Microscopic modeling for sustainable materials applications, 7.5hp

1. Course name and size
Microscopic modeling for sustainable materials applications, 7.5hp

2. Course organization
The course is a joint activity between WISE-universities Örebro University, Uppsala University, Luleå Technical University, and Lund University.

Course nodes
All course developers are lecturing courses in theory of condensed matter physics and mathematics at their respective university and at bachelor, masters, and PhD-level.
• Docent Dr. Danny Thonig, Örebro University University
• Docent Dr. Heike Herper, Dr. Alena Vishina, Uppsala University
• Dr. Corina Etz, Luleå Technical University
• Docent Dr. Erik van Loon, Lund University

3. Course description including intended learning outcome
The goal of this course is to provide an overview of state-of-the-art microscopic modeling techniques, their functionalities, capabilities, and limitations. Though the course focuses on computational methods, it addresses all PhD students within WISE, as measurements and simulations go hand in hand in many research areas, and assessment of the quality of computational modeling is essential for experimental scientists. We will encompass a wide array of theoretical models, including multi-parameter and first principles approaches, state-of-the-art computational methods and tools also relevant for experimental measurements. The applications of these models will be explored not only in the context of designing and analyzing sustainable materials but also in terms of their computational efficiency and sustainability. The theoretical principles taught in the course will be practically applied in hands-on exercise sessions, allowing students to directly engage with the material and with sustainable processes. We encourage the use of freely available software, such as *QuantumEspresso* or *Elk*, which students can use independently in future, to facilitate a deeper understanding and practical application of the course content.

4. Course plan

Pre-requisites and other conditions for access to the course
Master's degree in engineering or natural science or equivalent experience.

Education
The education consists of lectures and practical sessions via video link, group exercises and group project work.

Examination
The course is examined in the following way: writing short reports and peer-to-peer review of lab reports, written report and oral examination of a selected project work. There will be no written exam.

Course content
In line with the increasingly important role of sustainable technologies, materials modelling has become an inherent part of identifying new materials and is a valuable tool to understand the driving mechanisms behind functional materials from the atomic scale up. The goal of this course is to provide an overview of the state-of-the-art microscopic modelling techniques such as first-principles methods, the coupled dynamics of atoms, electrons and spins, data mining and machine learning. The course will discuss the ideas, capabilities, and limitations of these methods and hands-on sessions will let the students work with the techniques themselves. Applicability of the methods for various materials and different ambient conditions will be shown, which will allow the students to choose the best approach to use in their future research.
The real-life cases will be presented of these methods being applied to current-day sustainability issues. Examples will be given of theoretical calculations assisting and guiding the experimental search for materials with desired properties, e.g. permanent magnets and magnetocaloric materials. Modern software allowing to speed up the materials search and automatize the workflow will be touched upon, which can be utilised by the users without previous experience.
The course concludes with a short project where the students will use computational modelling to tackle concrete problems related to sustainable materials.
More in detail:

- Introduction to electronic structure description of solids.
- Overview, basic description, advantages, and limitations of different electronic structure calculation methods.
- Description of ground states and dynamics with (time-dependent) Density Functional Theory (DFT).

- Review of methods - Perturbation theory and system responses - for calculating excited states.
- Molecular Dynamics (MD) simulations
- Optimisation for sustainability: Monte Carlo (MC) simulations for materials behavior at higher temperatures
- Recent big data' methods applied to materials science, e.g. data-mining and machine learning
- Atom-Multiferroic Dynamics (AMfD) simulations
- Overview of various experimental methods used for investigating sustainable materials and the role of microscopic modeling in it.
- Applications of microscopic modelling for sustainable materials
- The examples of the above mentioned methods applied to recent sustainability challenges

Simulation will be performed on individual students' computers.

Learning goals

After completing the course the students are expected to:

i) Knowledge and understanding

- Explain the physical background of different electronic structure and microscopic modeling methods.
- Describe the implementation methods used in different electronic structure and microscopic modeling techniques.
- Exemplify what electronic structure and dynamics computational methods are used for and what kind of questions can be answered.
- Evaluate how computational physics fits into today's research in material and product development
- Name different experimental methods that provide information about the properties of interest for different systems

ii) Competence and skills

- Apply and use different computational techniques
- Design electronic structure calculations as well as dynamics simulations for model systems and real materials, in order to simulate their properties and predict technological applications
- Plan, execute, assess and present electronic structure and dynamics simulations
- Identify and correct the most common sources of error in calculations.
- Identify the appropriate method needed to describe different systems and properties.
- Analyze (evaluate and assess) results from simulations.

iii) Judgment and approach

- Determine which models and which approximations can be used in simulations, in order to generate meaningful results.

- Make a critical assessment of the used model and approximations, as well as of the results of simulations.
- Give a physical interpretation of the outcome of simulations.
- Relate and compare results of computational simulations to experimental data.

Tentative schedule

Lectures

The course will have a number of lectures introducing different approaches in microscopic modelling techniques, with a focus on applications to sustainable materials science. In addition to the theory, the lectures will also introduce the practical tools/codes that will be used in the labs (e.g., QuantumEspresso). The 16 lectures will be given online.

Course outline

Date & Time	**Module**	**Lecturer**
W47		
2024/11/18 10-12	Lecture 1. *Introduction to the course and Motivation/ Computing Aspects*	All
2024/11/20 10-12	Lecture 2. *Theoretical Foundations and Electronic structure methods*	Heike Herper
W48		
2024/11/25 10-12	Lecture 3. *Electronic structure methods*	Heike Herper
2024/11/27 10-12	Lecture 4. *Electronic structure methods*	Heike Herper
W49		
2024/12/02 10-12	Lecture 5. *Molecular Dynamics*	Danny Thonig
2024/12/04 10-12	Lecture 6. *Molecular Dynamics*	Danny Thonig
W50		
2024/12/09	Lecture 7. *Coupled Dynamics in Materials*	Erik van Loon
2024/12/11	Lecture 8. *Coupled Dynamics in Materials and Perturbation theory*	Erik van Loon
W51		
2024/12/16	Lecture 9. *First Principles Approach to Sustainable Materials*	Danny Thonig

2024/12/18	Lecture 10. *First Principles Approach to Sustainable Materials*	Erik van Loon
W2		
2025/01/07	Lecture 11. *Data-mining and machine learning*	Alena Vishina
2025/01/08	Lecture 12. *Optimisation for sustainable Materials*	Alena Vishina
W3		
2025/01/13	Lecture 13. *Multiferroics and Dynamics*	Corina Etz
2025/01/15	Lecture 14. *Multiferroics and Dynamics*	Corina Etz
W4		
2025/01/20	Lecture 15. *First Principles Approach to Sustainable Materials*	Alena Vishina
2025/01/22	Lecture 16. *Practical Applications and Case Studies*	Corina Etz

Practical Sessions

For the labs and project, we plan for the students to work in groups of 3-4, when possible localized at a single node so they can meet and work together in person. The course contains 5 labs and the final project. The labs will allow the students to test and try the methods/tools introduced in the preceding lecture.

For all the labs, each group will hand in a short report. Each group will then peer review a report of a different group. The lecturers will give feedback on the reports+peer reviews.

For the project, the groups will be given a list of small projects to choose from (based on, e.g., important papers from the field and allowing the students to utilize their acquired skills). Each project group will have an assigned teacher to help and provide feedback. The groups will present their project at the end of the course.

2024/11/25 13-15	Lab 1. *Electronic structure methods*	Heike Herper
2024/12/02 13-15	Lab 2. *Molecular dynamics*	Danny Thonig

2024/12/09 13-15	Lab 3. *Coupled Dynamics*	Erik van Loon
2024/12/16 13-15	Lab 4. *Data-mining and machine learning*	Alena Vishina
2025/01/13 13-15	Lab 5. *Multiferroics*	Corina Etz
On individual basis	Project - Introduction to the projects (and fixing residual issues from previous labs) - Consultations with assigned teacher	All
2025/02/10 13-15	Project: Oral presentations	All

Examination

3 assignments

- Written lab reports: exercises from Lab 1 to 5
- Peer-review on lab report of one other group
- Final Project and Oral presentation

Grading

All the assignments are mandatory. A passing grade is required for each assignment in order to pass the course.

The course is graded pass/fail (G/U).

5. Number of participants

The project work limits the number of participants. Each tutor is supposed to supervise two project groups with 4 students each. Hence, 5*4*2 = 40. The lectures are open for all.

6. Literature

Thijssen, J. M. “Computational Physics” ISBN 9780521833462, Cambridge University Press (2007)

Basic reading:

Sander, L. M. “Advanced Condensed Matter Physics” ISBN 978-0521872904, Cambridge University Press (2009)

Additional material from the course’s website: Canvas