

Name: Theoretical chemistry (C-PS.II1-TheoCH)

Name in Polish:

Name in English: Theoretical chemistry

Information on course:

Course offered by department: Faculty of Chemistry

Course for department: Faculty of Chemistry

Default type of course examination report:

Grading

Language:

English

Description:

LECTURE:

1. Repetition of the information related to the basics of quantum mechanics: genesis, postulates of quantum mechanics, simple models of quantum mechanics (particle in the box, harmonic oscillator, rigid rotor, hydrogen-like atom), approximation methods (variational and perturbational).
2. Many-electron systems. Total energy operator for the molecule and possibility of solving Schrodinger equation for the molecule.
3. Basic approximations of quantum chemistry leading to the Hartree-Fock method (HF) and Hartree-Fock-Roothaan method (HFR) for the closed-shell systems. Concept of basis set.
4. Basis of Density Functional Theory (DFT).

CLASSES:

During the seminar we discuss the topics introduced previously during the lecture and solve the exercises related with them. Additionally, students can run the quantum calculation PQS software, which will be used intensively in the second semester during lab classes.

Bibliography:

1. Notatki z wykładów.
2. T. Engel, W. J. Hehre, "Quantum chemistry and spectroscopy", Boston etc. : Pearson 2013.
3. J. P. Lowe, K. L. Peterson, "Quantum Chemistry", Elsevier 2006.
4. L. Pielak, "Ideas of Quantum Chemistry", Elsevier 2014.

Learning outcomes:

KNOWLEDGE

W1. Have basic knowledge of quantum chemistry. K_W08

W2. Have general knowledge about Hartree-Fock and Hartree-Fock-Roothaan methods. K_W08

SKILLS

U1. Should be able to demonstrate the necessity of quantum-mechanical description of microsystems and formulate the postulates of quantum mechanics. K_U04, K_U23

U2. Should be able to formulate and calculate exercises related to the problem discussed during the course. K_U01, K_U16

COMPETENCES

K1. Know the limitations of his/her knowledge and understand the need of further education. K_K01

K2. Be able to work in a team and understand the need of teamwork in research in the field of modern chemistry. K_K02

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Contact hours (work with an academic teacher)

lecture 15 hrs, laboratory 15 hrs,

Total number of hours with an academic teacher: 30 hrs

Number of ECTS points with an academic teacher: 1

Non-contact hours (students' own work)

Preparation for lectures 10 hrs

Preparation for seminar 10 hrs

Literature studies 10 hrs

Total number of non-contact hours: 30 hrs

Number of ECTS points for non-contact hours: 1

Total number of ECTS points for the module: 2

consultations: 2 hrs

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Final test - W1, W2, U1, U2
Activity - K1, K2

Requirements

Finished math course as well as the course on the basics of theoretical (quantum) chemistry

Course credits in various terms:**<without a specific program>**

Type of credits	Number	First term	Last term
European Credit Transfer System (ECTS)	2	15/16	