UNIVERSITY OF GOTHENBURG

DEPARTMENT OF PHYSICS

FYM320 Computational materials and molecular physics, 7.5 credits

Beräkningsmetoder för material- och molekylfysik, 7,5 högskolepoäng

Second Cycle

Confirmation

This course syllabus was confirmed by Department of Physics on 2019-11-04 and was last revised on 2023-05-08 to be valid from 2024-01-15, spring semester of 2024.

Field of education: Science 100%
Department: Department of Physics

Position in the educational system

The course is elective within the master program in physics.

The course can be part of the following programmes: 1) Complex Adaptive Systems, Master's Programme (N2CAS) and 2) Physics, Master's Programme (N2PHY)

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Main field of studies	*Specialization*
Physics	A1N, Second cycle, has only first-cycle course/s as entry requirements

Entry requirements

A Bachelor's degree in physics or equivalent, including 30 credits mathematics (including linear algebra and analysis), and programming.

Some knowledge of Computational physics and numerical methods is recommended.

Applicants must prove their knowledge of English: English 6/English B from Swedish Upper Secondary School or the equivalent level of an internationally recognized test, for example TOEFL, IELTS.

Learning outcomes

The aim of the course is to outline modern computational methods and schemes providing challenges for the future and to develop practical experience in carrying out high performance computing. The course introduces numerical methods and new areas of physics that can be studied with these methods. It gives examples of how physics can be applied in a much broader context than usually discussed in the traditional physics undergraduate curriculum and it teaches structured programming in the context of doing science.

On successful completion of the course the student will be able to:

- Comprehend and analyze different electronic structure methods, such as Hartree-Fock and Density Functional Theory
- Comprehend and apply MD simulation and Monte-Carlo technique to investigate material properties with the help of computers
- Use the objected-oriented scripting language Python to solve numerical problems and to steer and organize large scale computing tasks and to provide simple visualization
- Write technical reports where computational results are presented and explained
- Communicate results and conclusions in a clear way.

Course content

- Basics of Hartree-Fock and Density Functional Theory for the electronic structure problem
- Molecular dynamics and Monte-Carlo simulation technique for many-particle systems
- Python and in particular modular programing in Python

Form of teaching

Basic theory and methods are covered by a series of lectures. The students get training by applying the theory and methods in exercises and homework problems. An important part consists of practical training of carrying out large-scale computations using primarily preexisting molecular dynamics and/or electronic structure codes. This training includes also experience of using Python, an object-oriented scripting languages, as a common platform to steer and analyze and combine results from various codes.

Language of instruction: English

Assessment

The examination can be adjusted to previous background and interests. In general the examination consists of coding assignments, computing-lab assignments, theory assignments and more individualized projects with a report and a presentation. All examination parts will be graded.

If a student, who has failed the same examined element on two occasions, wishes to change examiner before the next examination session, such a request is to be submitted to the department in writing and granted unless there are special reasons to the contrary (Chapter 6, Section 22 of Higher Education Ordinance).

In the event that a course has ceased or undergone major changes, students are to be guaranteed at least three examination sessions (including the ordinary examination session) over a period of at least one year, though at most two years after the course has ceased/been changed. The same applies to work experience and VFU, although this is restricted to just one additional examination session.

Grades

The grading scale comprises: Pass with Distinction (VG), Pass (G) and Fail (U).

Course evaluation

The results of and possible changes to the course will be shared with students who participated in the evaluation and students who are starting the course.