7. Write description on the following :

(a) Polarization and diffuse functions 5

(b) Potential energy surfaces 5

(c) Time correlation functions. 5

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May 2026

M. Sc. (Chemistry) (Second Semester)

Computational Techniques (CHP-110-V)

Time : 3 Hours] [*Maximum Marks : 75*

Note : It is compulsory to answer all the questions (1.5 marks each) of Part A in short. Answer any *four* questions from Part B in detail. Different sub-parts of a question are to be attempted adjacent to each other.

Part A

1. (a) Differentiate between STO and GTO basis functions. **1.5**

(b) Define diffuse functions and discuss their applications. **1.5**

(c) What are Slater Type Orbitals (STOS) ? Mention their advantages and limitations. **1.5**

(d) Explain pair potentials with suitable examples. **1.5**

(e) What is basis set ? **1.5**

(f) Explain the significance of time-step selection in MD simulations. **1.5**

(g) Define mean-square displacement. **1.5**

(h) Differentiate between discrete and continuous random variables. **1.5**

(i) State Bayes theorem. **1.5**

(j) Explain the basic principles of MD algorithms. **1.5**

Part B

2. Discuss molecular dynamics algorithms and their applications in computational chemistry. **15**

3. Explain different types of thermostats and their role in temperature control during simulations. **15**

4. (a) Discuss the importance of basis set selection in quantum chemical calculations. **7.5**

(b) Discuss transition state theory and its significance in computational reaction dynamics. **7.5**

5. (a) Discuss the role of force fields in molecular simulations. **7.5**

(b) Discuss the Lennard-Jones potential and its applications in intermolecular interaction studies. **7.5**

6. Explain factors affecting stability and accuracy in molecular dynamics simulations. Describe periodic boundary conditions and minimum image convention in detail. **15**