



Uva Wellassa University, Sri Lanka  
Faculty of Science and Technology  
Science and Technology Degree Programme  
1<sup>st</sup> Semester Examination – March/April 2013



SCT 433-1 Multi-Scale Modeling Methods in Materials Science

PART II

1.

In the calculation of the single energy of a hydrogen fluoride (HF) molecule, a portion of an output file generated by a molecular modeling code is shown in page 04. Carefully examine it to the answer following questions.

- a. Indicate the theory used for the calculation. Write the wave function corresponding to MO-1. (25 marks)
- b. Indicate clearly the atomic orbitals participating in the formation of MO-1. Is MO-1 normalized? Justify your answer. (25 marks)
- c. Estimate the total electron density of the molecule. (25 marks)
- d. Calculate electron population in the fluorine 2s orbital. Verify your answer using the data shown under atomic orbital electron population data. (25 marks)

2.

- a. State major assumptions made in Hartree – Fock method. (25 marks)
- b. Define the following:  
(i) Basis function      (ii) Primitive Gaussian      (iii) Basis set      (25 marks)
- c. Suppose you are performing electronic structure calculations on the ethanol molecule. Describe the 6-31G basis set for ethanol, including the total number of atomic orbitals. (25 marks)
- d. 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). (25 marks)