第一原理計算材料物理學期末考試卷

Date: 2 January 2018; Return your answers by or on Jan. 15, 2018

(*Please note: 4 problems on 2 pages; Answers in both Chinese and English are OK.*)

1. (25 %) Structural and mechanical properties as well as pressure-induced structural phase transition of iron metal.

(a) (10 %) By using the volume optimization and GGA-PBE potential, determine the lattice constant a_0 (c/a) for nonmagnetic and ferromagnetic Fe in bcc, fcc and hcp structures. Calculate the total energy for several lattice constants (e.g., a_0, (1.0±0.01)a_0, (1.0±0.02)a_0, (1.0±0.03)a_0, (1.0±0.04)a_0) for each magnetic state and each structure.

(b) (8 %) Plot your total energy per atom and magnetic moment per atom as a function of volume per atom for all the magnetic and structural phases. By polynomial fitting, calculate all the bulk modulii. Also, calculate the phase transition pressure (in GPa) for the phase transition from ferromagnetic bcc to nonmagnetic hcp structure.

(c) (7 %) Make a table to list your results, together with available experimental results. Comments on **all** your results and available experimental data.

(Hint: Consult Guo, Wang, Chin. J. Phys. 38 (2000) 949).

2. (25 %) Optical properties of fcc Au and diamond-structure Si at lattice constant a = 4.08 Å (Au) and 5.43 Å (Si).

(a) (12 %) Calculate and plot band structure, density of states, joint density of states, dielectric function, energy loss function and absorption spectra of Au and Si. Compare and comment on the differences in the calculated results with previously published results.

(b) (13 %) Repeat (a) by including the spin-orbit coupling. Comment on the effects of the relativistic spin-orbit coupling on the calculated properties. Also compare your results with available experimental data.

3. (25 %) Phonon band structure and thermal properties of silicon.

(a) (5 %) Perform strucutural optimization using GGA-PBE exchange-correlation potential. Perform the self-consistent calculation for the theoretical lattice constant and then plot the electronic band structure. Compare your lattice constant and band structure with previous reports.

(b) (6 %) Calculate and plot phonon dispersion relations for the theoretical lattice constant using 2×2×2 supercell. Compare your results with experimental measurements.

(c) (6 %) Calculate and plot thermodynamic properties (internal energy, free energy, entropy and specific heat). Compare your results with previous experiments.

(d) (8 %) Repeat (b) and (c) using a larger supercell of 3×3×3.

4. (25 %) Effective magnetic coupling (exchange interaction) *J* in bcc Mn in GGA-PBE.
(a) (8 %) Perform two self-consistent total energy calculations for the ferromagnetic and antiferromagnetic states of Mn at lattice constant a = 2.89 Å , respectively.
(b) (10 %) Use the calculated total energy difference between the two magnetic configurations to estimate the effective nearest neighbor interaction parameter *J*. Estimate the magnetic phase transition temperature within the mean field approximation.
(c) (7 %) Do a literature search for previous related experimental and theoretical papers, and compare your predictions (spin magnetic moment, exchange coupling parameter and magnetic phase transition temperature) with the previous results. If there are discrepancies between your and previous results, please comment.