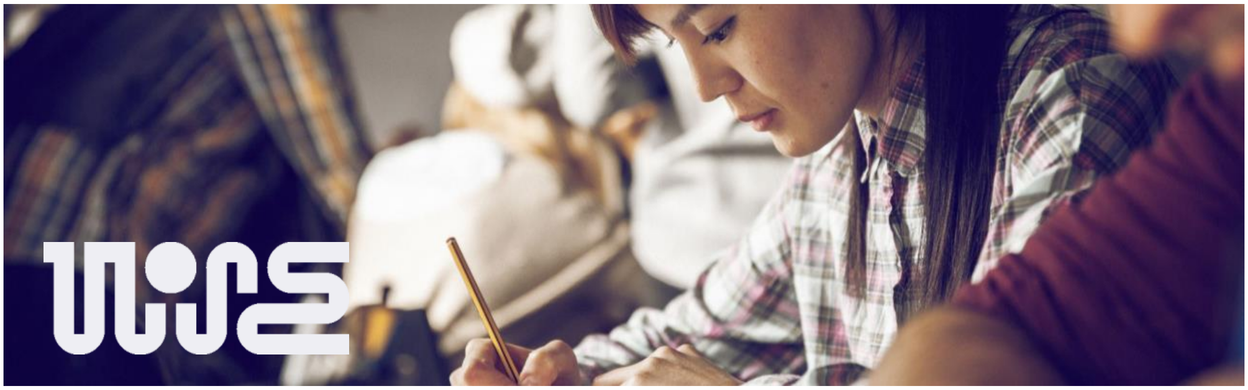

Microscopic modeling for sustainable materials applications, 7.5hp

Course guide autumn term 2024, a joint activity between WISE-universities Örebro University, Uppsala University, Luleå Technical University, and Lund University.

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Teacher:

Docent Dr. Danny Thonig, Örebro University
Docent Dr. Heike Herper, Uppsala University
Dr. Alena Vishina, Uppsala University
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Docent Dr. Erik van Loon, Lund University

Examinator: all teachers listed above.
Course organisations: The course is a joint activity between WISE-universities Örebro University, Uppsala University, Luleå Technical University, and Lund University.

Course purpose

The goal of this course is to provide an overview of state-of-the-art microscopic modeling techniques, their underlying basic theory, 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*, *Lammps, Phonopy*, *EPW*, and *UppASD*, which students can use independently in future, to facilitate a deeper understanding and practical application of the course content.

Course goal

Knowledge and Understanding

Upon completion of the course, the student should be able to:

- Explain the physical background of different materials modelling methods, including electronic structure and microscopic modeling methods.
- Exemplify what different materials modelling methods are used for and what kind of questions can be answered, in the application on sustainable materials.
- Evaluate how computational physics and microscopic modeling 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

Skills and Abilities

Upon completion of the course, the student should be able to:

- Apply and use different computational techniques for sustainable applications
- Design electronic structure calculations, spectroscopy, dynamics, phase transition, as well as high throughput simulations for real materials, to simulate their properties and predict sustainable applications
- Plan, execute, assess and present outcomes of microscopic modeling 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.

Judgment and Approach

Upon completion of the course, the student should be able to:

- 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.

Course content

The course covers the following topics:

- Introduction to first principles electronic structure modelling of materials
- Introduction to molecular dynamics
- Recent ‘big data’ methods applied to materials science, e.g. high-throughput simulations, data mining and machine learning
- Introduction to spectroscipy and linear response
- Review of methods - Perturbation theory and system responses - for calculating excited states.
- Optimization for sustainability: Monte Carlo (MC) simulations for materials behavior at higher temperatures
- Introduction to phase transition
- Developing basic knowledge for computation and programming in python and within jupyter notebooks
- Training with scientific codes such as Quantum Espresso, Lammps, EPW, and UppASD
- 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

Course Pre-requisites

Master’s degree in engineering or natural science or equivalent experience. Basic knowledge in condensed matter physics. No pre-knowledge in python programming required.

Course activities

The course is build from **16 Lectures** and **6 regular Practical sessions**. Furthermore, you are suppose to work on dedicated projects worth **6 sessions**. All course activities will be hold online, via Zoom.

The main zoom link is
https://oru-se.zoom.us/j/68549809932?pwd=RUhiMjhBSWxCYVk0dmlRU1ImMzJWQT09

Due to limitations of Zoom, each teacher has his/her own Zoom link:

Heike Herper: https://uu-se.zoom.us/j/65823674447

Danny Thonig: https://oru-se.zoom.us/j/68549809932?pwd=RUhiMjhBSWxCYVk0dmlRU1ImMzJWQT09

Erik van Loon: https://lu-se.zoom.us/j/68796470393?pwd=9TISQGbff9LWWU1F6uS5HNbKV6mw7D.1

Alena Vishina: https://uu-se.zoom.us/j/65823674447

Corina Etz: https://ltu-se.zoom.us/j/64058547042

Note that we were asked to trace the attendance at the course. We will do that using the canvas tool **RollCall.**

Rules in Zoom

We will record all lectures and labs and will provide them to the students in a Box folder, since Canvas has limited space. The link to the Box folder is https://uppsala.box.com/s/ap21gjcou4o8mm48mu24kkscreedl1ry

In Zoom, we leave it to the student to have the Camera on, but we ask you
- To be muted, except you have questions or comments,
- To have your full First- and Surname displayed as Zoom username.

In case you have questions, but you do not want to be recorded, please say so and we stop the recording for it.

The idea is that you will be able to do the labs and exercises on your own computer. In case you encounter substantial difficulties, it is possible to use the “remote control” feature in Zoom to get additional help, if you agree. Details can be found here https://support.zoom.com/hc/en/article?id=zm_kb&sysparm_article=KB0065790 .

Lectures

In the theoretical segment of this course, covered by the course lecture, students can expect to encounter basic underlying theoretical concepts of microscopic modelling that will be introduced, discussed, and possibly applied. The 16 lectures, 2 hours each, will delve into introducing different approaches in microscopic modelling techniques, with a focus on applications to sustainable materials science. To bolster students understanding, selected these models demonstrated with the help of well-established computational tools. While attendance at the lectures is not compulsory, it is highly recommended. The reason is that the course goes beyond the course literature during lectures, offering additional material such as diverse examples and valuable strategies that can facilitate meeting the course requirements.

The lectures will take place on Zoom. Students should always have their laptops or tablets ready at the class, with the following digital tools: i) provided Jupyter environment, ii) KTH Canvas iii) Padlet (distributed in advance), iv) Mentimeter. The first is necessary for hands-on engagement with provided code examples, while the others serve for rapid feedback and quizzes conducted during the lectures. If students wish to ask questions anonymously, feel free to use the course padlet.

In the tables below, you can see what will be covered during each session, which sections in the provided literature correspond to it (Table below).

Course outline (Literature is available further down in the text)

Date & Time	**Module**	**Lecturer**	**Literature**
W47			
2024/11/18 10-12	Lecture 1. *Introduction to the course and Motivation/ Computing Aspects*	All	
2024/11/20 10-12	Lecture 2. *Electronic structure methods*	HH	Thijssen, Chap. 3-5, Koch/Holthausen Chap. 1
W48			
2024/11/25 10-12	Lecture 3. *Electronic structure methods*	HH	Thijssen Chap. 5-6, Koch/Holthausen Chap. 4-5, advanced reading: Martin, Chap. 9
2024/11/27 10-12	Lecture 4. *Electronic structure methods*	HH	
W49			
2024/12/02 10-12	Lecture 5. *Molecular Dynamics*	DT	
2024/12/04 10-12	Lecture 6. *Molecular Dynamics*	DT	
W50			
2024/12/09 10-12	Lecture 7. *Coupled Dynamics in Materials*	EvL	

2024/12/11 10-12	Lecture 8. *Coupled Dynamics in Materials*	EvL	
W51			
2024/12/16 10-12	Lecture 9. *Molecular Dynamics for Sustainable Materials*	DT	
2024/12/18 10-12	Lecture 10. *Coupled Dynamics for Sustainable Materials*	EvL	
W2			
2025/01/07 10-12	Lecture 11. *Data-mining and machine learning*	AV	
2025/01/08 10-12	Lecture 12. *Data-mining and machine learning*	AV	
W3			
2025/01/13 10-12	Lecture 13. *Phase transition theory*	CE	
2025/01/15 10-12	Lecture 14. *Phase transition theory*	CE	
W4			
2025/01/20 10-12	Lecture 15. *Data-mining and machine learning for Sustainable Materials*	AV	
2025/01/22 10-12	Lecture 16. *Phase transition theory for Sustainable Materials*	CE	

Preparing for the lecture

Later lectures in a module start with a brief recap of the preceding lecture, either via discussions or tools like Mentimeter or Canvas quizzes. As such, students' active participation in recalling and discussing the prior lecture's content is not only encouraged but vital in contributing to the collection of information required for the summary. Additionally, students are encouraged to submit questions in advance of each lecture, either via Canvas, email or on the lecture's Padlet platform. These questions will be addressed by the lecturer during the summary segment.

Goals of the lecture:

The learning objectives for the theory part are as follows: After completing the course, the student should be able to:

- Understand basics about
    - Density functional theory
    - Molecular modelling on classical and quantum mechanical potentials
    - Light-matter interaction at the level of the Random Phase Approximation
- Understand how these concepts link to the modelling of sustainable materials
- Have a general idea of machine learning and data-mining approaches to materials modeling and discovery
-

The learning objectives are a summary of several fundamental sub-goals, to which a number of advanced sub-goals are added.

Among the fundamental sub-goals, the student should be able to:

- Understand the strengths and weaknesses of materials databases and use them to find the necessary materials properties
- ???

The advanced sub-goals include the ability to:

- Use their knowledge about different exchange-correlation functionals and when to apply them.
- Determine Hellman-Feynman forces from density functional theory
- Choose a suitable tool to automate their calculations for data mining
- ???

Computer Labs

Note that all computer labs will be performed on individual students' computers. The labs allow the students to test and try the methods/tools introduced in the preceding lecture.

Regular Labs

In the 5 regular computer labs, each lasting 2 hours, teachers demonstrate the use of different scientific software tools for microscopic modelling and apply it, mostly to simple test materials first. Weekly exercises will be shared before each occasion and time will be allocated to start solving these exercises with the gained knowledge of the respective lab. The computer labs are dedicated to the hands-on aspect of the course, with a particular emphasis on runing the software tools and understanding their in- and outputs. This practical training will be structured through a series of exercises (weekly), allowing you to actively engage with the course material. You will collaborate in small groups, typically comprising 3 students. These groups will be assigned randomly by the course tutor and will remain constant throughout the duration of the course and also for the project works. You can find your assigned group number in a separate document provided to you. The computer labs are not compulsory, but are highly recommend attending them. These occasions provide a place to meet for the group work as well as to interact with the teacher and ask questions. Your active participation in these lab sessions is encouraged and can greatly enhance your learning experience.

In order to make easily the scientific software available to all students, the container software Docker and, from within the container, Jupyter notebooks will be used. ***The student has the responsibility to install the docker and the provided container in advance of the course start and not later than the first week of the course.*** Details about the installation and use, can be found on the separate “computer lab website”

https://wise-course-modelling-2024-cahmd-db7774fb7ae62bb7ad65142223823a.gitlab.io/index.html

Make sure that you have also basic understandings of the underlying programming language Python. Tutorials and recommendations are also provided on the “computer lab website”. Please contact the tutors, in case you need support with the installation or if you have questions about the software, programming language etc..

Course scheme for the regular labs is

2024/11/25 13-15	Lab 1. *Electronic structure methods*	Heike Herper
2024/12/02 13-15	Lab 2. *Molecular dynamics*	Danny Thonig
2024/12/11 13-15	Lab 3. *Coupled Dynamics*	Erik van Loon
2025/01/07 13-15	Lab 4. *Data-mining and machine learning*	Alena Vishina
2025/01/13 13-15	Lab 5. *Phase transition theory*	Corina Etz

Project work and Consulting Labs

The main part of the computer lab module is the project work, which is mainly in the students responsibility. The projects are based on, e.g., important papers from the field. You, as a group (same group as for the regular labs), are suppose to select one project out of 5 projects. Each project is supervised by on of the teachers. To balance the projects and the amount of supervision for each teacher, maximum two groups can work on the same topic. A poll will be opened beginning of December, where you can register for a project following “first-come-first-serve” rule.

The projects are:
- Will be announce soon, supervised by Danny Thonig
- Will be announce soon, supervised by Corina Etz
- Will be announce soon, supervised by Heike Herper
- ‘Ferroelectric materials’, supervised by Erik van Loon
- ‘Finding the best Co3Mn2Ge-based permanent magnet’, supervised by Alena Vishina

The topics of the projects are balanced to cover at least 2 of the courses main topics. Each project as a dedicated teacher. You have about one month to actively work with the project. Students are responsible to schedule an introduction meeting with their supervisors. Here, even further details on the project will be presented. After, students are suppose to schedule consulting meetings with the supervisor on their need and progress, but you should have at least three meetings (no dedicated length).
The time table for the project work is

On individual basis	Project - Introduction to the projects (and	All

	fixing residual issues from previous labs) - Consultations with assigned teacher	
2025/02/10 13-17	Project: Oral presentations	All

Goals of the labs
The learning objectives for the computer laboratory part are as follows:

After completing the course, the student should be able to understand and use the some principle scientific software:
- Quantum Espresso
- Lammps incuding visualisation with VMD
- Phonopy
- EPW
- UppASD

The learning objectives summarize a number of fundamental sub-goals, to which a number of advanced sub-goals are added.
Among the fundamental sub-goals for the computer laboratory part, the student should be able to, based on the theoretical goals, evaluate:
- Models and software related to real-world applications
- Integratability with experimental methods
- Design and Conduct Simulations
- Present Outcomes Effectively
- Collaborative Problem Solving

Among the advanced sub-goals for the computer laboratory part, the student should be able to implement and, based on the theoretical goals, evaluate:
- Independent Problem-Solving in Simulations
- Independent adapting software input on problems in sustainable application simulations
- Foster Sustainable Innovation

The final sub-goals are for students to develop the ability to independently work out the selection of microscopic modelling, implement them into usable material, and present them to a group.

Literature

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

Basic reading:

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

Electronic structure

[3] Koch, W.; Holthausen, M. C. “A Chemist’s Guide to Density Functional Theory.” Wiley-VCH Verlag, Second Edition (2001)

[4] Martin, R. “Electronic structure: basic theory and practical methods.” Cambridge University Press (2004)

Molecular Dynamics

[5] D. Frenkel, B. Smit, “Understanding Molecular Simulation - From Algorithms to Applications”, ACADEMIC PRESS (2002)
[6] M. P. Allen and D. J. Tildesley, Computer Simulations of Liquids, Clarendon Press, 1989.
[7] J. M. Haile, Molecular Dynamics Simulation, John Wiley & Sons, 1992.

Additional material will be provided on Canvas.

Note: A digital copy of the literature is provided in our Box folder: https://uppsala.box.com/s/ap21gjcou4o8mm48mu24kkscreedl1ry .

Examination and Grades

Depending on how you registered for the coures, you have one of the following examinations:

i) **Theory and problem solving**, **2.5 hp** - for those with lectures only

or

ii) **Theory and problem solving + Computer-aided calculations, 7.5 hp**

Theory and Problem solving, 2.5 hp

Goal

The goal of the exam is that

- choose and apply an appropriate method to solve problems in sustainable materials modelling,
- argue for your approaches using concepts, relationships, and different theories in microscopic modelling, and present clear reasoning

Execution

For students taking the lectures only, the part Theory and Problem solving will be examined individually and orally in a 15min discussion with two teachers. For students performing also the **Computer-aided calculations (see below)**, examination form ii), the Theory and Problem solving examination will be integrated into the final project presentation (see below).
You are allowed to use course presentations, course scripts, course books etc. for the examination, as long as searching for answers are not hindering the examination process.

Grading criteria and grading
The grading for the examination is as follows: U (unsatisfactory), G (satisfactory). Criterias are

- Student knows and understand basic aspects of microscopic modelling
- Student has an understanding how the methods and the modelling in general can improve sustainability aspects

Computer-aided calculations, 5hp

Goals
Goals that which will be examined are

- develop notebooks and use scientific programs to visualize and solve microscopic modelling problems.
- develop sense for inputs and outputs as well as the applicability of certain codes for sustainability applications
- develop independence in microscopic model applications and sense how to tackle challenges in modelling.

Execution

Regular Labs
For the first five labs, there will be weekly assignment exercises that the students must solve in groups. These assignments are based on the topic of the weekly labs and contain mainly computational aspects and modifying Jupyter notebooks. The results must be reported, preferably in a modified Jupyter notebook, and submitted before a certain deadline. As part of the exercise, students are asked to peer-to-peer review the previous lab reports from the other groups. The allocations which groups reviews what others group report will vary and communicated for the individual assignments. The grading will be via 'U' or 'G'.

Project work and Consulting Labs
Main examination of the course is the project work (see above). The groups must submit a final report about their project and defend this project in front of a committee. The submission day is **Thursday, 6th of February 2025**.

There is no limit for the report length, but this time it will be not sufficient to just submit a Jupyter notebook. Evaluation criteria for the report:

- clear motivation for the use of certain codes and input setups
- scientific interpretation of the outputs
- adequate visualization of data
- reflection on aspects about sustainability
- engagement in supervision meetings

The report should contain also a minimum half page discussion about sustainability aspects of the project. Please remember that the project work is a group work and all in the team should be updated on the progress and achievements. Hence, together with the report submission, each individual student from the group must submit a 5min video pitch about the project. The videos coming from each group must be distinct from each other. Here, the individual understanding of the project

The project works need to be defended within a 20min presentation followed by a 20min defense where the committee, consisting out of three teachers and two other groups, can ask questions about the project but also aspects from the lecture. Students should make sure that each individual from the group is presenting certain part of the project work.

Grading criteria and grading

The grading for the examination is as follows: U (unsatisfactory), G (satisfactory). Criterias are

- Student knows and understand basic aspects of microscopic modelling
- Student manage to run certain scientific software tools for microscopic modelling and apply it for sustainability applications

- Students scientifically present and defend a project that includes microscopic modelling and linking it towards sustainability aspects.
- Individually pitching project works
- Active engangement in the supervision meetings and group work.

Final grade for the lab

To successfully finish the lab with a ‘G’, you need to pass 3 out of the 5 labs exercise with a ‘G’. Furthermore, your video pitch as well as the final project including the defense need to be approved with a ‘G’. Not satisfying these conditions gives you an ‘U’.

Final grade of the course

You pass the course if you have a ‘G’ in the “Theory and problem solving” for students registered just for (i) or a ‘G’ in the “Theory and problem solving + Computer-aided calculations” for students registered for (ii).