Lab 04 – Energy and *k*point convergence

1. **Convergence of *absolute energies* with respect to cutoff energies.**
    a. Using Quantum Espresso, calculate the energy of diamond as a function of cutoff energy. A good increment might be ~10 Ryd, in the range of 10-140 Ryd. When changing the cutoff, make sure to keep the other variables (lattice constant, *k* points, etc.) fixed. Record all relevant parameters such as lattice constant, *k* points, and so on. Record and plot your final results. Specify when you reach the level of convergence of ~5 meV/atom (convert this to Ryd).
    b. Do you see a trend in your calculated energies with respect to cutoff? If you see a trend, is this what you expect and why? If not, why?
    c. Deliverables:
        i. Table of DFT results (highlight converged energy cutoff)
        ii. Plot of total energy vs energy cutoff
        iii. Answer to part (b)
2. **Convergence of *absolute energies* with respect to *k*points.**
    a. Using PWSCF, calculate the energy as a function of *k* point grid size. For each grid, record the number of unique *k* points. This gives a measure of how long your calculation will take calculations scale as K, where K=number of unique *k* points. When changing the size of the *k* point grid, make sure to keep your other variables fixed (lattice constant, cutoff, etc.)
    b. Do you see a trend in your calculated energies with respect to grid size? If you see a trend, is this what you expect and why? If not, why?
    c. Deliverables:
        i. Table of DFT results (highlight converged number of kpoints)
        ii. Plot of total energy vs K
        iii. Answer to part (b)

3. **Convergence of *forces* with respect to cutoff energies.**
    a. Sometimes, we are interested in quantities other than energies. In this problem, we will be calculating forces on atoms. Displace a C atom +0.05 in the *z* direction (fractional coordinates). Keeping other parameters fixed, calculate the forces on C as a function of energy cutoff. A good force value would be converged to within ~10 meV/Angstrom (convert this to Ryd/bohr – PWSCF gives forces in Ryd/bohr). Don't forget to record relevant parameters (lattice parameter, *k* points, unique *k* points, etc.). A good *k* point grid to use is 4x4x4. Plot and record your results.
    b. Deliverables:
        i. Table of DFT results (highlight converged energy cutoff)
        ii. Plot of total force on C vs K
4. **Convergence of *forces* with respect to *k*points.**
    a. Using PWSCF, calculate the force on a C atom (displaced +0.05 *z* direction in fractional coordinates) as a function of *k* point grid size. Keep all other parameters fixed. Record your relevant conditions (lattice parameter, cutoffs, etc.)
    b. Deliverables
        i. Table of DFT results (highlight converged number of k-points)
        ii. Plot of total force on C vs K
5. **Convergence of *energy differences* with respect to energy cutoffs.**
    a. In practice only energy differences have physical meaning, as opposed to absolute energy scales, which can be arbitrarily shifted. Therefore, it is important to understand the convergence properties. Using PWSCF, calculate the energy difference between diamond structures at two lattice parameters as a function of cutoff. For example, you could

calculate the energy of diamond at the experimental lattice parameter (6.74 bohr), the calculate the energy at 6.70 bohr (or any lattice parameter close to the minimum), take the difference between the two, and repeat for many energy cutoffs. Make sure to keep your other variables (lattice constant, *k* points, etc.) fixed while changing the cutoff. Record all relevant parameters such as the lattice constant, *k* points, and so on. A good energy difference is converged to ~5 meV/atom (convert this to Ryd).

b. Deliverables
    i. Table of DFT results (highlight converged number of k-points)
    ii. Plot of energy difference vs energy cutoff

6. **Comparing Probs. 1, 2, 3, and 4, and 5**: How do the cutoff requirements change when looking at absolute energies vs. looking at forces vs. energy differences? How do the *k* point grid requirements change?