TOPICS IN COMPUTATIONAL PHYSICS AND MATERIAL SCIENCE

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Course description

This course is intended for graduate students in Physics, Chemistry and Material Science seeking to learn about the key concepts and practical applications of atomic-scale simulations. We begin with simple empirical potential calculations, which provide insight into basics of the supercell approach, modeling of defects, relaxation of atomic positions, lattice and molecular dynamics. The core part of the course is devoted to fundamentals of the density functional theory (DFT) and its application to studying physical properties of molecules and solids. More specifically, the course covers DFT calculations of cohesive and elastic properties, the phase diagram, properties of defects and surfaces.

Module 1 (weeks 1–3): Empirical potentials
- valence force field
- supercells
- geometry optimization
- defects
- vibrational properties (lattice dynamics)
- molecular dynamics

Module 2 (weeks 4–6): Tight-binding theory
- simplest molecules
- bonding in semiconductors
- energy bands
- impurities

Module 3 (weeks 7–9): Fundamentals of density functional theory
- general formulation and numerical methods
- atoms and molecules
- real and reciprocal space
- basis set
- reaction rates

Module 4 (weeks 10–12): Bulk properties of solids *ab initio*
- equilibrium phase diagrams
- elastic properties

– cohesive properties
– geometry optimization
– point defects (structure relaxation, formation energy, defect electronic states)
– planar defects

Module 5 (week 13): Surfaces
– slab model
– reconstruction
– surface energy

Evaluation

The final mark comprises of performance measurements during lectures and practical sessions as well as assignments (no final or midterm examinations).

Prerequisites

The course level is suitable for individuals from a variety of scientific backgrounds with no experience in atomic simulations. The course is well-suited for students who want to use atomic simulations in their work, but do not require extensive knowledge of theory and mathematical details. The material covered is largely self-contained, but an earlier exposure to quantum mechanics, solid state physics and programming is desirable.

Recommended texts

- Joseph M. Thijssen, *Computational physics* (Cambridge University Press, 2007).
- Walter A. Harrison *Electronic structure and the properties of solids: the physics of the chemical bond* (Dover Publications, 1989).
- David S. Sholl and Janice A. Steckel, *Density functional theory: a practical introduction* (John Wiley & Sons, 2009).
- Peter Y. Yu, Manuel Cardona, *Fundamentals of Semiconductors: Physics and Materials Properties* (Springer, 2010).
- Efthimios Kaxiras, *Atomic and electronic structure of solids* (Cambridge University Press, 2003).