JT 208 Computational Methods for Condensed Matter and Materials Science

Credits: 2:0 or 2:1 or Audit

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Atomistic Simulations

- Interatomic potentials or force fields
- A unified framework for structure-composition-properties relation
- First-principles density functional theory based methods of simulations: pseudopotentials, total energy, derivatives of total energy
- Boundary Conditions: Molecules, Clusters and Extended Systems
- Classical potentials; Ewald Summation

Optimization

- Variational principle: mapping of eigenvalue problems, differential equations
- Methods of optimization: Linear problems
- Methods of optimization: Nonlinear and highly nonlinear problems
- Singular Value Decomposition

Machine Learning

- Artificial Neural Networks, Deep Learning
- Kernel Regression methods
- Descriptors: Feature Selection

Simulations for Statistical Mechanical Analysis

- Sampling of phase space within different ensembles
- Monte Carlo Simulations
- Molecular Dynamics (MD) Simulations
- Error Analysis
- Free energies and Phase Transitions
- Fluctuations, Susceptibilities and Transport properties
- Coarse-graining

Desirable back-ground knowledge

- *Linux* operating system and *vi* editor
- Programming in any language
- Courses on Solid State Physics I or Physics of Materials

References

1. Electronic Structure by Richard Martin
2. www.electronicstructure.org
2. Computer Simulations of Liquids by Allen and Tildesley
3. Undersanding Molecular Simulations by Frenkel and Smit

Evaluation

- Three Homework assignments
- Mid-term examination
- Final examination
- A project involving simulations (for 2:1 credits only)