GDAŃSK UNIVERSITY OF TECHNOLOGY

Subject card

Subject name and code	Computational methods in nanotechnology, PG_00071033		
Field of study	Nanotechnology, Nanotechnology		
Date of commencement of studies	February 2027	Academic year of realisation of subject	2026/2027
Education level	second-cycle studies	Subject group	Obligatory subject group in the field of study Subject group related to scientific research in the field of study
Mode of study	Full-time studies	Mode of delivery	at the university
Year of study	1	Language of instruction	English
Semester of study	1	ECTS credits	5.0
Learning profile	general academic profile	Assessment form	exam
Conducting unit	Division of Physics of Disordered Systems -> Institute of Nanotechnology and Materials Engineering -> Faculty of Applied Physics and Mathematics -> Faculties of Gdańsk University of Technology		
Name and surname of lecturer (lecturers)	Subject supervisor	dr hab. inż. Jacek Dziedzic	
	Teachers		

Lesson types

Lesson type	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
Number of study hours	30.0	0.0	30.0	0.0	0.0	60
E-learning hours included: 0.0						

Learning activity and number of study hours

Learning activity	Participation in didactic classes included in study plan	Participation in consultation hours	Self-study	SUM
Number of study hours	60	2.0	63.0	125

Subject objectives

The aim of this course is to familiarise students with quantum-mechanical approaches that are widely used in the the computational and simulational analysis of nanoscale systems. Following a brief recap of the basics of quantum mechanics, we start from the assumptions of QM, and highlight the difficulties of trying to directly employ the Schroedinger equation and wavefunction methods. We then expose the avenues opened up by Hohenberg-Kohn theorems, and we cover the practicalities of the most popular *ab initio* approach used in engineering and research -- density functional theory (DFT).

Learning outcomes

Course outcome	Subject outcome	Method of verification
[K7_W02] has in-depth, theoretically grounded and detailed knowledge of phenomena, methods, and theories related to nanotechnology, as well as of related and allied fields of science or engineering	Has broadened and well-structured knowledge of simulation approaches used to study nanoscale systems through in silico experiments. Is able to use density functional theory to determine the electronic structure of uncomplicated systems.	[SW1] Assessment of factual knowledge
[K7_U05] is able to plan and carry out theoretical and numerical calculations as well as simulations of phenomena and processes, critically analyze their results, draw conclusions, and formulate well-founded opinions in nanotechnology and related physical and natural sciences	Is able to independently plan and carry out uncomplicated calculations in the field of electronic structure — both by solving simple, model problems analytically and by tackling more complex ones through computer simulation. Is able to critically evaluate the obtained results and draw conclusions from the computed values.	[SU1] Assessment of task fulfilment [SU4] Assessment of ability to use methods and tools [SU3] Assessment of ability to use knowledge gained from the subject [SU5] Assessment of ability to present the results of task
[K7_W05] has in-depth knowledge of mathematical, numerical, and simulation methods - both classical and quantum - used in the modeling of nanostructures	Demonstrates understanding of the theoretical background and mathematical apparatus used in quantum and classical modelling of nanostructures.	[SW1] Assessment of factual knowledge

Subject contents

Course content – lecture

1. Introduction: Why nanotechnology? Mechanisms responsible for the unique behaviour of nanoscale systems. Example uses and promises of nanotechnology. Difficulties of experimental studies of nanotechnology.
2. Problem statement: Interactions in matter. Questions and answers in theoretical investigations of nanostructures. Dynamical equation. Landscape of computational methods in physics.
3. Refresher in basics of quantum mechanics: wavefunction, statistical interpretation, Schroedinger equation, operators, expectation value, linear vector space, basis, inner product, orthogonality and orthonormality, operators as matrices, spaces with infinitely many dimensions.
4. First things first: Many-body systems. Molecular chemistry. Atomic units. Molecular Hamiltonian. Born-Oppenheimer approximation. Potential energy surface. Spin. Electronic Hamiltonian. External potential.
5. Orbital-free approach: Electron density. Hohenberg-Kohn theorems. Orbital-free (pure) density functional theory (OF-DFT). Lagrange multiplier approach. Exchange. Correlation. Thomas-Fermi model. Thomas-Fermi-Dirac model.
6. Kohn-Sham DFT (KS-DFT): Interacting vs. non-interacting electrons. Kohn-Sham electrons. Molecular orbital. Hartree product. Slater determinant. Effective potential. Exchange-correlation energy. Difficulties of KS-DFT. Diagonalisation. Self-consistency. Energy minimisation in KS-DFT.
7. Practicalities: Exchange and correlation: LDA, GGA, m-GGA, hybrid functionals. Pseudopotential.
8. Basis sets in DFT: Function basis. LCAO. Slater and Gaussian basis. Electronic integrals. Contractions. Minimal basis. Extended basis. Split-valence basis. Polarisation functions. Diffuse functions. Pople basis. Duning basis. Complete basis set limit. Basis set superposition error. Other bases: NAO, Daubechies wavelets, NGWF, plane waves, LMTO.
9. Post-HF methods (briefly).

Course content – laboratory

Atomic units. De Broglie waves. Time-dependent and time-independent Schroedinger equation. Expectation values. Function minimization with constraints, Lagrange multipliers. Variational principle for the wavefunction. Electrostatics of point charges and extended charge densities. Thomas-Fermi model. Dirac correction. Variational principle for the electronic density. Minimal basis. Slater and Gaussian orbitals. Plane wave basis. Overlap integrals. One-electron integrals. Basis set superposition error.

Prerequisites and co-requisites

Basic: Basics of calculus (Riemann integral, minimisation of a function, partial and total derivatives, differential). Basics of linear algebra (linear vector space, vector, basis, linear combination). Basics of classical mechanics (force, acceleration, potential) and quantum mechanics (wavefunction, Schroedinger equation, observables, superposition, operators). Basics of electrostatics (electric field, potential, work, Coulombic interaction). High-school-level chemistry (atom, molecule, orbital, chemical bond, hybridisation).

Additional: Numerical methods, variational calculus, statistical physics.

Assessment methods and criteria

Subject passing criteria	Passing threshold	Percentage of the final grade
Written exam	50.0%	50.0%
Lab reports	50.0%	50.0%

Recommended reading

Basic literature	1. David J. Griffiths, Introduction to Quantum Mechanics, 2nd ed, Pearson Prentice Hall, 2004. 2. Frank Jensen, Introduction to Computational Chemistry, Wiley, 2007. 3. R. Shankar, Principles of Quantum Mechanics, Springer, 2013. 4. N. M. Harrison, An Introduction to Density Functional Theory, Imperial College, London, 2025.
Supplementary literature	1. Tadmor, Miller, Modeling Materials, Cambridge, 2011.
eResources addresses	

Example issues/ example questions/ tasks being completed

1. What are the main differences between classical and quantum-mechanical methods for the computational study of nanoscale systems?
2. Write down the general formula for the total quantum-mechanical Hamiltonian of a molecule with Nat atoms and Nel electrons in units of your choosing. Define the symbols used. What does each of the terms represent?
3. Briefly derive the first Hohenberg-Kohn theorem.
4. Briefly compare three problems: a) interacting electrons, b) non-interacting electrons, c) Kohn-Sham electrons. What are the advantages and disadvantages of each model?
5. List and briefly characterise the main difficulties of Kohn-Sham DFT.
6. Briefly discuss the rungs of Jacob's ladder that you are familiar with. What can be found on each of the ends of the ladder?
7. What does it mean that a pseudopotential is non-local? Semi-local? Local?
8. Compare Slater and Gaussian orbitals. Give expressions, advantages, disadvantages. Describe the symbols used.
9. Write down everything you know about Pople bases.
10. Explain how the plane-wave basis set works and when it is suitable.

Practical activites within the subject

Not applicable