Silicon Carbide

Group 1A and 1B

1 Input set-up

Silicon carbide (SiC) is a semiconductor containing silicon and carbon in the unit cell. The beta modification (β-SiC) has a zinc blende FCC crystal structure (similar to diamond), with an experimental lattice parameter of 4.358 Å.

- generate an input file for an SCF computation: you should decide which pseudopotential you will use (norm-conserving, ultrasoft, PAW) and the approximation for the exchange-correlation potential (LDA, PBE, PBE-sol).
- visualize your crystal structure with the software XCRYSDEN. This will help you understand if you are going to simulate the correct system or not with the input file you have written!

2 Convergence tests

- Set a sufficiently high grid sampling in k-space (e.g. $6 \times 6 \times 6$) and vary the value of E_{cut}. Be careful that you must also change the value of E_{rho} if you are using US or PAW pseudopotentials! Then plot the total energy per atom as a function of E_{cut}. We say that the energy is converged when its variations are ≤ 1 mRy. What is your converged E_{cut}?
- Now set E_{cut} to the value which assures convergence as found at precedent point. Vary the k-point grid and plot the total energy per atom as a function of the number of k-points. What is your converged k-point grid?

3 Equilibrium geometry

- Perform an automatic cell+ion relaxation: what is the new lattice parameter? what are the new ions' positions?
- Now manually modify the lattice parameter from its experimental value in a range of $\sim \pm 5\%$. Plot the results and fit the E vs alat curve with a second or higher order polynomial: the equilibrium lattice parameter is found as the minimum of this curve. What is the new lattice parameter? From this new lattice parameter you can now perform only a ion relaxation and see if atoms change position
- Plot the E vs volume curve and compute the bulk modulus which is defined as:

$$B = V_0 \Big(\frac{d^2 E}{dV^2} \Big)_{V=V_0}$$

  where V_0 is the equilibrium volume of the primitive cell. What is the value of the bulk modulus? Remember that $V_{\text{primitive cell}} = V_{\text{unit cell}}/4$. The result will be in Ry/bohr^3 which can be converted in Pa multiplying by 1.47×10^{13}. The experimental value for SiC is $B_{exp} = 250$ GPa.
- Compare both the theoretical lattice parameter and the theoretical bulk modulus with their experimental counterparts. What is the error? What is the cause?

4 Electronic structure

Starting from either the theoretical relaxed structure or the experimental structure, both with the converged parameters:

- Perform a band computation and extract the electronic dispersion relation. From this you can obtain the direct and/or the indirect energy band gaps: compare with the experimental value $E_g = 2.36$ eV. Moreover, by fitting band minima or maxima with a parabola you can extract the effective masses of carriers.
- Perform a non-self consistent computation with increasing value of the k-point grid and extract the electron density of states until convergence is reached. Plot the converged result and discuss if the system can be considered free-electron like.

5 Vibrational properties

- Perform a convergence test for phonons at $q = \Gamma$: change the k-grid in the SCF cycle and for each case perform a phonon computation until convergence of phonon frequencies is reached.
- With the converged k-grid, perform a phonon computation on a coarse grid of q-points, for example you can start with $2 \times 2 \times 2$. Extract the phonon dispersion relation and the phonon density of states. From this you can fit acoustic modes with lines, whose slope will give you the sound velocity. Moreover, from the density of states you can get an estimate of both the Debye and Einstein temperature.
- Now increase the grid of q-points and see if phonon dispersion relation and density of states change.