University of Gdańsk

Subject card

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|---|---|---|---|
| Subject name and code | Quantum chemistry in practice, PG_00054865 | | |
| Field of study | Chemistry | | |
| Date of commencement of studies | October 2024 | Academic year of realisation of subject | 2024/2025 |
| Education level | postgraduate studies | Subject group | Obligatory subject group in the field of study |
| Mode of study | full-time studies | Mode of delivery | at the university |
| Year of study | 1 | Language of instruction | English<br>English |
| Semester of study | 1 | ECTS credits | 3.0 |
| Learning profile | academic | Assessment form | |
| Conducting unit | Katedra Chemii Teoretycznej -> Faculty of Chemistry | | |
| Name and surname of lecturer (lecturers) | Subject supervisor | prof. dr hab. Piotr Skurski | |
| | Teachers | prof. dr hab. Piotr Skurski | |

**Lesson types**

| Lesson type | Lecture | Tutorial | Laboratory | Project | Seminar | SUM |
|---|---|---|---|---|---|---|
| Number of study hours | 30.0 | 0.0 | 0.0 | 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 | 40.0 | 75 |

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| Subject objectives | Acquainting students with the possibilities of using quantum chemistry methods and quantum chemistry software to solve chemical problems |

**Learning outcomes**

| Course outcome | Subject outcome | Method of verification |
|---|---|---|
| [CHEMMU2_U02] Critically assesses the results of conducted, performed observations and theoretical calculations and discusses errors. | Student critically assesses the results of performed theoretical calculations and discusses them in the context of predicted properties of molecules | [SU1] oral statement/conversation/ discussion<br>[SU4] test/exam - oral or written |
| [CHEMMU2_W05] Has extended knowledge in the field of the specialisation studied. | Student has extended knowledge in the field of quantum chemistry tools and techniques | [SW4] test/exam - oral or written |
| [CHEMMU2_K01] Knows the limitations of her/his own knowledge; understands the need for further education and can inspire other people to do so. | Student knows the limitations of her/his own knowledge; understands the need for further education | [SK4] test/exam - oral or written |
| [CHEMMU2_U04] Applies acquired knowledge of chemistry and related scientific disciplines. | Student applies acquired knowledge of the structure and properties of molecules, general chemistry and related scientific disciplines | [SU4] test/exam - oral or written |
| [CHEMMU2_W08] Demonstrates knowledge of theoretical computational and IT methods used to solve problems in chemistry. | Student demonstrates in-depth knowledge of the ability of solving various chemical problems by using quantum chemistry tools | [SW4] test/exam - oral or written<br>[SW1] oral statement/ conversation/discussion |
| [CHEMMU2_W07] Selects experimental and theoretical techniques to the extent necessary to understand the description and modelling of medium complexity chemical processes. | Student selects suitable computational tools to the extent necessary to study various types of chemical problems | [SW4] test/exam - oral or written |

**Subject contents**

Basic knowledge concerning various types of chemical problems that might be solved using quantum chemistry methods and software, the use of software designed to evaluating physicochemical properties of molecules, defining the problem that is to be solved, the ability to perform desired calculations using computers, the ability to properly interpret the results and formulate conclusions, preparing input data files for QM software, 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), determining stationary points on the potential energy surface.

**Prerequisites and co-requisites**

Basic knowledge in chemistry and physics

**Assessment methods and criteria**

| Subject passing criteria | Passing threshold | Percentage of the final grade |
|---|---|---|
| Written final exam | 51.0% | 100.0% |

**Recommended reading**

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| Basic literature | An Introduction to Theoretical Chemistry, Jack Simons, Cambridge University Press, 2003<br><br>Molecular Quantum Mechanics, P. W. Atkins, R. S. Friedman, Oxford University Press Inc., New York (2011)<br><br>Energetic Principles of Chemical Reactions, J. Simons, Jones and Bartlett Publishers, Inc., 1983. |
| Supplementary literature | Quantum Mechanics in Chemistry, J. Simons, J. Nichols, Oxford University Press (1997)<br><br>Geometrical Derivative of Energy Surfaces and Molecular Properties, P. Jorgensen, J. Simons, D. Reidel Publ. Company, 1985 |
| eResources addresses | Adresy na platformie eNauczanie: |

**Example issues/ example questions/ tasks being completed**

Describe the computational steps which must be undertaken to determine the Gibbs free reaction energy of the Gly-Ala dipeptide formation (using Gly and Ala substrates) at T=297 K and p=1 atm.

**Work placement**

Not applicable

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