Uva Wellassa University of Sri Lanka
Faculty of Science and Technology
Science and Technology Degree Programme
4th Year First Semester Examination – July 2016
SCT 433-1 Multiscale Modeling Techniques in Materials Science

Uva Wellassa University

Instructions to candidates
Duration: One (01) hour
Number of questions: Two (02)
Mark allocation: 100 marks
Answer all questions

1.

a. Explain the difference between a "functional" and a "function" using an example. (5 marks)

b. State the two Hohenberg-Kohn theorems. (6 marks)

c. According to the density functional theory (DFT), the ground state energy of a real system is given by

$$E_0 = \sum_{A=1}^{M} \int \frac{Z_A}{|r - R_A|} \rho(r) dr - \frac{1}{2} \sum_{i=1}^{2n} \int \psi_i^{*(KS)}(r) \nabla^2 \psi_i^{(KS)}(r) dr + \frac{1}{2} \iint \frac{\rho_0(r1)\rho_0(r2)}{r_{12}} dr_1 dr_2 + \Delta\langle T[\rho_0] \rangle + \Delta\langle V_{ee}[\rho_0] \rangle$$

(1) (2) (3) (4) (5) (6)

i. Explain the meaning of each term (1), (2), (3), (4), (5), (6) (12 marks)

ii. What is the special name given to {term (5) + term (6)} ? (2 marks)

d. Briefly explain the following

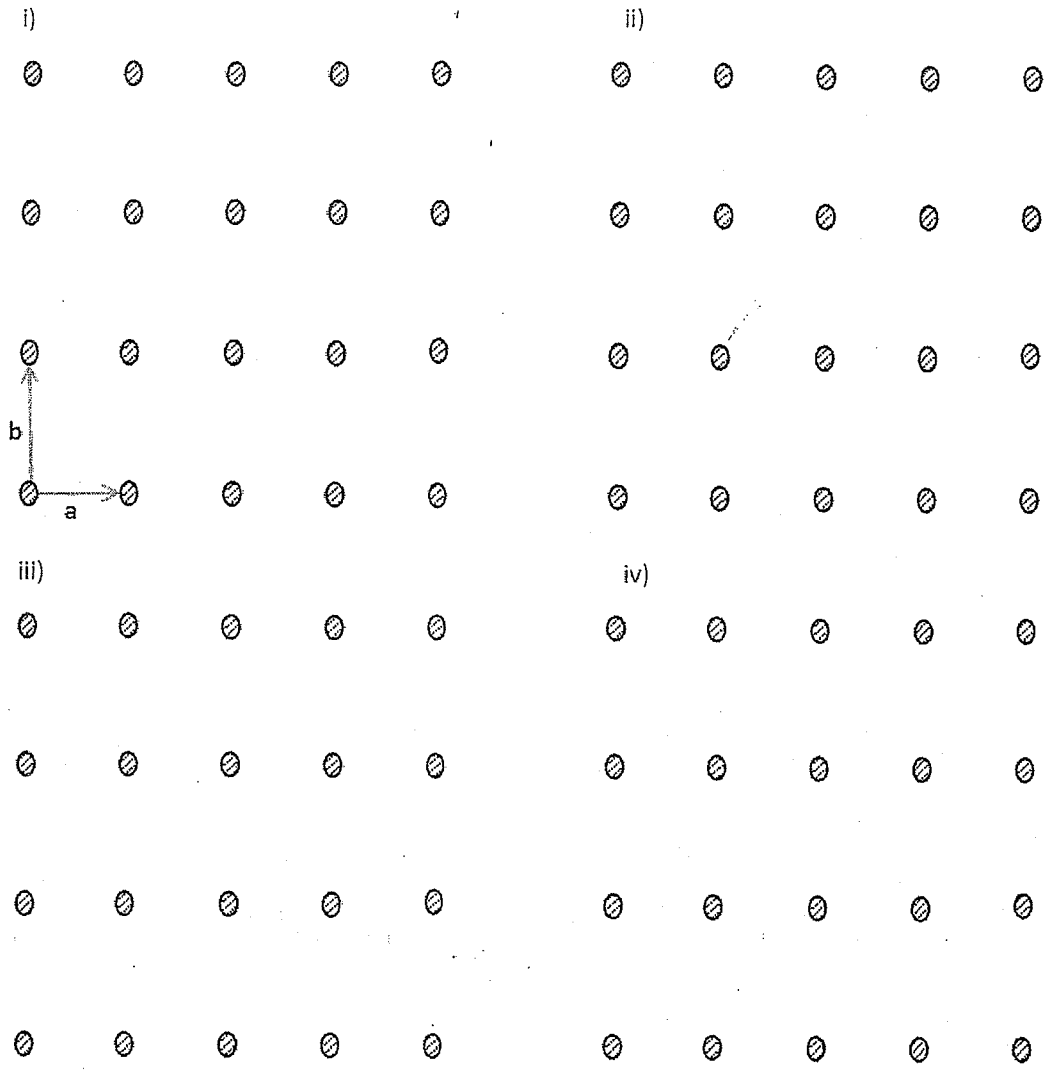
i. Generalized gradient approximation (GGA) (5 marks)
ii. Hybrid functionals (5 marks)

2.

a. Using the 2D lattice given below draw planes corresponding to

i. (0 1 0) (4 marks)
ii. (2 0 0) (4 marks)
iii. (1 1 0) (4 marks)
iv. (1 2 0) (4 marks)

(6) (69)



b. X-rays with wavelength 1.54 Å are reflected from the (1 1 0) planes of an orthorhombic crystal with unit cell a = 8.2 Å, b = 9.4 Å, c = 7.5 Å. Calculate the Bragg angle, θ, for orders of reflection n = 1 and n = 2. (10 marks)

c. Palladium (Pd) crystallizes in a face-centered cubic unit cell. Its density is 12.023 g/cm^3. Molar mass of Pd is 106.42 g mol^{-1}. Calculate the atomic radius of Pd. Consider Avogardro's number = 6.022 x 10^{23} mol^{-1} (10 marks)

d. Briefly explain the following

i. Miller indices (4 marks)
ii. Bravais lattices (4 marks)
iii. Space groups (4 marks)

e. Write short notes on the following

i. Multiscale modeling (4 marks)
ii. "Continuum" in materials science (4 marks)
iii. Coarse Graining (4 marks)

f. Arrange the following computational techniques/methods in a schematic diagram of increasing length scale vs time scale: quantum mechanics, molecular dynamics, molecular coarse graining, continuum theory. (5 marks)