off equal to 4, 6, or 8 times the cut-off for the wavefunctions. Discuss how the results change. For this calculation use a smearing parameter 0.02 Ry and a **k**-point mesh equal to $(12, 12, 8)$.

2. At the cut-offs determined at the previous point, study the convergence of the energy with the **k**-point sampling. Repeat the calculation for smearing parameters 0.02 Ry, 0.01 Ry, and 0.005 Ry. Discuss the convergence of the results and, if necessary, decrease or increase further the smearing.

3. Using the option `calculation='vc-relax'` determine the equilibrium values of a and c/a at zero pressure. Discuss their convergence with the kinetic energy cut-offs and **k**-point sampling.

4. At the equilibrium values of a and c/a determine the phonon frequencies at the point Γ, K, M, and A of the Brillouin zone. Study their convergence with the kinetic energy cut-offs and **k**-point sampling.

5. Using the parameters for which previous frequencies are converged within 3 cm^{-1} plot the complete phonon dispersions of Scandium comparing with the experimental data in Phys. Rev. B **44**, 6794 (1991).

6. (optional) Now apply a strain ϵ_{11} and show that the strained solid can be described by a base-centered orthorombic lattice with two atoms in the unit cell. Compute the phonon dispersions of the strained solid for two small values of the strain (one positive and one negative) and use the computed frequencies to calculate numerically the Grüneisen parameters of this solid.