Uva Wellassa University, Sri Lanka
End Semester Examination – March 2011
SCT 433-1 Multi-Scale Modeling Methods in Materials Science

Time: One (01) hour

Total **three (03)** questions
Answer **all** questions
You may use standard symbols/ abbreviations without a definition

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01) a. Write short notes on:
   i. Phase space;
   ii. Autonomous system;
   iii. Equi-partition theory

(20 marks)

b. "Phase trajectories of particles in an autonomous system do not intersect each other" Explain briefly.

(20 marks)

c. Plot phase trajectories of a particle moving under $V(q) = -\frac{1}{2} m\omega^2 q^2$ potential field.

(20 marks)

d. Draw a trajectory of a particle moving under simple harmonic motion.

(20 marks)

e. Write a mathematical expression to calculate the number of micro states of the system examined under section (d).

(20 marks)

02) a. What is meant by an ergodic system? Write mathematical expressions to calculate ensemble and time averages of an observable 'A'.

(20 marks)

b. Prove that $S = k.log\ [\Omega(N,V,E)]$. State similar expressions in terms of relevant partition functions for the calculation of Helmholtz and Gibb's free energies (no derivations are needed).

(20 marks)

c. Derive expressions in terms of micro-canonical partition function for the calculation of temperature, pressure and chemical potential of a system.

(20 marks)

d. Verlet algorithm is widely used in Molecular Dynamics (MD) simulations. Briefly explain the theory behind it. State the order of accuracy of the method.

(20 marks)

e. In MD simulations how the required inter-potential functions are calculated?

(20 marks)

03) a. Briefly explain following terms:

i. Variation principle;

ii. 6-31 G (d) basis set.

(20 marks)

b. State the HF equation for *n*-electrons system. State Columbic and Exchange operators.

(20 marks)

c. Derive the Roothaan equation for N electron system. Why the solutions to Roothaan equation are treated self consistent?

(40 marks)

d. In DFT (Density Functional Theory), what is the property (quantity) of interest? Why DFT is more useful than traditional HF (Hatree Fock) theory for calculating molecular properties?

(20 marks)