A COURSE SYLLABUS – DOCTORAL SCHOOLS

REGARDING THE QUALIFICATION CYCLE FROM 2019 TO 2023

REGARDING THE QUALIFICATION CYCLE FROM 2020 TO 2024

GENERAL INFORMATION ABOUT COURSE	
Course title	**Selected issues of computational methods of condensed matter physics**
Name of the unit running the course	Doctoral School of University of Rzeszów
Type of course *(obligatory, optional)*	obligatory
Year and semester of studies	2-nd and 3-rd year; summer semester 2021/2022
Discipline	Physics
Language of Course	English
Name of Course coordinator	Dr hab. Małgorzata Sznajder, prof. UR
Name of Course lecturer	Dr hab. Małgorzata Sznajder, prof. UR
Prerequisites	Completed course on the foundations of condensed matter physics, in particular knowledge of quantum-mechanical description of electronic states in crystals, knowledge of basic approximations in the band theory of solids.

BRIEF DESCRIPTION OF COURSE **(max 300-400 words)**
The aim of the lecture is to present the idea of quantum-mechanical computations carried out within the electron density functional theory, in the Kohn-Sham formulation. Particular emphasis is placed on the presentation of the foundations of the theory and the development of methods enabling the determination of the electronic structure of a solid. Discussion of the approximations used to describe the exchange and correlation interactions and their limitations. Presentation of the practical possibilities of numerical codes, with the implemented algorithm for solving the Kohn-Sham equation in a self-consistent manner. Getting to know different types of functionals, discussing their advantages and disadvantages. Presentation of the methods of selecting numerical parameters for the selected numerical code (Siesta), tests of these parameters, construction and selection of the size of supercells, methods of system geometry relaxation and calculation of the band structure.

COURSE LEARNING OUTCOMES AND METHODS OF EVALUATING LEARNING OUTCOMES				
Learning outcome	The description of the learning outcome defined for the course	Relation to the degree programme outcomes (symbol)	Learning Format (Lectures, classes,...)	Method of assessment of learning outcomes (e.g. test, oral exam, written exam, project,...)
Knowledge (no.)				
1	The doctoral student knows and understands the world achievements covering the theoretical foundations of the electron density functional theory of a system of many interacting particles,	P8S-WG/1	L	report
2	knows and understands the idea of Kohn-Sham of replacing the system of interacting particles with an auxiliary system of independent particles and reducing the multi-body effects to the form of an exchange-	P8S-WG/1	L	report

	correlation functional,			
3	knows the development of approximations used in the construction of exchange-correlation functionals used in the quantum theory of solids,	P8S-WG/2	L, c	report, project
4	knows and understands self-consistent methods of solving the Kohn - Sham equation.	P8S-WG/2	L	discussion
5	knows and understands the methodology of research in the discipline of physical sciences	P8S-WG/3	L	discussion
Skills (no.)				
1	The doctoral student is able to use the knowledge of condensed matter physics and quantum chemistry to solve the problem of determining the electronic band structure of crystalline bodies, is able to define the purpose and subject of research, formulate a research hypothesis, creatively use the known techniques and research tools to achieve the assumed goal,	P8S-UW/1	L, c	report, discussion, project
2	is able to critically analyze and evaluate the results of scientific research in the discipline of physical sciences	P8S-UW/2	L, c	report, discussion, project
3	is able to initiate a debate and participate in the scientific discourse on selected computational methods of condensed matter physics.	P8S-UK/3, P8S-UK/4; P8S-UK/1; P8S-UK/5	L, c	report, discussion, project
Social competence (no.)				
1	The PhD student is ready to recognize the importance of the accumulated knowledge in solving practical problems of condensed matter physics	P8S-KK/3	L	discussion
2	The PhD student is ready to critically evaluate accomplishments within the discipline of physical science	P8S-KK/1	L	discussion
3	The PhD student is ready to act in the public interest	P8S-KO/2	L	discussion

LEARNING FORMAT – NUMBER OF HOURS						
Semester (no.)	Lectures	Seminars	Lab classes	Internships	others	ECTS
IV and VI	5	10	——	——	—	0

METHODS OF INSTRUCTION

LECTURE: A LECTURE SUPPORTED BY A MULTIMEDIA PRESENTATION, DISCUSSION
CLASSES: WORK WITH NUMERICAL CODE, PRACTICAL PROJECT, DISCUSSION

COURSE CONTENT

1. **Lectures/ Seminars:**

    1. Fundamentals of the electron density functional theory. The Thomas-Fermi-Dirac approximation, example of a functional. The Hohenberg - Kohn theorems.
    2. The Kohn - Sham auxiliary system. The Kohn-Sham variational equations. E_{xc}, V_{xc}, and the exchange-correlation hole. Meaning of the eigenvalues.
    3. Functionals for the exchange and correlation interaction. LDA and GGA approximations. Hybrid functionals. Tests of functionals.
    4. Solving Kohn - Sham equations.

2. **Seminars / Lab classes/ others:**

Generation and optimization of pseudopotentials for numerical computations within the density functional theory using Siesta software. Selection and tests of numerical parameters. System geometry relaxation. Calculations of the electronic band structure of a crystalline system and density of states function.

COURSE ASSESSMENT CRITERIA

The condition for passing the lecture is to present a written report containing a discussion of the most important conclusions from the issues discussed during the lecture.
The condition for passing the exercises is to obtain over 51% of points from the project consisting in presenting comprehensive results of the calculation of the band structure of the selected crystalline material, carried out using the *ab-initio* method within the Kohn-Sham density functional theory. The project will include the generation of pseudopotentials, their test, selection of numerical parameters for the Siesta code, construction of a supercell adequate to the given problem (e.g. crystal containing point defects), relaxation of the geometry of the system, definition of the Brillouin zone, determination of the E(***k***) relationship and the density of states function.
The final grade will be issued depending on the number of points obtained for the project (the correctness and completeness of individual elements of the project are assessed):
poor; 3.0 (51 - 60)% pkt.,
satisfactory; 3.5 (61 - 70)% pkt.,
good; 4.0 (71 - 80)% pkt.,
very good; 4.5 (81 - 90)% pkt.,
excellent; 5.0 (91 - 100)% pkt.

TOTAL PhD STUDENT WORKLOAD REQUIRED TO ACHIEVE THE INTENDED LEARNING OUTCOMES – NUMBER OF HOURS AND ECTS CREDITS

Activity	Number of hours
Scheduled course contact hours	15
Other contact hours involving the teacher (consultation hours, examinations)	1
Non-contact hours – student`s own work (preparation for classes or examinations, project, etc.)	20
Total number of hours	36
Total numer of ECTS credits	

INSTRUCTIONAL MATERIALS	
Compulsory literature:	1. R. M. Martin, Electronic structure. Basis Theory and Practical Methods, Cambridge University Press, New York, 2009 2. Walter A. Harrison, Solid State Theory, Dover Publications, UK, 2012 3. Parr, R.G and Yang, W., Density-Functional Theory of Atoms and Molecules, Oxford University Press New York, 1989 4. Koch, W. and Holthasuen, M.C., A Chemists' Guide to Density Functional Theory, Wiley-VCH, Weinheim, 2001
Complementary literature:	1. Hohenberg, P. and Kohn, W "Inhomogeneous electron gas", Phys. Rev. 136:B864-871, 1964 2. Kohn W. and Sham, L.J. "Self-consistent equations including exchange and correlation effects", Phys. Rev. 140:A1133-1138, 1965 3. Mermin, N.D. "Thermal properties of the inhomogeneous electron gas" Phys. Rev. 137:A 1441-1443, 1965 4. Kohn, W. "Nobel lecture: electronic structure of matter wave functions and density functionals" Rev. Mod. Phys. 71:1253, 1999 5. Jones, R.O. and Gunnarsson, O. "The density functional formalism, its applications and prospect", Rev. Mod. Phys. 61:689-746, 1989 6. Casida, M.E. in Recent Developments and Applications of Density Functional Theory, ed. by J.M. Seminario, Elsevier, Amsterdam, 1996, p. 391 7. Staedele, M., Moukara, M., Majewski, J.A., Vogl, P., and Gorling, A., „Exact exchange Kohn-Sham formalism applied to semiconductors", Phys. Rev. B 59:1001-10043, 1999

29.10.2021 Małgorzata Sznajder
Date and signature of the Course lecturer

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Approved by the Head of the Department or an authorised person