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

7.	**General information about the module**
Module name	**Materials modeling**
Module code	W4-TC-S1-5-MM
Number of the ECTS credits	2
Language of instruction	Polish
Purpose and description of the content of education	Moduł Modelowanie materiałów ma za zadanie zapoznanie studentów z podstawowymi pojęciami i metodami chemii obliczeniowej skupiając się przede wszystkim na rozwijaniu umiejętności korzystania z chemii obliczeniowej jako zaawansowanej metody badawczej, alternatywnej wobec tradycyjnych eksperymentów. Student zostanie zapoznany z ważniejszymi możliwościami wykorzystania metod mechaniki molekularnej i metod kwantowo-chemicznych do opisu struktury i własności cząsteczek chemicznych, a także do opisu zjawisk spektroskopowych. Treści zajęć: Zastosowanie obliczeń kwantowych w zielonej chemii: Wykorzystanie obliczeń kwantowo-chemicznych do analizy struktury i właściwości molekularnych; Badania energetyczne i strukturalne molekuł przy użyciu metod kwantowo-chemicznych; Optymalizacja warunków reakcji za pomocą podejścia teoretycznego. Projektowanie Zrównoważonych Materiałów: Wykorzystanie metod chemii teoretycznej do projektowania materiałów o mniejszym wpływie środowiskowym; Badania właściwości materiałów przy użyciu narzędzi obliczeniowych.
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-TC-S1-5-MM_01	Zna i rozumie podstawowe pojęcia mechaniki kwantowej .	TCh_W01	4
W4-TC-S1-5-MM_02	Zna metody mechaniki klasycznej i kwantowej wykorzystywane w modelowaniu molekularnym.	TCh_W01	4
W4-TC-S1-5-MM_03	Umie wyjaśnić budowę cząsteczek chemicznych, rozumie naturę wiązania chemicznego i potrafi scharakteryzować różne jego typy.	TCh_U01	4
W4-TC-S1-5-MM_04	Zna i rozumie metodykę przeprowadzenia obliczeń metodami kwantowo-chemicznymi i mechaniki molekularnej.	TCh_W01	3
W4-TC-S1-5-MM_05	Wykazuje znajomość podstawowych pakietów chemii kwantowej i mechaniki molekularnej.	TCh_W05	3
W4-TC-S1-5-MM_06	Ma podstawową wiedzę na temat planowania i wykonania eksperymentu numerycznego w zakresie metod kwantowo-chemicznych i mechaniki molekularnej.	TCh_W07	3

W4-TC-S1-5-MM_07	Posiada wiedzę na temat zasad projektowania układów molekularnych i reakcji z zachowaniem zasad zielonej chemii i zrównoważonego rozwoju.	TCh_W09	3
W4-TC-S1-5-MM_08	Potrafi zastosować wybrany program obliczeniowy do wyznaczenia struktury elektronowej oraz optymalnej geometrii molekuły.	TCh_U01	4
W4-TC-S1-5-MM_09	Potrafi wyznaczyć strukturę stanu przejściowego reakcji.	TCh_U01	4
W4-TC-S1-5-MM_10	Planuje i realizuje eksperyment numeryczny z zastosowaniem metod kwantowo-chemicznych zgodnie z zasadami zielonej chemii.	TCh_U05	3
W4-TC-S1-5-MM_11	Ma świadomość komplementarności badań teoretycznych i doświadczalnych i ich roli w poznawaniu struktury materii.	TCh_K04	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*
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*

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-TC-S1-5-MM_sf_1	lecture	15	exam	W4-TC-S1-5-MM_01, W4-TC-S1-5-MM_02, W4-TC-S1-5-MM_04, W4-TC-S1-5-MM_05, W4-TC-S1-5-MM_06, W4-TC-	a01, a03, c07

				S1-5-MM_07, W4-TC-S1-5-MM_11	
W4-TC-S1-5-MM_sf_2	laboratory classes	30	course work	W4-TC-S1-5-MM_03, W4-TC-S1-5-MM_04, W4-TC-S1-5-MM_06, W4-TC-S1-5-MM_08, W4-TC-S1-5-MM_09, W4-TC-S1-5-MM_10, W4-TC-S1-5-MM_11	c07, d01, e01

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
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 well as from the notes or other materials/artifacts made in class*	No
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.