

NPTEL Video Lecture Topic List - Created by LinuXpert Systems, Chennai

NPTEL Video Course - Chemistry and Biochemistry - NOC:Computational Chemistry and Classical Molecular Dynamics

Subject Co-ordinator - Prof. B.L. Tembe

Co-ordinating Institute - IIT - Bombay

Sub-Titles - Available / Unavailable | MP3 Audio Lectures - Available / Unavailable

- Lecture 1 - Introduction to Computational Chemistry
- Lecture 2 - Writing Simple Programs
- Lecture 3 - Programming Techniques 1 - Evaluating the sine function
- Lecture 4 - Programming Techniques 2 - Do loops and if statements
- Lecture 5 - Programming Techniques 3 - Roots of a quadratic equation and arrays
- Lecture 6 - Programming Techniques 4 - Arrays and matrices
- Lecture 7 - Practical Session of Programming 1
- Lecture 8 - Programming Techniques 5 - Formats, Functions and Subroutines
- Lecture 9 - Programming Techniques 6 - Functions and Subroutines, arranging numbers in as ascending order
- Lecture 10 - Programming Techniques 7 - Functions and Subroutines, and the common statement
- Lecture 11 - Numerical Methods. Analysis of errors
- Lecture 12 - Practical Session on Programming 2 - The exponential function
- Lecture 13 - Practical Session on Programming 3 - Functions and Subroutines
- Lecture 14 - Interpolation Methods-1
- Lecture 15 - Interpolation Methods-2
- Lecture 16 - Errors in interpolation, Matrix operations
- Lecture 17 - Gauss elimination method for matrix inversion
- Lecture 18 - Matrix diagonalization, Similarity transformations
- Lecture 19 - Matrix inversion, Matrix diagonalization
- Lecture 20 - Curve fitting, Newton Raphson method
- Lecture 21 - Random numbers, Numerical integration using Simpson's rule
- Lecture 22 - Numerical Integration and Differential Equations
- Lecture 23 - Practical Session on Programming 3
- Lecture 24 - Scilab-2
- Lecture 25 - Scilab-3
- Lecture 26 - Scilab-4
- Lecture 27 - Scilab-5
- Lecture 28 - Scilab-6
- Lecture 29 - Classical Molecular Dynamics-2, Force Fields and Equations of Motion

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- Lecture 30 - Classical Molecular Dynamics-3, Force Fields and MD Algorithms
- Lecture 31 - Classical MD-4 Thermodynamic Properties and Distribution Functions.
- Lecture 32 - Classical MD-5, Execution of programs on liquid argon
- Lecture 33 - Molecular Dynamics using Gromacs-1
- Lecture 34 - Molecular Dynamics using Gromacs-2
- Lecture 35 - Molecular Dynamics using Gromacs-3
- Lecture 36 - Molecular Dynamics using Gromacs-4
- Lecture 37 - Molecular Dynamics using Gromacs-5
- Lecture 38 - Molecular Dynamics using Gromacs-6
- Lecture 39 - Molecular Dynamics using Gromacs-7
- Lecture 40 - Molecular Dynamics using Gromacs-8
- Lecture 41 - Molecular Dynamics using Gromacs-9