Computational Chemistry - Web course

COURSE OUTLINE

This course deals with different aspects of computational chemistry. Some fundamental computational techniques such as interpolation, matrix methods, the Newton - Raphson method, Fourier transforms and curve fitting are considered in the first part.

The second part deals with quantum mechanical calculations for molecular structures. . Ab initio methods are introduced at the Hartree Fock level and extensions at higher levels of are outlined through explicit examples.

The further extensions of these calculations in explicit solvent models is considered next. Calculations of molecular frequencies, thermodynamic functions and NMR frequencies is also outlined. Methods employed in geometry optimization and computations of transition states is also described.

The next part of the course deals with computations that deal with the applications of statistical mechanics of chemical problems. The molecular dynamics method, constrained dynamics and simulations on liquid Ar and water are considered in detail.

The Monte Carlo method for thermodynamic properties and its applications for the evaluation of integrals is considered next. Biomolecular simulations include applications to polypeptide conformations and structures of RNA and DNA.

COURSE DETAIL

Module No.	Topic/s
1	**Introduction and Numerical Methods:** 1. Introduction 2. Basic Programming Techniques 3. Interpolation and Curve Fitting 4. Roots of Equations 5. Matrix Methods 6. Differential Equations 7. Numerical Integration 8. Integral Transforms
2	**Quantum mechanical calculations** 9. Ab initio methods –I (Hartree Fock) 10. Ab initio methods - II (Post Hartree Fock) 11. Density functional methods 12. Softwares for quantum mechanical calculations 13. Different forms of inputs for Ab initio calculations

NP-TEL

NPTEL

http://nptel.iitm.ac.in

Chemistry and Biochemistry

Pre-requisites:

Chemical thermodynamics, chemical bonding, statistical mechanics, quantum chemistry.

Even exposure to the two later courses may serve as a good starting point.

Coordinators:

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	14. Computation of single point energies 15. Geometry optimization 16. Electron densities and electrostatic potentials 17. Analysis of output for Gausian programmes – I 18. Analysis of output for Gausian programmes - II 19. Molecular frequencies 20. Modeling in solutions - I 21. Modeling in solutions - II 22. Thermodynamic functions 23. NMR frequencies 24. QSAR 25. Transition states
3	**Classical Simulations** 26. Potential Models 27. Concept of Periodic Boundary Conditions (PBC) 28. Generalized coordinates 29. Solution of equations of motions using Finite Difference Methods 30. Basics of Statistical Mechanics - concept of ensemble; time average vs. ensemble average properties 31. Concept of Temperature in simulations 32. Development of a molecular dynamics (MD) code for Lennard-Jones fluids 33. Monte Carlo (MC) method 34. Development of a MC code 35. Analysis of simulated data
4	**Biomolecular simulations** 36. Polypeptide conformations (Aqueous and non aqueous media) – I 37. Polypeptide conformations – II 38. Polypeptide conformations – III 39. Structure of DNA and RNA-I 40. Structure of DNA and RNA-II

References:

Introductory books on quantum chemistry, statistical mechanics and computer programming fundamentals.