Exercise: calculate the equation of state for silicon

1. **Calculate the total energy for different values (~7-10) of the lattice constant around the equilibrium value**. Hint: create a separate subfolder for each calculation
2. **Create a text file** with two columns reporting (Hint, use “grep lattice” and “grep !”):
   - The lattice parameter (in a.u.)
   - The total energy (in Ry)
3. **Fit the equation of state with ev.x**

   Lattice parameters or Volume are in (au, Ang) > au
   Enter type of bravais lattice (fcc, bcc, sc, hex) > fcc
   Enter type of equation of state :
   1=birch1, 2=birch2, 3=keane, 4=murnaghan > 4
   Input file > a_e.dat
   Output file > eos.dat

$$E(V) = E_0 + V\left(\frac{B}{B'}\right)\left[\left(\frac{V_0}{V}\right)^{B'/(B'-1)} + 1\right] - \frac{BV_0}{(B'-1)}$$

$$P(V) = \left(\frac{B}{B'}\right)\left[\left(\frac{V_0}{V}\right)^{B'} - 1\right]$$

Homework: diamond

Assignment to do at home: **calculate the band structure and equation of state of diamond**.
Some hints:

- Use the SCF input for silicon as a template
- You need to check the Bravais lattice of diamond, is it the same of silicon?
- You need to modify the lattice constant and atomic positions for diamond
- You need to change the pseudopotentials and adjust the wavefunction and charge density cutoffs!
- What qualitative differences do you expect w.r.t. to silicon as regards the:
  - Band structure
  - Equation of state

Use the documentation available at https://www.quantum-espresso.org/Doc/INPUT_PW.html

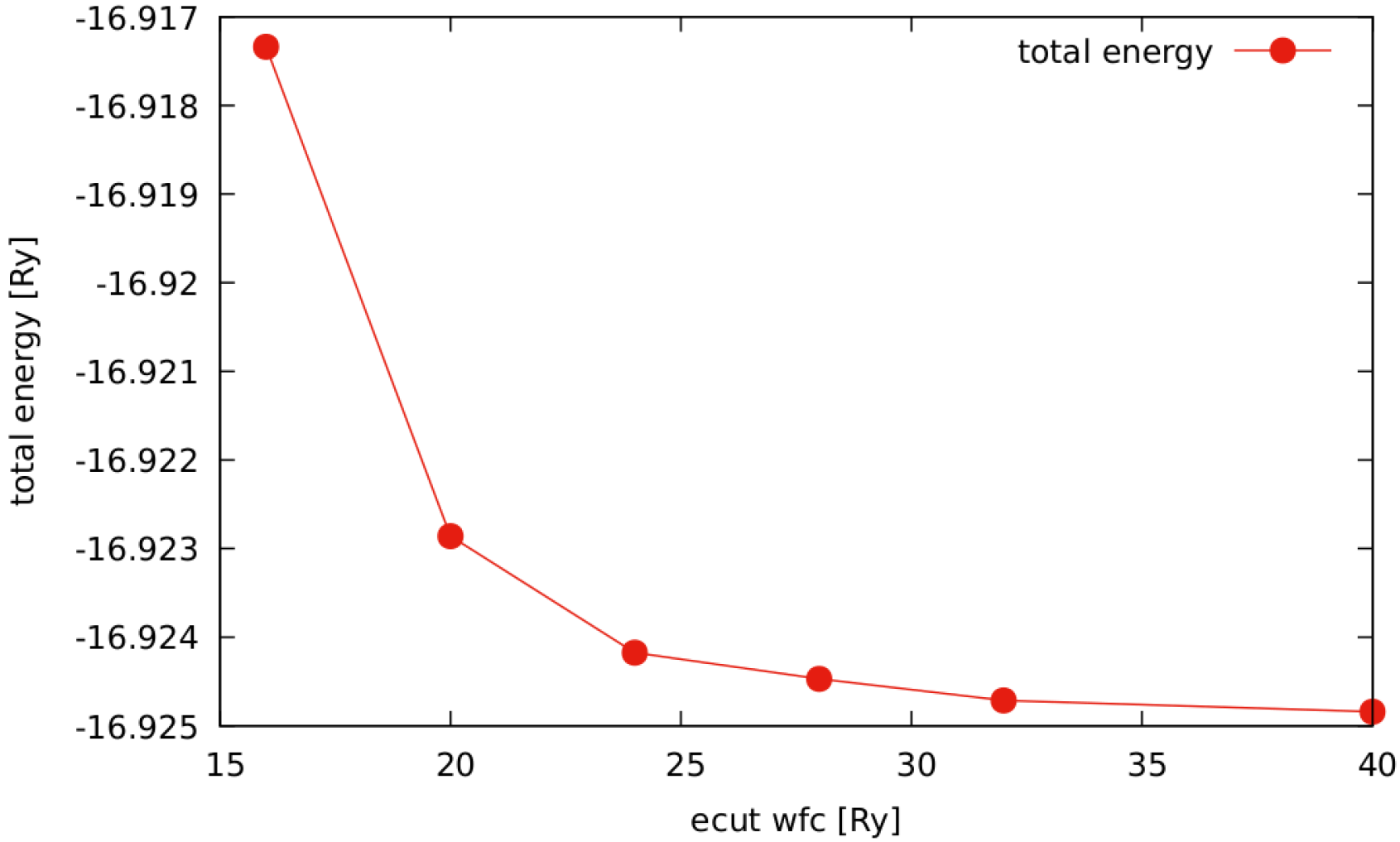
Convergence tests

- The numerical value of **electronic-structure properties** calculated with DFT (or any other method) **needs to be converged with respect to key input parameters** of the calculation. In addition, **thresholds** on iterative algorithms (e.g. diagonalisation) need to be **strict enough to ensure the result is sufficiently accurate** (in QE see e.g. “etot_conv_thr”, “forc_conv_th”). Consider also the possibility of magnetic systems.

- For a DFT, the key input parameters to be converged are
  - **Wavefunction cutoff** (in QE “ecut”, expressed in Ry): determines number of plane waves needed to represent the Kohn-Sham orbitals
  - **Charge-density cutoff** (in QE “ecut_rho”): number of plane waves needed to represent the electronic charge density NB: for norm-conserving pseudopotentials, the exact value would be 4 times the wavefunction cutoff.
  - **K-points sampling**: determines the set k-points used to perform k-space integrals over the Brillouin zone, often a uniform mesh is used (e.g. 6x4x4 grid, nowadays often Gamma-centered)

Exercise: convergence of the wavefunction cutoff

- Calculate the total energy of silicon for a range of wavefunction cutoffs and plot the results with gnuplot



Exercise: convergence of the k-points mesh

- Calculate the total energy of silicon for a different k-point grids and plot the results with gnuplot