

**2005 JAWAHARLAL NEHRU TECHNOLOGICAL UNIVERSITY**

**IV B.TECH I SEMESTER REGULAR EXAMINATIONS  
MOLECULAR MODELLING AND DRUG DESIGN  
(BIO-TECHNOLOGY)**

NOVEMBER 2005

**TIME: 3 HOURS  
MAX MARKS: 80**

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**Answer any FIVE Questions  
All Questions carry equal marks**

1. What is polarization? What is its importance in molecular modeling?
2. Explain the following :
  - (a) simple water models
  - (b) flexible water models.
3. What is a computer simulation? How does it help in understanding molecular systems? What are the two basic types of molecular simulations? How do they differ from each other?
4. Describe how various properties are monitored during the equilibrium phase of a computer simulation of a molecular system.
5. Describe very briefly any four integration methods used in molecular dynamics simulation of molecules with continuous potentials.
6. What are time correlation coefficients? Describe briefly how molecular dynamics simulation can be used to calculate them.
7. Explain the following :
  - (a) Monte Carlo method
  - (b) Metropolis method
  - (c) Markov chain
  - (d) random number generator.
8. Explain the following :
  - (a) cut off region
  - (b) preferential sampling procedure
  - (c) force-bias Monte Carlo method
  - (d) Smart Monte Carlo method.