COMPUTATIONAL PHYSICS TFYA90

PART I: MOLECULAR DYNAMICS & MONTE CARLO
Davide Sangiovanni

02/11/2020 Lecture 1: Introduction to atomistic simulations. Statistical mechanics – Molecular Dynamics (MD) and Monte Carlo (MC) methods – examples of applications.

04/11/2020 Lecture 2: Molecular dynamics. Classical molecular dynamics and beyond. Examples of implementations, kinetics of physical/chemical reactions.

09/11/2020 Lecture 3: Stochastic sampling. Monte Carlo techniques, Metropolis algorithm and Simulated Annealing, Kinetic Monte Carlo, Parameter Optimization.

23/11/2020 Lab: Molecular dynamics simulations applied to bulk crystal properties and thin-film growth.

Home assignments: Questions based on concepts from the lectures (deadline for submission is the 23rd of November, 23:30).

Lecture Notes, lab's description and home assignments are available on Lisam.

PART II: THEORY OF MANY-PARTICLE SYSTEMS
Iryna Yakymenko

11/11/2020 Lecture 1: Variational Approach in Quantum Mechanics. Wave function and Hamiltonian for many-particle systems (pp. 90-96 in Lecture Notes).

18/11/2020 Lecture 2: Hartree Equations. Hartree-Fock Equations (pp. 96-100 in Lecture Notes).

20/11/2020 Lecture 3: Jellium model and Thomas-Fermi Approximation. Examples and preparation for lab (pp. 101-105 in Lecture Notes).

30/11/2020 Lab: Modelling of the helium atom within Hartree-Fock approximation.

Home assignments: Modelling of a helium atom using different approximative methods (deadline for submission is the 15th of December, 23:30).

Lecture Notes, lab's description and home assignments are available on Lisam.

PART III: DENSITY FUNCTIONAL THEORY AND IT'S APPLICATIONS
Björn Alling

25/11/2020 Lecture 1: Quantum Mechanics and Density Functional Theory (DFT).
Introduction to modern Density Functional Theory with examples, strengths, and weaknesses.

02/12/2020 Lecture 2: Thermodynamics, vibrations, and phase stability based on DFT.

07/12/2020 Lab: Density functional theory calculations of Aluminium and Silicon.

09/12/2020 Lecture 3: Configurational Thermodynamics and metastable phases.

Home assignments: Questions based on concepts from the lectures (deadline for submission is the 8th of January 2021, 23:30).

Lecture Notes, lab's description and home assignments are available on Lisam.