GDAŃSK UNIVERSITY OF TECHNOLOGY

Subject card

Subject name and code	Density functional approaches to the many-body problem, PG_00060061		
Field of study	Technical Physics		
Date of commencement of studies	October 2020	Academic year of realisation of subject	2022/2023
Education level	first-cycle studies	Subject group	Optional subject group 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	3	Language of instruction	English
Semester of study	6	ECTS credits	2.0
Learning profile	general academic profile	Assessment form	assessment
Conducting unit	Zakład Metod Obliczeniowych Fizyki Chemicznej -> Instytut Fizyki i Informatyki Stosowanej -> Faculty of Applied Physics and Mathematics		
Name and surname of lecturer (lecturers)	Subject supervisor	dr Simone Taioli	
	Teachers	dr Simone Taioli	

Lesson types and methods of instruction

Lesson type	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
Number of study hours	30.0	0.0	0.0	0.0	0.0	30

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	30	0.0	0.0	30

Subject objectives

The lectures introduce the density functional approach to the many-body problem and show its applications in condensed matter

Learning outcomes

Course outcome	Subject outcome	Method of verification
[K6_U09] Can use technical literature in English.	The student is able to find information about the content of the subject in the recommended publications written in English.	[SU3] Assessment of ability to use knowledge gained from the subject
[K6_W02] Has systematized knowledge of the basics of physics, including mechanics, thermodynamics, electricity and magnetism, optics, atomic and particle physics, solid-state physics, nuclear and elementary particle physics.	The student has basic knowledge about the time-dependent quantum mechanics and knows its applications	[SW1] Assessment of factual knowledge

Subject contents	1. Essential of Quantum Mechanics The time-independent Schrödinger equation and the variational principle Wave mechanics of non-interacting fermions Basis vectors and representations Periodic boundary conditions Local orbitals The jellium model Pseudopotentials 2. Essential of Density Functional Theory What is a functional? Functional derivatives The HohenbergKohn theorems The Thomas-fermi model The Kohn-Sham equations 3. The variational principle at work The Hellmann-Feynman theorem Perturbation theory with the density Second order HohenbergKohn-Sham functional 4. Linear response theory The response function and its relationship to the Kohn-Sham density functional The dielectric function and the Ritchie theory Linear response and Greens functions Linear response in jellium and in crystals 5. Modelling atoms within solids Cohesive energy Elastic constants

	Phonons and lattice dynamics Pairwise potentials in molecules and solids Tight-binding approach 6.Time-dependent density functional theory (maybe) Fundamentals theorems The time-dependent Kohn-Sham scheme Time-dependent observables Linear response and excitation energies 7. The computational way (exercises) Computational minimum Tight-binding approach to electronic structure calculations Plane-wave density functional calculations Density functional calculations with atomic orbitals Real-space density functional calculations Time-dependent density functional calculations (maybe)
Prerequisites and co-requisites	Basics of quantum mechanics Mathematics (integration, differential equation) Basic working knowledge of high-level programming (Fortran 90 and shell script)
Assessment methods and criteria	Subject passing criteria: quiz; Passing threshold: 50.0%; Percentage of the final grade: 100.0%
Recommended reading	Basic literature: Lecture notes taken during the lessons are enough to survive the exam.

	Supplementary literature	or a deeper knowledge the following texts can be adopted: Electronic structure: Basic Theory and Practical Methods by Richard M. Martin, Cambridge University Press, 2nd edition, 2020, ISBN: 9781108555586 Computational Nanoscience by Kálmán Varga & Joseph A. Driscoll, Cambridge University Press, 2012 ISBN: 9780511736230
	eResources addresses	Uzupełniające Adresy na platformie eNauczanie:
Example issues/ example questions/ tasks being completed	Use a numerical code based on DFT to calculate the electronic band structure of simple solids, such as silicon, diamond and graphite	
Work placement	Not applicable	