SUBJECT NO-CY60101, SUBJECT NAME- Computational Chemistry

LTP- 3-0-0,CRD- 3

SYLLABUS :-

Prerequisite : CY41003, CY41002Geometry optimization, Basis set, Frequency analysis, Population analysis, Global and local descriptors.Classical Molecular Dynamics (MD): Lagrangian, Hamiltonian, and Newtonian equations of motions, Various integration algorithms, Periodic boundary conditions and minimum image convention, Potential truncation and shifted-force potentials, Neighbor list, Force calculations, Special methods to handle long range interactions.Classical Monte Carlo (MC): Random numbers, Evaluating integrals using random numbers, Importance sampling, Metropolis algorithm, Smart MC techniques.Analysis of simulated trajectories: Estimation of various distribution functions and transport properties of simulated model systems.Special techniques for simulation of biomolecules and polymers. Ab-initio computing.Books: Computer Simulation of Liquids, by M. P. Allen and D. J. Tildesley; Clarendon Press (Oxford). Understanding Molecular Simulations: From Algorithms to Applications, by D. Frenkel and B. Smit (Academic Press). Quantum Chemistry: (Ref: Hehre, Radom, Schleyer, Pople)