Combined hands-on excises+ homework No. 3

Issued 16 Oct. 2017 and due 6 Nov. 2017

1. *Ab initio* calculation of bulk moduli of Na and Al and compare your results with the prediction of Hartree-Fock approximation of free electron gas.
(1) Using the volume optimization to determine the lattice constant a_0 for fcc Al.
(2) Calculate the total energy for several lattice constants (e.g., a_0, $(1.0\pm0.01)a_0$, $(1.0\pm0.02)a_0$, $(1.0\pm0.03)a_0$).
(3) Plot total energy as a function of volume and then fit a polynomial to the total energy versus volume curve. Evaluate the lattice constant a_0 and bulk moduli B_0 of Al using the obtained polynomial.
(4) Estimate the r_s for fcc Al. Use the Hartree-Fock results for a free electron gas in Problem 2 in Homework Sheet 2 to evaluate the lattice constant a_0 and bulk moduli B_0. Compare these results with those of (3).
(5) Repeat (1)-(4) for bcc Na.

2. Comparison of the ground state crystal and magnetic structures of bcc Fe of the LDA and GGA calculations.
(1) LDA calculations. (a) Using the volume optimization to determine the lattice constant a_0 for nonmagnetic fcc Fe. (b) Calculate the total energy for several lattice constants (e.g., a_0, $(1.0\pm0.01)a_0$, $(1.0\pm0.02)a_0$, $(1.0\pm0.03)a_0$, $(1.0\pm0.04)a_0$). (c) Repeat the calculations of (a) and (b) for nonmagnetic and ferromagnetic bcc Fe. (d) Plot all the total energies and spin magnetic moment as a function of volume, and find the ground state magnetic and crystal structure including the lattice constant.
(2) Repeat the calculations of (1) using GGA.
(Consult (i) Wang et al., PRL 54 (1985) 1852 and (ii) Guo, Wang, Chin. J. Phys. 38 (2000) 949).

3. GGA band gaps of typical semiconductors versus the experimental values.
(1) (a) Using the volume optimization to determine the lattice constant a_0 for Si in diamond structure. (b) Calculate and plot the band structure and density of states (using the tetrahedron method) using the obtained a_0. Then read the band gap from both the calculated energy bands and density states. (c) Compare your theoretical lattice constant a_0 and band gap Eg with the experimental values.
(2) Repeat the calculations of (1) for Ge and GaAs.

4. Comparison of GGA and GGA+U calculations of NiO in the AF-II magnetic structure

(Consult Terakura et al., PRB 30 (1984) 4734 for the AF-II magnetic structure).
(1) (a) Use the experimental fcc lattice constant to perform the selfconsistent GGA AF-II calculation. (b) Use the converged charge density (CHGCAR) to calculate band structure as well as total and atom-decomposed densities of states. (c) Plot the band structure and also the densities of states. Find out the calculated band gap as well as total and Ni magnetic moments. (d) Use VESTA to plot the crystal and magnetic structures.
(2) Repeat the calculations using GGA+U with effective U_{eff} = 7.0 eV. Then compare the results from (1) and (2) with comments.