Course Syllabus

Skoltech

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Contact Person	Alexander Kvashnin
Contact Person's E-mail	a.kvashnin@skoltech.ru
Course Title (in English)	Computational Methods in Atomistic Simulations
Course Title (in Russian)	Вычислительные методы в атомистическом моделировании
Lead Instructor	Kvashnin, Aleksandr

Here's a structure of the form below:

1. Annotation
2. Basic Information
3. Course Content
4. Learning Outcomes
5. Assignments and Grading
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1. Annotation

Course Description

Course will cover both classical and modern topics of computational methods in atomistic simulations of condensed matters. We will begin from classical representations of electric and heat transport in condensed matter and will finish with modern theories covering the molecular dynamics methods coupled with density functional theory and applications of machine learning. Practical part of the course will be devoted to hands-on sessions where students will apply these theories on practice by performing calculations of real materials. This will give an entire picture of applied computational methods allowing the solution of various tasks like calculations of mechanical properties of solid-state compounds, lattice dynamics, thermal conductivity etc.

Аннотация

Курс будет охватывать как классические, так и современные темы вычислительных методов в атомистическом моделировании конденсированных сред. Курс начнется с классических представлений переноса электричества и тепла в конденсированном веществе и закончится современными теориями, охватывающими методы молекулярной динамики в сочетании с теорией функционала электронной плотности и приложениями машинного обучения. Практическая часть курса будет посвящена практическим занятиям, на которых студенты будут применять эти теории и методы на практике, выполняя расчеты реальных материалов. Это даст полное представление о прикладных вычислительных методах, позволяющих решать различные задачи, такие как расчеты механических свойств твердых тел, динамики решетки, теплопроводности и т.д.

2. Basic Information

Course Academic Level MSc PhD

Course Academic Level Master-level course suitable for PhD students

Number of ECTS credits 6

Course Prerequisites / Recommendations

Students should be familiar with basics of materials science, classical mechanics, basic programming skills. Ideally it should follow an introductory course in Materials Science and Introduction to Solid State Physics.

Type of Assessment Graded

Grading Scale

A: 86

B: 76

C: 66

D: 56

E: 46

Course Term (in context of Academic Year) Term 2

Students of Which Programs do You Recommend to Consider this Course as an Elective?

BSc Programs: , Masters Programs: Advanced Manufacturing Technologies
Applied Computational Mechanics
Materials Science, PhD Programs: Computational and Data Science and Engineering
Materials Science and Engineering

Maximum Number of Students

	Maximum Number of Students
Overall:	14
Per Group (for seminars and labs):	

Course Stream Science, Technology and Engineering (STE)

3. Course Content

ECTS Credit System – Reference Tool

Topic: Introduction to quantum mechanics, Summary of Topic: Introduction to quantum mechanics, Contact Hours: Lectures: 2, Contact Hours: Seminars: 0, Contact Hours: Labs: 0, Non-contact Hours: Student's Independent Study: 8
Topic: Description of materials, Summary of Topic: Classical representation; Quantum mechanical representation; Thermal properties of materials; Debye model, Sommerfeld model; Wiedemann-Franz law in quantum and classical representations; Electronic properties of materials; density of states; conductivity; electronic contribution to thermal conductivity;, Contact Hours: Lectures: 6, Contact Hours: Seminars: 0, Contact Hours: Labs: 0, Non-contact Hours: Student's Independent Study: 8
Topic: Methods for atomistic simulations, Summary of Topic: Interactions in materials; Classical molecular mechanics and dynamics; introduction to quantum mechanical methods; Basics of Hartree-Fock and density functional theory; Pseudopotentials; Kohn-Sham equations, Contact Hours: Lectures: 8, Contact Hours: Seminars: 4, Contact Hours: Labs: 4, Non-contact Hours: Student's Independent Study: 16
Topic: Mechanical properties of materials, Summary of Topic: Basic definitions, young’s modulus; bulk and shear moduli; Hooke’s law; Definition and determination of elastic tensor; symmetry and mechanical properties; Elastic waves in crystals; elastic and mechanical properties of 2D materials; non-linear characteristics; hardness and fracture toughness; computational models for hardness; , Contact Hours: Lectures: 6, Contact Hours: Seminars: 2, Contact Hours: Labs: 2, Non-contact Hours: Student's Independent Study: 16
Topic: Mechanical properties from atomistic simulations, Summary of Topic: Deformations; stresses; Algorithms for relaxations and calculations; Recommended strategy and parameters; pre- and post-processing of the data; Scripting , Contact Hours: Lectures: 4, Contact Hours: Seminars: 6, Contact Hours: Labs: 6, Non-contact Hours: Student's Independent Study: 24
Topic: Advanced methods for mechanical properties determinations, Summary of Topic: Machine learning for mechanical properties; ML potentials for description of mechanical properties; mechanics of complex solids; polycrystals; composites; multi-phase systems; AI models towards high-throughput screening for materials; symbolic regression; , Contact Hours: Lectures: 6, Contact Hours: Seminars: 6, Contact Hours: Labs: 4, Non-contact Hours: Student's Independent Study: 24

4. Learning Outcomes

Please specify course intended learning outcomes using Skoltech Learning Outcomes Framework.

Skoltech Learning Outcomes are indicated as per Skoltech Learning Outcomes Framework.

1. FUNDAMENTAL KNOWLEDGE 1.1. KNOWLEDGE OF MATHEMATICS AND NATURAL SCIENCES

1.4. INTERDISCIPLINARY THINKING

KNOWLEDGE STRUCTURE AND INTEGRATION

2. PERSONAL AND GENERAL PROFESSIONAL SKILLS AND ATTRIBUTES:

2.1. COGNITION AND MODES OF REASONING

2.1.1. Analytical reasoning and problem solving

2.1.2. System thinking

2.1.4. Decision making (with ambiguity urgency etc.)

2.2. ATTITUDES AND LEARNING PROCESS

2.2.2. Willingness to make decisions in the face of uncertainty

2.2.3. Responsibility intensity perseverance urgency and will to deliver

2.2.6. Development and support of teaching and learning community

2.3. ETHICS, EQUITY AND OTHER RESPONSIBILITIES

2.3.1. Ethical action integrity and courage

2.3.4. Trust and loyalty

3. INTERPERSONAL SKILLS

3.1. COMMUNICATIONS IN INTERNATIONAL ENVIRONMENTS

3.1.1. Communications strategy and structure

3.1.2. Written electronic and graphical communication

3.1.3. Oral presentation and discussion

3.1.5. Communications in English in scientific business and social settings

4. LEADING THE INNOVATION PROCESS

4.1. MAKING SENSE OF GLOBAL SOCIETAL ENVIRONMENTAL AND BUSINESS CONTEXT

4.1.1. Appreciating the potential and limitations of science and technology their role in society and society's role in their evolution

4.2. VISIONING — INVENTING NEW TECHNOLOGIES THROUGH RESEARCH

4.2.1. The research process — hypothesis

evidence and defense

4.2.2. Basic research leading to new scientific discovery

4.2.4. Imagining utility of new science and technology

4.3. VISIONING — CONCEIVING AND DESIGNING SUSTAINABLE SYSTEMS

4.3.2. Identifying and formulating objectives and goals

5. Assignments and Grading

In-person Attendance Requirement 80

In-person Attendance Requirement Comment

Students should actively participate in the working process during the classes rather than just presenting

Assignment Type: Class participation, Assignment Summary: Active participation in seminars, asking questions throughout the course, and answering the questions., % of Final Course Grade: 50
Assignment Type: Computer Labs, Assignment Summary: Student successfully finished all tasks in the Lab, % of Final Course Grade: 20
Assignment Type: Final Project, Assignment Summary: Final project is the presentation according to the topic which student defines at the beginning of the course. Information from lectures and computer labs should help for preparation of the final project presentation., % of Final Course Grade: 30

6. Assessment Criteria

Select Assignment 1 Type Class participation

Sample Assigment 1:

Input Sample of Assignment 1 or Share a Link to Assignment 1

Active participation in seminars, asking questions throughout the course, and answering questions.
Discussing your course project during the course and at any other convenient time.
You should enjoy to learn new things

Assessment Criteria for Assignment 1

Participation in at least 80% of all classes of the cource. 100% of computer labs should be participated

Input example in the text box or upload a file, for the next assignment to appear.

Select Assignment 2 Type Computer Labs

Sample of Assigment 2:

Input Sample of Assignment 2 or Share a Link to Assignment 2

Choose bulk single crystal, 2D material for lab work.
Determine the parameters for calculations by performing the convergence tests.
Calculations of mechanical properties of single crystals by writing scripts for pre- and post-processing
Analyse and Present the obtained results

Assessment Criteria for Assignment 2

Obtain results according to the task.
Convergence test should be done before the final results.
Comparison with published experimental or other reference and related data, if possible.

Results should be presented as 1-2 page report or 5-min presentation of everything that you consider nontrivial in your work.

Select Assignment 3 Type Final Project

Sample of Assigment 3:

Input Sample of Assignment 3 or Share a Link to Assignment 3

The final project can be related to your current or future research or can be given by instructor or supervisor.

It should be presented as conference-style presentation: 20-min, 15-30 slides including Introduction, Methods, Results, and Conclusion sections
Article-style report: 5-10 pages of original text + unlimited number of figures and tables + at least 10-20 references

Assessment Criteria for Assignment 3

Well prepared presentation about your project where you will discuss the results, methods that you used, and discussion why your result is similar to reference ones or not, explain possible explanation of that.

Sample of Assigment 4:

Sample of Assigment 5:

Sample of Assigment 6:

Sample of Assigment 7:

Sample of Assigment 8:

Sample of Assigment 9:

7. Textbooks and Internet Resources

You can request at most two required textbooks. Additionaly, you can suggest up to nine recommended textbooks.

Required Textbooks: Solid State Physics by Neil W. Ashcroft, N. David Mermin, ISBN-13 (or ISBN-10): 978-0030839931

8. Facilities

Software: Quantum Espresso, python

Equipment: Room equipped with audio, video, WiFi

9. Additional Notes

Is this syllabus complete? Yes, the syllabus is a final draft waiting for approval by Education Department

The proposed course 1) has explicit academic content and requirements for receiving credits, 2) is in alignment with the program's learning outcomes, 3) adheres to policies and Skoltech regulations.	Lead Instructor confirms
Syllabus status	Approved by the Education Department