

**Subject card**

|  |  |  |                          |                                     |                        |            |     |
|--|--|--|--------------------------|-------------------------------------|------------------------|------------|-----|
| <b>Subject name and code</b>                       | Statistical mechanics of biological macromolecules, PG_00119777  |  |                          |                                     |                        |            |     |
| <b>Field of study</b>                              | Chemistry  |  |                          |                                     |                        |            |     |
| <b>Date of commencement of studies</b>             | October 2024   | <b>Academic year of realisation of subject</b>           |                          |                                     | 2025/2026              |            |     |
| <b>Education level</b>                             | Master's studies   | <b>Subject group</b>                                     |                          |                                     | Optional subject group |            |     |
| <b>Mode of study</b>                               | full-time studies  | <b>Mode of delivery</b>                                  |                          |                                     | at the university      |            |     |
| <b>Year of study</b>                               | 2  | <b>Language of instruction</b>                           |                          |                                     | English<br>no comments |            |     |
| <b>Semester of study</b>                           | 3  | <b>ECTS credits</b>                                      |                          |                                     | 2.0                    |            |     |
| <b>Learning profile</b>                            | academic   | <b>Assessment form</b>                                   |                          |                                     |                        |            |     |
| <b>Conducting unit</b>                             | Faculty of Chemistry -> Rector   |  |                          |                                     |                        |            |     |
| <b>Name and surname of lecturer (lecturers)</b>    | <b>Subject supervisor</b>  |  | prof. dr hab. Józef Liwo |                                     |                        |            |     |
|  | <b>Teachers</b>  |  |                          |                                     |                        |            |     |
| <b>Lesson types</b>                                | <b>Lesson type</b>   | Lecture  | Tutorial                 | Laboratory                          | Project                | Seminar    | SUM |
|  | <b>Number of study hours</b>   | 0.0  | 30.0                     | 0.0                                 | 0.0                    | 0.0        | 30  |
|  | E-learning hours included: 0.0   |  |                          |                                     |                        |            |     |
| <b>Learning activity and number of study hours</b> | <b>Learning activity</b>   | Participation in didactic classes included in study plan |                          | Participation in consultation hours |                        | Self-study | SUM |
|  | <b>Number of study hours</b>   | 30   |                          | 5.0                                 |                        | 15.0       | 50  |
| <b>Subject objectives</b>                          | The aim of the course is to familiarize students with the basics of statistical mechanics of biopolymers, with particular emphasis on the conditions and mechanisms their structure formation. |  |                          |                                     |                        |            |     |

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|---|---|--|---|
| Learning outcomes   | Course outcome  | Subject outcome  | Method of verification  |
|   | [CHEMMU2_K06] Undertakes research tasks consciously and responsibly, understanding the social aspects of the practical application of the acquired knowledge and skills and the responsibility related to it.   | The student applies statistical mechanics in the description of biological macromolecules.   | [SK1] oral statement/conversation/discussion<br>[SK4] test/exam - oral or written<br>[SK5] implementation of a problem task |
|   | [CHEMMU2_W05] Has extended knowledge in the field of the specialisation studied.  | The student applies extended knowledge in the statistical mechanics of biological macromolecules.  | [SW4] test/exam - oral or written<br>[SW1] oral statement/conversation/discussion   |
|   | [CHEMMU2_W06] Applies mathematics to the extent necessary to understand, describe and model chemical processes of medium complexity.  | The student applies calculus to statistical mechanical description of macromolecules.  | [SW4] test/exam - oral or written<br>[SW1] oral statement/conversation/discussion<br>[SW5] implementation of a problem task |
|   | [CHEMMU2_U02] Critically assesses the results of conducted, performed observations and theoretical calculations and discusses errors.   | The student critically evaluates applications of statistical mechanics in the description of the structure and energetics of biological macromolecules.                          | [SU1] oral statement/conversation/discussion<br>[SU5] implementation of a problem task                                      |
|   | [CHEMMU2_K01] Knows the limitations of her/his own knowledge; understands the need for further education and can inspire other people to do so.   | The student knows the limitations of her/his knowledge in calculus, statistical physics, and the physical chemistry of biological molecules and knows the ways of completing it. | [SK4] test/exam - oral or written<br>[SK5] implementation of a problem task   |
| [CHEMMU2_U11] Communicates in English in accordance with the requirements specified for level B2 of the Common European Framework of Reference for Languages. | The student learns English vocabulary in statistical physics and the physical chemistry of biological macromolecules.   | [SU1] oral statement/conversation/discussion   |   |
| Subject contents  | Elements of statistical mechanics: ensembles, ensemble averages, thermodynamic connection. Statistical-mechanical models of polymers chains. Potentials of mean force. Structure formation and self-organization in biopolymers as a phase transition. One-dimensional case: helix-coil transition. Solvent-mediated interactions in the formation and stabilization of biopolymer structure. Polymers in a good and in a bad solvent. Global minimum of a potential and of the free energy and stability of polymer structure. Foldability. Simple lattice models to study foldability. Free-energy landscapes of biological macromolecules and methods for their investigation. Coarse-grained force fields for biopolymer simulations as potentials of mean force. |  |   |
| Prerequisites and co-requisites   | Knowledge of the applications of statistical mechanics in chemistry.  |  |   |
| Assessment methods and criteria   | Subject passing criteria  | Passing threshold  | Percentage of the final grade   |
|   | Completing assignments  | 51.0%  | 50.0%   |
|   | Test  | 51.0%  | 50.0%   |
| Recommended reading   | Basic literature  | D. McQuarrie: Statistical mechanics<br><br>A. Leach: Molecular modeling: principles and applications   |   |
|   | Supplementary literature  | T. Schlick: Molecular dynamics and simulations   |   |
|   | eResources addresses  | Adresy na platformie eNauczanie:   |   |
| Example issues/<br>example questions/<br>tasks being completed  | <p>1. Calculate the energy of a protein molecule represented by the HP model on cubic lattice.</p> <p>2. Using UNRES server run energy minimization of the crambin molecule and interpret the deviations from the experimental structure.</p> <p>3. Using UNRES server determine the thermal heat-capacity profile of tryptophan cage and interpret the maximum in this profile.</p>  |  |   |
| Work placement  | Not applicable  |  |   |

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