University of Gdańsk

Subject card

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|---|---|---|---|
| Subject name and code | Computer instead of chemistry laboratory, PG_00080800 | | |
| Field of study | Chemical Business | | |
| Date of commencement of studies | October 2026 | Academic year of realisation of subject | 2028/2029 |
| 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 | 3 | Language of instruction | Polish |
| Semester of study | 5 | ECTS credits | 2.0 |
| Learning profile | academic | Assessment form | credit |
| Conducting unit | Department of Theoretical Chemistry -> Faculty of Chemistry -> Rector | | |
| Name and surname of lecturer (lecturers) | Subject supervisor | prof. dr hab. Piotr Skurski | |
| | 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

**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**

Acquainting students with the possibilities of using quantum chemistry software to solve chemical problems

**Learning outcomes**

| Course outcome | Subject outcome | Method of verification |
|---|---|---|
| [BCHINŻ_U04] In the course of carrying out engineering tasks, s/he uses basic statistical methods, IT techniques and uses application software packages to describe chemical processes and experimental data. | Student performs calculations using computational quantum chemistry methods. | [SU5] implementation of a problem task |
| [BCHINŻ_W03] Describes the techniques of higher mathematics and IT tools necessary to describe and model chemical phenomena and technological processes. | Student solves advanced problems related to computational chemistry methods. | [SW1] oral statement/ conversation/discussion<br>[SW5] implementation of a problem task |
| [BCHINŻ_W04] Describes the role of experiment and computer simulation in the design process of engineering issues. | Student selects and chooses proper algorithms and software packages which enable performing the calculations and solve a given problem. | [SW1] oral statement/ conversation/discussion<br>[SW5] implementation of a problem task |
| [BCHINŻ_U09] Using the acquired knowledge, skills and various sources of scientific information independently prepares written papers and oral presentations. | Student interprets the results using own knowledge | [SU1] oral statement/conversation/ discussion<br>[SU5] implementation of a problem task |
| [BCHINŻ_K02] Works individually demonstrating initiative and independence in actions, and effectively cooperates in a team, performing various roles in it. | Student works as a team member, respects the lecturer and other team members. | [SK1] oral statement/conversation/ discussion |

<table>
<tr><td>Subject contents</td><td>Preparing input data files, graphical interpretation of the results, determining the equilibrium structures of molecules,simulating IR, NMR, and UV spectra, evaluating physicochemical parameters (energy, Gibbs free energy, entropy, heat capacity, dipole and quadrupole moments, polarizability and hyperpolarizability), chemical reaction modeling (determining reaction mechanism, estimating activation barriers, calculating the reaction rate).Knowledge acquainted by the students after attending the lectures: basic knowledge concerning the types of problems that could be solved by using quantum chemistry methods and software, the ability of choosing proper theoretical approach to given problems, the ability of interpreting the results that come from quantum chemistry calculations.Knowledge acquainted by the students after attending the seminars: the knowledge concerning input data preparation (for quantum chemistry software packages), the ability of performing calculations resulting with obtaining molecular structure, simulated IR, NMR and UV spectra, multipole moments, polarizabilities and hyperpolarizabilities, energy, Gibbs free energy, and entropy; the ability of chemical reaction modeling by locating the transition state structures, intermediate products and reaction products, estimating the height of the activation barriers, calculating the rate of the overall process.</td></tr>
<tr><td>Prerequisites and co-requisites</td><td>Ability to use a PC computer (basic level).</td></tr>
<tr><td>Assessment methods and criteria</td><td>
<table>
<tr><th>Subject passing criteria</th><th>Passing threshold</th><th>Percentage of the final grade</th></tr>
<tr><td>Activity during classes</td><td>51.0%</td><td>25.0%</td></tr>
<tr><td>Reports documenting solved problems</td><td>51.0%</td><td>75.0%</td></tr>
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<tr><td>Recommended reading</td><td>
<table>
<tr><td>Basic literature</td><td>Molecular Quantum Mechanics (P. Atkins, R. Friedman)</td></tr>
<tr><td>Supplementary literature</td><td>Ideas of Quantum Chemistry (L. Piela)</td></tr>
<tr><td>eResources addresses</td><td></td></tr>
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<tr><td>Example issues/ example questions/ tasks being completed</td><td>Propose a path (series of steps) aiming to determine the ionization potential and electron affinity of a given molecule (using any chosen quantum chemistry method).</td></tr>
<tr><td>Work placement</td><td>Not applicable</td></tr>
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