SYLLABUS

Computational Methods for Nanomaterials 7.5 credits F7051T

Beräkningsmetoder för nanomaterial

Course syllabus admitted: Autumn 2023 Sp 1 - Present

DECISION DATE
2023-02-15

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LULEÅ TEKNISKA UNIVERSITET

Computational Methods for Nanomaterials 7.5 credits F7051T

Beräkningsmetoder för nanomaterial

Second cycle, F7051T

Education level	Grade scale	Subject	Subject group (SCB)
Second cycle	U G#	Fysik	Physics

Entry requirements

M0047M Differential Calculus, M0048M Linear algebra and integral calculus, M0049M Linear algebra and differential calculus; F0047T Quantum physics; F7045T Solid state physics or equivalent. Be able to write simple computer programs (e.g. D0009E). Good knowledge in English, equivalent to English 6.
It is beneficial to be able to use Matlab or Gnuplot for data analysis, and have studied F7035T Statistical Physics and Thermodynamics as well as M0014M Mathematical Physics, or equivalent.

Selection

The selection is based on 30-285 credits

Course Aim

After a successfully completed course, the student should be able to:

1. Knowledge and understanding

- Explain the physical background of different electronic structure and dynamics computational methods.
- Describe the implementation methods used in different electronic structure and dynamics simulations 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

2. 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.

3. Judgement 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 computational simulations to experimental data.

Contents

Introduction to electronic structure description of solids and nanostructures. Overview of different methods of electronic structure calculations.
Basic description, advantages and limitations for different computational methods.
Overview of various experimental methods used for investigating solids and nanostructures.
Use of different methods depending on the system's length-scale and the excitations' time-scale.
Description of ground states with Density Functional Theory (DFT) and review of methods for calculating excited states.
Monte Carlo (MC) simulations
Atom-Spin Dynamics (ASD) simulations
Molecular Dynamics (MD) simulations

Introduction to and usage of supercomputers (e.g. Kebnekaise vid HPC2N, Umeå) for simulations.

Realization

Each course occasion´s language and form is stated and appear on the course page on Luleå University of Technology's website.

The theoretical part of the course will be taught in form of lessons, as well as material for individual study. The practical part of the course consists of hands-on computer tutorials and exercises, when the student has the opportunity to put in practice the theoretical part covered by the lectures. The outcome of the practical sessions will be complemented by homework assignments and the result shall be summarized by the student in written reports. The reports need to be well structured, have the standard of a scientific report and have the main focus on the analysis and physical interpretation of the results obtained in simulations.
In order to reach the course aims, we suggest the student to attend and actively participate to the lessons and practical sessions, as well as study the recommended material.

Examination

If there is a decision on special educational support, in accordance with the Guideline Student's rights and obligations at Luleå University of Technology, an adapted or alternative form of examination can be provided.

Compulsory laboratory work with written reports summarizing the results from the practical sessions.

Unauthorized aids during exams and assessments

If a student, by using unauthorized aids, tries to mislead during an exam or when a study performance is to be assessed, disciplinary measures may be taken. The term “unauthorized aids” refers to aids that the teacher has not previously specified as permissible aids and that may assist in solving the examination task. This means that all aids not specified as permissible are prohibited. The Swedish version has interpretative precedence in the event of a conflict.

Course offered by

Department of Engineering Sciences and Mathematics

Modules

Code	Description	Grade scale	Cr	Status	From period	Title
0005	Practical sessions and written reports	U G#	7.5	Mandatory	A23	

Study guidance

Study guidance for the course is to be found in our learning platform Canvas before the course starts. Students applying for single subject courses get more information in the Welcome letter. You will find the learning platform via My LTU.

Last revised

by Mats Näsström, Head of Undergraduate Education 2023-02-15

Syllabus established

by Mats Näsström 2018-02-15