GDAŃSK UNIVERSITY OF TECHNOLOGY

Subject card

Subject name and code	Theoretical basis of nanotechnology, PG_00069740		
Field of study	Teoretyczne podstawy nanotechnologii		
Date of commencement of studies	February 2026	Academic year of realisation of subject	2025/2026
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	Polish
Semester of study	1	ECTS credits	4.0
Learning profile	general academic profile	Assessment form	assessment
Conducting unit	Division of Physics of Disordered Systems -> Institute of Nanotechnology and Materials Engineering -> Faculty of Applied Physics and Mathematics -> Wydziały Politechniki Gdańskiej		
Name and surname of lecturer (lecturers)	Subject supervisor	dr hab. inż. Jacek Dziedzic	
	Teachers	dr hab. inż. Jacek Dziedzic	

Lesson types	Lesson type	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
	Number of study hours	30.0	0.0	15.0	0.0	0.0	45
	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	45	5.0	50.0	100

Subject objectives	The aim of this course is to familiarise students with quantum-mechanical approaches that are widely used in the theoretical analysis and computer simulation 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 enhanced, theoretically supported, detailed knowledge of selected branches of nanotechnology and, according to the needs, within the scope of related fields of science and technology.	The student has acquired extended and well-ordered knowledge pertaining to theoretical and simulation-based quantum-mechanical approaches to the study of nanoscale systems. The student is able to employ density functional theory to obtain the electronic structure of straightforward systems.	[SW1] Ocena wiedzy faktograficznej
[K7_W04] has practical and theoretical knowledge of physical and chemical experimental methods of nanotechnology.	Possesses advanced and well-structured knowledge of simulation-based approaches to studying nanoscale systems using in silico experimental methods. Is able to apply the density functional theory method to determine the electronic structure of uncomplicated systems.	[SW1] Ocena wiedzy faktograficznej
[K7_U01] can learn individually, obtain knowledge and integrate information from literature, databases and other properly selected sources (in Polish and English). Has the ability of critical analysis and selection of information.	The student is able to acquire, on their own, relevant information from literature sources and to critically analyze them.	[SU2] Ocena umiejętności analizy informacji [SU3] Ocena umiejętności wykorzystania wiedzy uzyskanej w ramach przedmiotu

Subject contents

1. Why nanotechnology?
2. Mechanisms responsible for the unique behaviour of nanoscale systems.
3. Example uses and promises of NT.
4. Difficulties of experimental studies of NT.
5. Interactions in matter.
6. Questions that we want answered in theoretical investigations of nanostructures.
7. Answers that we must have in theoretical investigations of nanostructures.
8. Dynamical equation.
9. Landscape of computational methods in physics.
10. 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.
11. Many-body systems. Molecular chemistry. Atomic units.
12. Molecular Hamiltonian.
13. Born-Oppenheimer approximation. Potential energy surface.
14. Spin.
15. Electronic Hamiltonian. External potential.
16. Electron density.
17. Hohenberg-Kohn theorems.
18. Orbital-free (pure) density functional theory (OF-DFT).
19. Exchange. Correlation.
20. Thomas-Fermi model. Thomas-Fermi-Dirac model.
21. Kohn-Sham DFT (KS-DFT).
22. Interacting vs. non-interacting electrons. Kohn-Sham electrons.
23. Molecular orbital. Hartree product. Slater determinant.
24. Effective potential. Exchange-correlation energy.
25. Difficulties of KS-DFT. Diagonalisation. Self-consistency.
26. Energy minimisation in KS-DFT.
27. Exchange and correlation: LDA, GGA, m-GGA, hybrid functionals.
28. Jacob's ladder of functionals.
29. Core-valence approximation.
30. Pseudopotential.
31. Motivation for using pseudopotentials, difficulties associated with their use.
32. Transferability of a pseudopotential. Hard and soft pseudopotentials.
33. Function basis. LCAO. Slater and Gaussian basis. Electronic integrals. Contractions.
34. Minimal basis. Extended basis. Split-valence basis. Polarisation functions. Diffuse functions.
35. Pople basis. Duning basis.
36. Complete basis set limit.
37. Basis set superposition error.
38. Other bases: NAO, Daubechies wavelets, NGWF, plane waves, LMTO.
39. Post-HF methods (briefly).

Creating simple input structures. Choice of key parameters in electronic structure calculations: kinetic energy cutoff, number of orbitals in the minimal basis set, size of the simulation box. Self-consistency. Energy minimization methods used for systems with and without an energy gap. Visualization.

Prerequisites and co-requisites

Basics of calculus (Riemann integral, minimisation of a function of one variable, partial and total derivatives, differential). Basics of linear algebra (linear vector space, vector, basis, linear combination). Basics of classical mechanics (force, acceleration, energy, potential) and quantum mechanics (wavefunction, Schrödinger 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
lab reports	50.0%	50.0%
written exam	50.0%	50.0%

Recommended reading

Basic literature	1. Lucjan Piela, Ideas of Quantum Chemistry, PWN, 2011. 2. Frank Jensen, Introduction to Computational Chemistry, Wiley, 2007. 3. Christopher Cramer, Essentials of Computational Chemistry, Wiley, 2004.
Supplementary literature	1. Tadmor, Miller, Modeling Materials, Cambridge, 2011. 2. Scharoch, Peisert, Metody obliczeniowe ab initio w fizyce struktur atomowych (skrypt). 3. Grimme, Density functional theory with London dispersion corrections, WIREs Computational Molecular Science 1 (2011). 4. Rick, Stewart, Reviews in Computational Chemistry, Volume 18, Polarizability in computer simulations.
eResources addresses	

Example issues/ example questions/ tasks being completed	1. Briefly explain the difficulties associated with experimental analysis of nanostructures. 2. Explain why nanoscale systems behave differently from macroscale systems. Give examples of responsible mechanisms. 3. Give several examples of materials or nanostructures with atypical properties, briefly explain the reasons for their atypical behaviours. 4. Which of the four fundamental interactions are significant, and which are insignificant at the nanoscale? Why? 5. What is the dynamical equation? Briefly describe the four main regions and corresponding dynamical equations, depending on the masses and velocities of the studied particles. 6. What are the main differences between classical and quantum-mechanical methods for the computational study of nanoscale systems? 7. Describe the interpretation of expectation value in quantum mechanics. How can we measure the expectation value of an observable? How can we calculate it? 8. When is a set of vectors in a linear vector space linearly dependent, and when is it linearly independent? 9. What is the projection operator? What is its form? What is the result of acting this operator on a vector? Write down and interpret the completeness relation. 10. 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? 11. What assumptions and simplifications lead to the Born-Oppenheimer approximation? Name a situation where the usual simplifications fail. 12. What are the consequences of assuming the Born-Oppenheimer approximation? Explain the concept of potential energy surface (PES). 13. Given a wavefunction of a system of Nel interacting electrons, what formula would we use to determine the electronic energy? And the electron density? 14. Write down the quantum-mechanical Hamiltonian of the methane molecule (CH4) in atomic units. Define the symbols used. What does each of the terms represent? 15. What are the main consequences of electrons having spin? 16. In the context of an electronic problem, what is the external potential? Write down the formula for the external potential for an N2O molecule. Define the symbols used. 17. What information can we deduce from the electron density of a molecule? How can we deduce it? 18. Can we determine, in an exact fashion, the energy of a molecule knowing only its electron density? Why so, or why not? 19. What does the first Hohenberg-Kohn theorem say? 20. Briefly derive the first Hohenberg-Kohn theorem. 21. What is Hohenberg-Kohn's universal functional? What does universality mean in this context? 22. Write down and briefly comment on the variational principle for wavefunctions and the variational principle for electron densities. What are their consequences? 23. Into what three components is the electron-electron interaction energy usually decomposed? Describe them and the original energy (the one being decomposed). Give formulas wherever possible. 24. Describe the energy minimisation procedure in pure (orbital-free) DFT. The minimum of what functional do we seek in practice? 25. Write down the expression for the Thomas-Fermi density functional. Briefly characterise each of the terms. 26. What are the main simplifications assumed in the Thomas-Fermi midel? What are its predictions? 27. Briefly describe the improvements to the Thomas-Fermi model proposed by Dirac and Weizsäcker. 28. What are the main assumptions of pure (orbital-free) DFT? What difficulties does this model encounter in practice? 29. Briefly describe Kohn and Sham's idea which enables working around the main difficulty of pure (orbital-free) DFT. 30. How do we solve the non-interacting electron problem? 31. How do a) Hartree, b) Slater wavefunctions for a system of non-interacting electrons look like? What is wrong with Hartree's wavefunction? 32. What is the expression for the electron density of a system of non-interacting electrons described by a Slater wavefunction? What simplification is necessary to obtain this expression? 33. What is the effective potential in Kohn-Sham's model? What is its role? 34. What is the Hartree potential in Kohn-Sham's model? 35. What is the exchange-correlation potential in Kohn-Sham's model? What is its role? 36. Briefly compare three problems: a) interacting electrons, b) non-interacting electrons, c) Kohn-Sham electrons. What are the advantages and disadvantages of each model? 37. How does the expression for the electronic kinetic energy differ depending on the assumed model: a) interacting electrons in wavefunction methods, b) electrons in Hohenberg-Kohn's model (pure DFT), c) electrons in the Kohn-Sham model? 38. Characterise the exchange-correlation energy term (Exc) in Kohn-Sham's model. 39. List and briefly characterise the main difficulties of Kohn-Sham DFT. 40. Discuss the energy minimisation in Kohn-Sham DFT. The minimum of what functional do we seek in practice? 41. How does Kohn-Sham DFT differ from pure (orbital-free) DFT? What are the advantages and disadvantages of each of these approaches? 42. How do we deal with the issue of quadratic increase of the number of Lagrange multipliers that we encounter during minimisation in Kohn-Sham DFT? What are the difficulties associated with this workaround? 43. What is the self-consistency procedure in Kohn-Sham DFT? Why do we need this procedure? 44. What is the local density approximation (LDA) in Kohn-Sham DFT? How would you rate the quality of this approximation? 45. What is the generalised gradient approximation (GGA) in Kohn-Sham DFT? How would you rate the quality of this approximation? 46. What are the main differences between exchange-correlation functionals stereotypically used by chemists and those used by physicists? 47. What are meta-GGA functionals? 48. What are hybrid exchange-correlation functionals? What are their main advantages and disadvantages? 49. 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? 50. What does it mean that an exchange-correlation functional is non-local? Semi-local? Local? 51. What is the motivation behind using the pseudopotential approximation? What does this approximation entail?

	52. What do we expect from a good pseudopotential? 53. What are the difficulties associated with working in the pseudopotential approximation? What are the difficulties of not using this approximation? 54. What does it mean that a pseudopotential is non-local? Semi-local? Local? 55. What does it mean for a pseudopotential to be soft? Hard? What are the advantages and disadvantages of soft/hard pseudopotentials? 56. Briefly describe techniques for mitigating the pseudopotential approximation. 57. What is the LCAO approximation and what is it used for? 58. Compare Slater and Gaussian orbitals. Give expressions, advantages, disadvantages. Describe the symbols used. 59. What are overlap integrals? Give expressions and interpretations. 60. What are one-electron integrals? Give expressions and interpretations. 61. What are the differences between a) radial Gaussian functions, b) primitive Gaussian functions, c) contracted Gaussian orbitals? 62. What does Gaussian orbital contraction entail? Why would we use it? 63. What is a minimal basis? What are the advantages and disadvantages of using a minimal basis? 64. What is an extended basis? What is the difference between a DZ basis and a VDZ basis? 65. What are polarisation basis functions? What are they used for? 66. What are diffuse basis functions? What are they used for? 67. Write down everything you know about Pople bases. 68. Write down everything you know about correlation-consistent bases. 69. How do we deal with the fact that in practice we must use non-complete bases? 70. Describe the basis superposition error (BSSE). How can we deal with this problem? 71. What are numerical atomic orbitals (NAO)? What are the advantages and disadvantages of using them as a function basis? 72. Write down everything you know about non-orthogonal generalised Wannier function (NGWF) bases. 73. What is *in situ* basis optimisation? What are the advantages and disadvantages of such optimisation? 74. Briefly explain what the eggbox effect is. 75. Enumerate the advantages and disadvantages of the plane wave basis compared to real-space bases. 76. Explain how the plane-wave basis set works and when it is suitable. 77. What is the kinetic energy cutoff in a plane wave basis? Why is it used? 78. Briefly explain how the LMTO approach works. What are the difficulties associated with using it? 79. Give examples of computer codes enabling DFT calculations in (a) a plane wave basis, (b) in a GTO basis, (c) in an NAO basis. 80. Briefly summarise what you know about correlated (post-HF) electronic structure methods. 81. When do we term an interaction a short-range interaction, and when do we term it a long-range interaction? Give two examples of each. 82. When do we use Ewalds method? What does it achieve? Give a brief overview of how it works. Use diagrams to support your argument. 83. Describe the Ewald method in as much detail as you can. 84. What do implicit solvent methods achieve? How do they work in general? 85. Compare explicit and implicit solvation. What are the advantages and disadvantages of each? 86. What are the main contributions to energy (interactions) in the solvation process? Describe each of them. 87. How, in general, are the polar and non-polar terms to the free energy of solvation calculated? 88. What is the solute cavity? What are the different ways of constructing solute cavities? What are their advantages and disadvantages? 89. Briefly describe implicit solvent methods in the context of classical MD simulations. 90. Compare the Polarizable Continuum Model (PCM) and Fattebert-Gygis minimal parameter model. 91. What are the main difficulties associated with Fattebert-Gygis minimal parameter IS model? 92. Explain the origin of dispersion interactions. What length-scales are involved in dispersion interactions? Why does standard DFT struggle with describing dispersion? 93. What are some typical examples of systems where dispersion interactions are important? Why does standard DFT struggle with describing dispersion? 94. Briefly describe the four classes of approaches that can be used to correct DFT calculations to take dispersion into account. 95. What is DFT-D (also known as DFT+D)? How does it take dispersion into account? What are the advantages and disadvantages of this approach? 96. What are van der Waals density functionals (vdW-DF)? Name some examples. How do they take dispersion into account What are the advantages and disadvantages of vdW-DF? 97. When is the calculation of forces useful in DFT? What difficulties are associated with calculating forces in DFT? 98. Derive the expression for the Hellmann-Feynman force in DFT. What assumption needs to be taken in the derivation? 99. What are Pulay forces? When are they important and when do they vanish (become zero)?
Practical activites within the subject	Not applicable