ECS289K Introduction to Quantum Simulations 2016-05-04

Homework 3 due Fri 2016-05-13 at 23:55

Create a pdf file containing your report and upload it to Smartsite. Add your program as a text attachment. By uploading your files, you attest that they contain your individual work.

Electronic structure of cubic silicon carbide

Cubic silicon carbide (3C-SiC) crystallizes in the zincblende structure. This structure is similar to that of silicon (diamond structure) except that every other Si atom is replaced with a C atom. Note that SiC also crystallizes in hexagonal structures (4H-SiC and 6H-SiC) that we will not consider here. See https://en.wikipedia.org/wiki/Silicon_carbide . All calculations in this assignment will be carried out using Quantum Espresso.

SiC lattice constant

1) Using a 2-atom FCC primitive cell and 10 k-points in the irreducible Brillouin zone, compute the total energy of 3C-SiC in the range of lattice constants [7.5-9.0]. Use the Si.pz-vbc.UPF pseudopotential for silicon (as used in Si examples) and the carbon pseudopotential C.pz-vbc.UPF from the quantum-espresso.org web site.
a) Plot the energy vs lattice constant *E(a)* for various values of the plane wave energy cutoff chosen according to the convergence of the results.
b) Use a quadratic fit of the *E(a)* data to determine the equilibrium lattice constant of 3C-SiC. Give an estimate of the accuracy of your result using data obtained with various plane wave energy cutoffs. Compare your result with the LDA result listed in the paper of Haas (posted on SmartSite), and with the experimental value (listed in the same paper).

Band structure of SiC

2) Using a 2-atom FCC primitive cell and the lattice constant and plane wave energy cutoff determined in (1), compute the band structure of 3C-SiC including a total of 8 bands (4 valence + 4 conduction).
a) Plot the band structure along the path L-Gamma-X in the FCC Brillouin zone.
b) Identify the valence band maximum (VBM) energy and the conduction band minimum (CBM) energy and compute the value of the band gap (Eg). Compare you result with DFT-LDA computed values and experimental values taken from the literature.