



**RAJARATA UNIVERSITY OF SRI LANKA
FACULTY OF APPLIED SCIENCES**

**B.Sc. Honours in Chemistry/ B.Sc. Honours in Chemistry and Physics
Fourth Year - Semester I Examination – January / February 2021**

CHE 4201 – COMPUTATIONAL CHEMISTRY

Time: Two (2) hours

Answer all Questions

1. a) Describe the following terms:

- i. Minimum image convention
- ii. Periodic boundary condition

(40 marks)

b) Two spherical particles are at the positions A and B with coordinates (x_1, y_1, z_1) and (x_2, y_2, z_2) respectively. Dispersion interaction of these particles is represented by Lennard-Jones (12-6) potential function,

$$U(r) = 4\epsilon \left[\frac{\sigma^{12}}{r_{12}^{12}} - \frac{\sigma^6}{r_{12}^6} \right]$$

where r_{12} is the distance between two particles.

Evaluate an expression for the force acting on the particle 2 in the X-direction.

$$\left[r_{12} = \sqrt{(x_2 - x_1)^2 + (y_2 - y_1)^2 + (z_2 - z_1)^2} \right]$$

(40 marks)

c) Write down the main steps of a Monte Carlo simulation in a molecular system.

(20 marks)

2. a) i. Compare the Slater type orbital and Gaussian type orbital
 ii. Identify the pople style Basis Set 6-31G(d) (20 marks)
- b) Explain full Hamiltonian for the Schrodinger equation $\hat{H}\Psi=E\Psi$ is given by,

$$H = - \sum_i^{\text{electronic}} \frac{\hbar^2}{2m_e} \nabla_i^2 - \sum_k^{\text{nuclei}} \frac{\hbar^2}{2m_k} \nabla_k^2 - \sum_i^{\text{electronic}} \sum_k^{\text{nuclei}} \frac{Z_k e^2}{r_{ik}} + \sum_{k < l}^{\text{nuclei}} \frac{e^2 Z_l Z_k}{r_{kl}} + \sum_{i < j}^{\text{electronic}} \frac{e^2}{r_{ij}}$$

Typically, the approximation is made that the 2nd term can be ignored and that the 4th term becomes a constant. What is the name for this approximation? Briefly explain your answer and account for the advantage in computational calculations. (30 marks)

- c) What is LCAO approximation? (20 marks)
- d) Differentiate global maximum from a saddle point. (20 marks)
- e) Write down representation of Methanol molecules in Z-matrix form to be used in Gaussian software. (10 marks)

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