Cracow University of Technology

Course syllabus

binding for the doctoral students of the CUT Doctoral School commencing their studies in the academic year 2022/2023

Information on the course

Name of the course in Polish	Modelowanie molekularne
Name of the course in English	Molecular modelling
Number of the ECTS points	1
Language of instruction	Polish
Category of the course	Mandatory
Field of education	Engineering and Technology
Discipline of education	Chemical Engineering
Person responsible for the course Contact	Prof. Jarosław Handzlik, *doctus hab.*, DSc jaroslaw.handzlik@pk.edu.pl

Type of course, number of hours in the study programme curriculum

Semester	Credit type (G / NG)*	Lecture	Practical class	Laboratory	Computer laboratory	Project class	Seminar
3	G	15	0	0	0	0	0

*G – graded credit, NG – non-graded credit

Course objectives

Code	Objective description
Objective 1	To acquaint doctoral students with the possibilities of applying modern methods of theoretical chemistry for modelling chemical systems and processes at the molecular level.
Objective 2	To acquaint doctoral students with the basics of computational methods in theoretical chemistry.

Learning outcomes

Code	Description of the learning outcome adjusted to the specific characteristics of the discipline	Learning outcome symbol in the CUT SD	Methods of verification
OUTCOMES RELATED TO KNOWLEDGE			
EKW1	The doctoral student knows and understands the most important computational methods in theoretical chemistry applied to the issues of molecular modeling.	E_W01, E_W02	An oral assignment
EKW2	The doctoral student knows and understands the methods of theoretical prediction of the structure, properties and reactivities of chemical systems.	E_W01, E_W02	An oral assignment
EKW3	The doctoral student knows and understands the methods of materials modelling.	E_W01, E_W02	An oral assignment

OUTCOMES RELATED TO SKILLS			
EKU1	The doctoral student is able to communicate on topics related to molecular modelling, using appropriate terminology.	E_U04	An oral assignment; discussion

Course outline

No.	Contents	Learning outcomes for the course	No. of hours
LECTURE			
W1	General introduction to molecular modelling. Static and dynamic calculations. Software used in calculations.	EKW1, EKW2, EKW3, EKU1	3
W2	Computational methods in theoretical chemistry: molecular mechanics, *ab initio* methods, semi-empirical methods, methods based on density functional theory.	EKW1, EKW2, EKW3, EKU1	6
W3	Theoretical prediction of the structure, properties and reactivities of substances.	EKW2, EKU1	2
W4	Solid state modelling – claster and periodic models. Hybrid methods (QM/MM, QM/QM).	EKW3, EKU1	2
W5	Examples of the application of computational methods of theoretical chemistry in the modelling of chemical systems and processes.	EKW1, EKW2, EKW3, EKU1	2

The ECTS points statement

WORKING HOURS SETTLEMENT	
Type of activity	Average number of hours (45 min.) dedicated to the completion of an activity type
SCHEDULED CONTACT HOURS WITH THE ACADEMIC TEACHER	
Hours allotted in the syllabus	15
Consultations	1
Examination / course credit assignment	2
HOURS WITHOUT THE PARTICIPATION OF THE ACADEMIC TEACHER	
Independent study of the course contents	12
Preparation of a paper, report, project, presentation, discussion	0
ECTS POINTS STATEMENT	
Total number of hours	30
The ECTS points number	1

Preliminary requirements

No.	Requirements
1	Knowledge of general chemistry.
2	Knowledge of physical chemistry.

Course credit assignment conditions / method of the final grade calculation

No.	Description

COURSE CREDIT ASSIGNMENT CONDITIONS	
1	Obtaining a satisfactory grade in the oral assignment.
METHOD OF THE FINAL GRADE CALCULATION	
Evaluation of the oral assignment.	

Additional information

None

The course reading list

1	Jensen F., *Introduction to Computational Chemistry*, 2017, Wiley.
2	Cramer C.J., *Essentials of Computational Chemistry. Theories and Models*, 2013, Wiley.
3	Young D.C., *Computational Chemistry. A Practical Guide for Applying Techniques to Real World Problems*, 2001, Wiley.
4	Piela L., *Idee chemii kwantowej*, 2021, PWN.
5	Scientific articles related to molecular modelling.

Approval of the course syllabus

Person responsible for the course	
Director of the CUT DS	
Place, date	