MH3623: *Seminar Course in Atomic-scale Materials Science*
PhD course 6.0 credits

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Recommended prerequisites: basic quantum mechanics and statistical physics courses or equivalents.

Goal of the course

The course is intended for PhD students specializing in Materials Science. Its main goal is to give students the necessary knowledge and experience in the development of atomic-scale models of solid materials (metallic and semiconductor alloys) as well as atomistic models of kinetic processes in such materials.

As a result of this course the student should be able to:

1. Specify the basic assumptions and the application limits of the existing theoretical models in solid state physics.
2. Decide whether a quantum- or a classical-mechanical modeling is applicable to a particular problem in materials science and engineering.
3. Choose an optimal model (in terms of accuracy *versus* complexity) for a given material or process.
4. Apply the model and critically assess the model predictions by relating them to experimental observations on real materials.
5. Rationalize experimental data obtained on complex systems in terms of simple atomistic models.

Content of the course

Computer-aided theoretical modeling of atomic-scale processes in materials is nowadays widely used in materials research, complementing the traditional research approaches (experiment and theory). An introduction into the techniques of atomic-scale modeling will be given within the present course. The main emphasis will be made on so-called first-principles calculations, in which the studied system is considered quantum-mechanically as a collection of electrons and nuclei, and atomistic simulations such as Monte Carlo method and molecular dynamics.

The course consists of a seminar series in Atomic-scale Materials Science (AMS), with regular participation of senior scientists, postdocs, and PhD students. The seminars are held weekly by all the seminar participants, according to the schedule maintained by the appointed Secretary (normally a PhD student). Presentations by senior researchers are to be short lectures on relevant subjects within AMS, literature reviews, or research news. Each student is given the task to review the periodic literature or a set of textbook chapters on a specific

topic of first-principles or atomic-scale modeling (by agreement with the Teachers) and prepare at least 3 seminar presentations (45 min. each) about the topic.

Examination:

To successfully pass the Course a student should:

- attend min. 15 seminars,
- prepare and deliver min. 3 presentations withstanding questions from the audience.

Grading system is P (pass). Failure is not an option.

Recommended literature:

1. E. B. Tadmor and R. E. Miller, *Modeling Materials: Continuum, Atomistic and Multiscale Techniques*, (Cambridge University Press, Cambridge, 2011). http://www.cambridge.org/9780521856980

2. G. Grosso and G. Pastori Parravicini, *Solid State Physics*, 2nd edition (Academic Press, 2013). http://www.sciencedirect.com/science/book/9780123850300

3. D. Frenkel and B. Smit, *Understanding molecular simulation: from algorithms to applications*, (Academic Press: San Diego, 1996). http://www.sciencedirect.com/science/book/9780122673511

4. W. Cai W. D. Nix, *Imperfections in Crystalline Solids*, (Cambridge Univ. Press, 2016). http://www.cambridge.org/9781107123137

5. *Handbook on Materials Modeling, Part A. Methods*, Edited by S. Yip, (Springer, Dordrecht, 2005). https://link.springer.com/book/10.1007%2F978-1-4020-3286-8

6. *Handbook on Materials Modeling. Methods: Theory and Modeling*, Edited by W. Andreoni and S. Yip, (Springer Nature Switzerland AG 2020). https://link.springer.com/referencework/10.1007%2F978-3-319-44677-6

7. Presentation handouts and supplementary course material, to be distributed to the seminar participants via e-mail.

Appendix: Sample topics from the previous years

- Interatomic potentials for metals
- Interatomic potentials for non-metals
- Tight binding (TB) method and TB potentials
- Basis sets and electronic structure methods
- Real-space formulation and techniques for electronic structure calculations
- Density Functional Theory
- Hybrid and van der Waals functionals
- Van der Waals functionals within DFT formalism
- Dynamical Mean-field Theory (DMFT): Introduction
- Dynamical Mean-field Theory (DMFT): Examples
- Debye-Grüneisen model
- Lattice dynamics: Density Functional Perturbation Theory
- Force and Stress in Quantum Systems
- Molecular dynamics: Basics
- *Ab initio* Molecular Dynamics
- Molecular dynamics: Ensembles
- Pseudopotentials and the Projector Augmented Wave (PAW) method
- Monte Carlo method from a general perspective
- Free energy modelling, thermodynamic integration
- Hubbard model and strong correlations
- Cluster expansion
- Mean-field methods in statistical physics
- High-throughput methods for materials discovery
- Green's function method for electronic structure calculations
- Crystal plasticity model and its applications
- Introduction to finite-element method (FEM)
- Discrete dislocation dynamics (DDD)
- Atomistic modeling of dislocations
- Modeling of diffusion
- The crystal structure prediction code: USPEX
- Lattice dynamics at temperature: The TDEP approach
- Multiple phase fields and order parameters
- Modeling of paramagnetic state
- Coherent potential approximation: Introduction
- Thermodynamic properties up to melting point: *Ab initio* based approaches
- Structure and Energy of Grain Boundaries
- Molecular Dynamics in Various Ensembles
- Elastic Behavior of Interfaces