Introduction to Computational Studies of Electronic Structure of Nanosystems

Educational subject description sheet

Basic information

Study programme Fizyka **Speciality** INFORMACJA KWANTOWA I SPINTRONIKA **Organizational unit** Faculty of Physics **Study level** Second-cycle programme **Study form** Full-time **Education profile** General academic	**Didactic cycle** 2023/24 **Subject code** 04FIZIKSS.24KU.04365.23 **Lecture languages** English **Course type** Elective **Block** Complementary major subjects

Subject coordinator	Konrad Kapcia
Lecturer	Konrad Kapcia

Period	**Activities and hours**	**Number of ECTS points**
Semester 3	• Lecture: 30, Exam • Seminar: 15, Graded credit	4

Goals

Code	Goal
C1	Providing knowledge of the fundamentals of the methods of computations of electronic structure of matter, including the density functional theory as well as other first principle approaches
C2	Providing knowledge of specific aspects of the computational methods in applications to nanostructures
C3	Developing the ability for understanding of advanced computation methods for first principles description of solids
C4	Practicing the use of literature sources

Subject learning outcomes

Code	Outcomes in terms of	Learning outcomes	Examination methods
Knowledge – Student:			
W1	knows the mathematical formulation of the first principles approaches and basic theorems upon which the methods are based	FIZ_K2_W01, FIZ_K2_W02, FIZ_K2_W03, FIZ_K2_W04	Oral exam, Multimedia presentation
W2	knows the methodology of various ab initio computational packages	FIZ_K2_W02, FIZ_K2_W03, FIZ_K2_W06	Oral exam, Multimedia presentation
Skills – Student:			
U1	is able to understand physical theoretical concepts used in computational methods of electronic structure of matter	FIZ_K2_U01, FIZ_K2_U02, FIZ_K2_U03, FIZ_K2_U05	Oral exam, Multimedia presentation
U2	can evaluate the computational methods as concerns their scope and effectiveness, precision and complexity and to make a proper choice of a method to use for the specific research problem	FIZ_K2_U01, FIZ_K2_U03, FIZ_K2_U04, FIZ_K2_U05	Oral exam, Multimedia presentation
U3	is able to practically use the computational package of choice to study the electronic structure of simple nanostructures and analyze the results of the computations in physical terms	FIZ_K2_U01, FIZ_K2_U03	Oral exam, Multimedia presentation
Social competences – Student:			
K1	can prepare a summary reporting the results in a form of oral seminar and/or journal article based on published papers in the field of nanoscience	FIZ_K2_K01, FIZ_K2_K02	Multimedia presentation
K2	can explain the role of ab initio methods in physics to people outside the field	FIZ_K2_K03, FIZ_K2_K05	Multimedia presentation

Study content

No.	Course content	Subject learning outcomes	Activities
1.	A review of fundamental interactions relevant for the electronic structures of atoms, molecules and condensed matter systems.	W1, U1	Lecture
2.	A concept of electronic correlations.	W1, W2, U1	Lecture

No.	Course content	Subject learning outcomes	Activities
3.	A formulation of basic principles of the Hartree-Fock method and the density functional theory (within the self-consistent approach).	W1, W2, U1	Lecture, Seminar
4.	Various choices of basis of functions in first principles approaches.	W1, W2, U1, U2	Lecture, Seminar
5.	The pseudopotential method.	W1, W2, U1, U2	Lecture
6.	Methods of optimizing the spatial structures of molecules and condensed matter systems: molecular dynamics, conjugate gradients methods.	W1, W2, U2, U3	Lecture
7.	Lattice dynamics - harmonic approximation and anharmonicity.	W1, W2, U1, U2	Lecture, Seminar
8.	Overview of available implementations of first principles approaches (SIESTA, Quantum Espresso, Abinit, VASP, Wien2k).	W2, U2, U3	Lecture, Seminar
9.	Detailed analysis of simple case studies performed with a help of the selected computational packages (including nanosystems modelling).	W2, U2, U3, K1, K2	Lecture, Seminar

Additional information

Activities	Teaching and learning methods and activities
Lecture	Lecture with a multimedia presentation of selected issues, Discussion
Seminar	Conversation lecture, Work with text, Case study

Activities	Credit conditions
Lecture	Oral examination: several open questions (maximum 100%). Grading scale with applied percentage distribution: excellent (5.0): achievement of the student's expected learning outcomes at a minimum of 92.0%. very good (4.5): achievement by the student of the desired learning outcomes ranging from 84.0% - 91.9%. good (4.0): achievement of student learning outcomes 76.0% - 83.9%. average (3.5): achievement of student learning outcomes 68.0% - 75.9%. satisfactory (3.0): attainment of the student learning outcomes within 60.0% - 67.9%. unsatisfactory (2.0): failure of the student to achieve the expected learning outcomes below 60.0%.
Seminar	Preparation of the presentation about selected topic associated with the framework of the lecture (max. 100%). Grading scale with applied percentage distribution: excellent (5.0): achievement of the student's expected learning outcomes at a minimum of 92.0%. very good (4.5): achievement by the student of the desired learning outcomes ranging from 84.0% - 91.9%. good (4.0): achievement of student learning outcomes 76.0% - 83.9%. average (3.5): achievement of student learning outcomes 68.0% - 75.9%. satisfactory (3.0): attainment of the student learning outcomes within 60.0% - 67.9%. unsatisfactory (2.0): failure of the student to achieve the expected learning outcomes below 60.0%.

Literature

Obligatory

1. Parr, R. G.; Yang, W. (1989). Density-Functional Theory of Atoms and Molecules. New York: Oxford University Press.
2. Axel D. Becke. Perspective: Fifty years of density-functional theory in chemical physics. J. Chem. Phys. 140, 18A301 (2014).
3. M.C. Payne, M.P. Teter, D.C. Allan, T.A. Arias and J.D. Joannopoulos. Iterative minimization techniques for ab initio total-energy calculations: molecular dynamics and conjugate gradients. Rev. Mod. Phys. 64, 1045 (1992).

Optional

1. J. M. Soler et al. The SIESTA method for ab initio order-N materials simulation. J. Phys.: Cond. Mat. 14, 2745 (2002).

Calculation of ECTS points

Activities	**Activity hours***
Lecture	30
Seminar	15
Reading the indicated literature	25
Preparation of a multimedia presentation	15
Preparation for the exam	20
Preparation for classes	15
Student workload	**Hours** 120
Number of ECTS points	**ECTS** 4

* academic hour = 45 minutes

Efekty uczenia się dla kierunku

Kod	Treść
FIZ_K2_K01	The graduate is ready to critically evaluate own knowledge and received content
FIZ_K2_K02	The graduate is ready to recognize the importance of knowledge in solving cognitive and practical problems and seeking expert opinion (also from other scientific disciplines) to overcome difficulties during independent problem solving
FIZ_K2_K03	The graduate is ready to fulfill social obligations, inspire and organize activities for the benefit of the social environment and initiate activities in the public interest
FIZ_K2_K05	The graduate is ready to responsibly perform professional roles, incorporating changing social needs, including advancing the achievements of the profession and maintaining its ethos, as well as the observance and development of the principles of professional ethics and actions to comply with these principles
FIZ_K2_U01	The graduate can use their knowledge to formulate and solve complex and unusual problems in the field of physical sciences; select and apply appropriate methods and tools necessary to solve a given problem (including advanced IT techniques), as well as adapt existing methods and tools or develop completely new ones
FIZ_K2_U02	The graduate can find the necessary information in the professional literature, databases and other sources, in particular in scientific journals basic to physics, and perform critical analysis, synthesis and creative interpretation of the collected information
FIZ_K2_U03	The graduate can formulate and test hypotheses related to simple research problems in physics (plan and perform observations, experiments, theoretical calculations or computer simulations and critically evaluate and discuss the results obtained)
FIZ_K2_U04	The graduate can prepare, for various audiences, oral presentations and written studies presenting specialized topics in the field of physical sciences in a communicative way, as well as debate on such topics
FIZ_K2_U05	The graduate can use English in accordance with the requirements set out for level B2+ of the Common European Framework of Reference for Languages, as well as specialist English terminology in the field of physical sciences
FIZ_K2_W01	The graduate knows and understands in-depth selected facts, phenomena, concepts and theories specific to physics and complex relationships between them (constituting advanced general knowledge in the field of physical sciences and representing both key and other selected issues in the field of advanced detailed knowledge in this discipline)
FIZ_K2_W02	The graduate knows and understands in-depth selected research methods and tools as well as mathematical models used in physics
FIZ_K2_W03	The graduate knows and understands in-depth selected computational methods and information technology tools and techniques used to solve complex problems in physics
FIZ_K2_W04	The graduate knows and understands main development trends in the discipline of physical sciences
FIZ_K2_W06	The graduate knows and understands basic concepts and principles in the area of industrial property protection and copyright