University of Gdańsk

Subject card

| | | | |
|---|---|---|---|
| Subject name and code | Introduction to molecular modeling, PG_00033259 | | |
| Field of study | Chemistry | | |
| Date of commencement of studies | October 2024 | Academic year of realisation of subject | 2025/2026 |
| Education level | Bachelor's studies | Subject group | Optional subject group |
| Mode of study | full-time studies | Mode of delivery | at the university |
| Year of study | 2 | Language of instruction | Polish<br>Some of the resources used (e.g. manuals for some programs) are only available in English. |
| Semester of study | 3 | ECTS credits | 2.0 |
| Learning profile | academic | Assessment form | credit |
| Conducting unit | Laboratory of Carbohydrate Chemistry -> Department of Organic Chemistry -> Faculty of Chemistry -> Rector | | |
| Name and surname of lecturer (lecturers) | Subject supervisor | dr hab. Rafał Ślusarz | |
| | Teachers | | |

**Lesson types**

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

E-learning hours included: 0.0

Additional information:

- experiment designing
- analysis of critical events (cases)
- conducting experiments
- blended learning (on-line and stationary classes)

Methods:

- problem study with issues for independent learning
- discussion in the course forum
- exercises in the computer lab (stationary)

**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 | 5.0 | 15.0 | 50 |

**Subject objectives**

Introduction of the student to the subject of molecular modeling.

## Learning outcomes

| Course outcome | Subject outcome | Method of verification |
|---|---|---|
| [CHEML3_U05] Uses basic statistical methods and IT techniques to describe chemical processes and analyse experimental data. | student names the projection methods and defines the scope of the transmitted information in selected molecular systems | [SU2] presentation/project/paper/ report |
| [CHEML3_W09] Describes the practical applications of IT tools (computer programmes) for chemical calculations and data analysis. | student illustrates changes occurring in systems, selects tools specialized in measurement, construction or analysis of collected data | [SW2] presentation/project/paper/ report |
| [CHEML3_W08] Demonstrates knowledge of basic computational methods to solve problems in chemistry, physics, mathematics. | student calculates simple profiles of energy changes, constructs correct queries to bioinformatics databases, indicates the causes of conformation changes | [SW2] presentation/project/paper/ report |
| [CHEML3_U09] Is able to learn independently. | student assesses the usefulness of types of representations in the presentation of results, proposes the best methods of visualization of chemical compounds, shows creativity in the preparation of chemical presentations | [SU2] presentation/project/paper/ report |

## Subject contents

- learning to visualize chemical structures in various computer programs
- preparation of two- and three-dimensional representations of structures of chemical compounds
- simple computer simulations of dynamics and geometry optimization of modeled chemical compounds

## Prerequisites and co-requisites

A basic knowledge of English and a general understanding of the structure of chemical compounds is required.

## Assessment methods and criteria

| Subject passing criteria | Passing threshold | Percentage of the final grade |
|---|---|---|
| student prepares a report for each exercise performed; each such report is assessed separately; the final grade is the arithmetic mean of the partial grades obtained | 51.0% | 100.0% |

## Recommended reading

| | |
|---|---|
| Basic literature | none |
| Supplementary literature | none |
| eResources addresses | |

## Example issues/ example questions/ tasks being completed

- identify and measure all valence angles in an aspirin molecule
- prepare 1,2-dichloroethane z-matrix
- draw up and interpret selected bond-rotation energy profile

## Work placement

Not applicable

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