

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

NPTEL Video Course - Mechanical Engineering - NOC:Foundations of Computational Materials Modelling

Subject Co-ordinator - Dr.Narasimhan Swaminathan

Co-ordinating Institute - IIT - Madras

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

Lecture 1 - Introduction to the course
Lecture 2 - Some applications of MD simulations
Lecture 3 - Introduction to Bravais lattices and constructing simple crystals with MATLAB
Lecture 4 - Introduction to symmetry - 1
Lecture 5 - Symmetry Elements - 1
Lecture 6 - Symmetry elements - 2
Lecture 7 - Plane groups and their Hermann-Mauguin (HM) symbols
Lecture 8 - Glide reflection; Examples of writing point group symbols; Wyckoff positions
Lecture 9 - Generating 2D crystal with MATLAB using Bilbao crystallography website
Lecture 10 - Symmetry of space groups
Lecture 11 - Hermann maugin symbols of space groups
Lecture 12 - Translational symmetry operators
Lecture 13 - The Space groups
Lecture 14 - Generation of crystals
Lecture 15 - Generation of monoclinic lattice
Lecture 16 - Introduction to Statistical Mechanica - 1
Lecture 17 - Introduction to Statistical Mechanica - 2
Lecture 18 - Introduction to Statistical Mechanics - 3
Lecture 19 - Statistical mechanics - 1
Lecture 20 - Statistical mechanics - 2
Lecture 21 - Basic introduction to mechanics
Lecture 22 - Introduction to phase space
Lecture 23 - Introduction to phase average and time average
Lecture 24 - Canonical ensemble; Partition function
Lecture 25 - Basic introduction to MD
Lecture 26 - Input script for LAMMPS - 1
Lecture 27 - Input script for LAMMPS - 2
Lecture 28 - Input script for LAMMPS - 3
Lecture 29 - Input script for LAMMPS - 4

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Lecture 31	-	LAMMPS exercises	-	2
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