University of Silesia in Katowice

1.	Field of study	Chemistry
2.	Faculty	Faculty of Science and Technology
3.	Academic year of entry	2024/2025 (winter term)
4.	Level of qualifications/degree	second-cycle studies
5.	Degree profile	general academic
6.	Mode of study	full-time

7.	General information about the module	
Module name		**Theoretical chemistry**
Module code		W4-CH-S2-1-CHT
Number of the ECTS credits		6
Language of instruction		Polish
Purpose and description of the content of education		Moduł Chemia teoretyczna ma za zadanie zapoznanie studentów z ważniejszymi pojęciami chemii teoretycznej, w szczególności wyrobienie umiejętności posługiwania się chemią obliczeniową jako metodą alternatywną do badań eksperymentalnych. Główny akcent kładzie się na zastosowanie metod chemii kwantowej, na różnych poziomach dokładności, do określania charakterystyki spektralnej i właściwości związków chemicznych oraz do opisu struktury połączeń chemicznych na gruncie chemii teoretycznej.
List of modules that must be completed before starting this module (if necessary)		not applicable

8.	Learning outcomes of the module			

Code	Description	Learning outcomes of the programme	Level of competenc (scale 1-5)
W4-CH-S2-1-CHT_01	Zna klasy metod obliczeniowych: DFT (związane z pojęciem gęstości elektronowej) i WFT (związane z pojęciem funkcji falowej).	CH_W01 CH_W06	3 5
W4-CH-S2-1-CHT_02	Rozumie rolę przybliżenia jednoelektronowego w metodach kwantowochemicznych. Zna metodę Hartree-Focka.	CH_W06	4
W4-CH-S2-1-CHT_03	Zna pojęcie korelacji elektronowej i potrafi wskazać metody obliczeniowe uwzględniające efekty korelacyjne.	CH_W06	3
W4-CH-S2-1-CHT_04	Zna metodę DFT w ujęciu Kohna-Shama.	CH_W06	4
W4-CH-S2-1-CHT_05	Zna elementy teorii grup w zakresie umożliwiającym opis i klasyfikację stanów kwantowych cząsteczek.	CH_W03	4
W4-CH-S2-1-CHT_06	Zna obowiązujące teorie wyjaśniające naturę oddziaływań międzycząsteczkowych oraz potrafi je scharakteryzować i sklasyfikować.	CH_W01 CH_W05	2 3
W4-CH-S2-1-CHT_07	Umie zastosować wybrane programy dostępne w pakietach komercyjnych do obliczeń w zakresie chemii kwantowej.	CH_U02	3

W4-CH-S2-1-CHT_08	Umie zastosować metody kwantowochemiczne do badania struktury i energetyki molekularnej.	CH_U02	5
W4-CH-S2-1-CHT_09	Umie wybrać i dostosować bazy funkcyjne do realizowanych obliczeń.	CH_U02	3
W4-CH-S2-1-CHT_10	Umie scharakteryzować konfiguracje i stany elektronowe.	CH_U02	2
W4-CH-S2-1-CHT_11	Umie zastosować metody obliczeniowe chemii kwantowej do opisu oddziaływań międzycząsteczkowych.	CH_U02	3
W4-CH-S2-1-CHT_12	Ma świadomość komplementarności badań teoretycznych i doświadczalnych i ich roli w poznawaniu struktury materii.	CH_K01	2

9.	Methods of conducting classes	

Code	Category	Name (description)
a01	Lecture methods / expository methods	**Formal lecture/ course-related lecture** *a systematic course of study involving a synthetic presentation of an academic discipline; its implementation assumes a passive reception of the information provided*
a03	Lecture methods / expository methods	**Description** *a description of objects, phenomena, processes or people; it involves specifying the structure and characteristic features of the object, phenomenon, or process being described; it is usually accompanied by a demonstration of the described object or by its models, drawings, tables, charts, etc.; a description may take the form of an explanation, classification, justification or comparison*
b01	Problem-solving methods	**Problem-based lecture** *an analysis of a selected scientific or practical problem accompanied by its assessment and an attempt to provide a solution to the issues presented in the lecture as well as the indication of the consequences of the proposed solution*
b02	Problem-solving methods	**Lecture-discussion** *transmission of content involving interaction with the lecture audience; discussion of lecture-related issues is one of its elements or constitutes its follow-up*
c07	Demonstration methods	**Screen presentation** *a presentation of synthetic image content using computer graphics, e.g., a series of slides or other multimedia forms, usually accompanied by a commentary; typical components of a screen presentation include text organized into bulleted points, charts, images and animations, sometimes sound effects or music; a multimedia illustration of course content presented in the form of a projected image*
d01	Programmed learning methods	**Working with a computer** *e.g., Webquest; implementation of educational tasks using electronic and digital devices, computer programs and Internet applications; the academic teacher acts as a consultant; students' work is carried out step by step according to the plan laid own by the person teaching the course and following his instructions, and proceeds towards producing the indicated results within the set deadline*
e01	Practical methods	**Laboratory exercise / experiment** *[also conducted as fieldwork] a method of practical application of knowledge; implemented in three stages: the recognition of a problem induced by the task content, the formulation of the problem and the attempt to solve it accompanied by the assessment of the effects; the goal is to acquire skills, abilities and habits, and to consolidate the acquired knowledge so that it becomes operational; the laboratory method assumes greater independence of learners than carrying out an experiment*
e05	Practical methods	Internship

		including professional and individual training; gaining skills and experience in real-life conditions, e.g., in the environment, institution or workplace the student is preparing for by following a specific study programme; training in real working conditions

10.	Forms of teaching					
Code	**Name**		**Number of hours**	**Assessment of the learning outcomes of the module**	**Learning outcomes of the module**	**Methods of conducting classes**
W4-CH-S2-1-CHT_fs_1	lecture		30	exam	W4-CH-S2-1-CHT_01, W4-CH-S2-1-CHT_02, W4-CH-S2-1-CHT_03, W4-CH-S2-1-CHT_04, W4-CH-S2-1-CHT_05, W4-CH-S2-1-CHT_06, W4-CH-S2-1-CHT_07, W4-CH-S2-1-CHT_10, W4-CH-S2-1-CHT_11	a01, a03, b01, b02, c07
W4-CH-S2-1-CHT_fs_2	laboratory classes		45	course work	W4-CH-S2-1-CHT_07, W4-CH-S2-1-CHT_08, W4-CH-S2-1-CHT_09, W4-CH-S2-1-CHT_10, W4-CH-S2-1-CHT_11, W4-CH-S2-1-CHT_12	c07, d01, e01, e05

11.	The student's work, apart from participation in classes, includes in particular:			
Code	**Category**		**Name (description)**	**Is it part of the BUNA?**
a03	Preparation for classes		Developing practical skills *activities involving the repetition, refinement and consolidation of practical skills, including those developed during previous classes or new skills necessary for the implementation of subsequent elements of the curriculum (as preparation for class participation)*	No
a04	Preparation for classes		Consulting materials complementary to those indicated in the syllabus *agreeing on materials complementary to those indicated in the syllabus, supporting the implementation of tasks resulting from or necessary for class participation*	Yes
b01	Consulting the curriculum and the organization of classes		Getting acquainted with the syllabus content *reading through the syllabus and getting acquainted with its content*	No
b02	Consulting the curriculum and the organization of classes		Verification / adjustment / discussion of syllabus provisions *consulting the content of the syllabus, possibly in the presence of the year tutor or members of the class group, and, if necessary, reassessing the provisions concerning special conditions for class participation, e.g., space and time requirements, technical and other requirements, including conditions for participation in classes outside the walls of the university, classes organized in blocks, organized online, etc.*	Yes
c01	Preparation for verification of learning outcomes		Determining the stages of task implementation contributing to the verification of learning outcomes *devising a task implementation strategy embracing the division of content, the range of activities, implementation time and/or the method(s) of obtaining the necessary materials and tools, etc.*	Yes
c02	Preparation for verification of learning outcomes		Studying the literature used in and the materials produced in class *exploring the studied content, inquiring, considering, assimilating, interpreting it, or organizing knowledge obtained from the literature, documentation, instructions, scenarios, etc., used in class as*	No

		well as from the notes or other materials/artifacts made in class	
c03	Preparation for verification of learning outcomes	Implementation of an individual or group assignment necessary for course/phase/ examination completion *a set of activities aimed at performing an assigned task, to be executed out of class, as an obligatory phase/element of the verification of the learning outcomes assigned to the course*	No
d01	Consulting the results of the verification of learning outcomes	Analysis of the corrective feedback provided by the academic teacher on the results of the verification of learning outcomes *reading through the academic teacher's comments, assessments and opinions on the implementation of the task aimed at checking the level of the achieved learning outcomes*	Yes
d02	Consulting the results of the verification of learning outcomes	Development of a corrective action plan as well as supplementary/corrective tasks *reviewing and selecting tasks and activities enabling the elimination of errors indicated by the academic teacher, their verification or correction resulting in completing the task with at least the minimum passing grade*	Yes

Information on the details of the module implementation in a given academic year can be found in the syllabus available in the USOS system: https://usosweb.us.edu.pl.