***Computational Chemistry and Chemical Bond Theory – dr. hab. Cina Foroutan-Nejad***

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| Title | **Computational Chemistry and Chemical Bond Theory** |
| Lecturer | **Dr. Cina Foroutan-Nejad** |
| Name of the unit | Institute of Organic Chemistry PAS |
| Number of ECTS credits assigned to the course | **1 ECTS** |
| Form | Lecture, 5 h/semester |
| Language | English |
| Learning outcomes for the subject in terms of: knowledge, skills and social competences | Introduction to main concepts: Basis set, Functional, Wavefunction<br>-In the first lecture I will introduce all terms that are frequently used in the terminology of computational chemistry to make sure that students are familiar with the concepts that are widely used in the manuscripts.<br>Potential Energy Surface<br>-In the second lecture I will introduce the concept of PES and how computational tools should be used to locate local minima, transition states and simple mathematical concepts behind them.<br>Chemical Bonds in Quantum Mechanics<br>-In the last lecture I will make a bridge between the chemical concepts used by experimental chemists and the concepts used by computational chemists. I will briefly explain the dilemma of chemical bonding and the misunderstandings between theory and experiment when it comes to classical concepts. |
| Implementation method | Lectures will be presented by PowerPoint. |
| Prerequisites and additional requirements | Basic knowledge of chemistry |
| Didactic methods used | Lectures will introduce basic concepts to the students. |
| Methods of checking and assessing the learning outcomes obtained by doctoral students | Oral exam. |
| The form and conditions of passing the course | Pass/fail |
| Course content | The course is tuned to cure part of the knowledge of the PhD students that is built on the basis of old concepts in chemistry. The lectures will hopefully help them to shed obsolete knowledge and replace them with state-of-the-art knowledge in computational and physical chemistry. Basic concepts like potential energy surface or the concepts of chemical bond, orbitals, and distinction between ground-, response-, and excited-state properties will be discussed. |
| List of basic and supplementary literature | 1. Computational Organic Chemistry, Steven M. Bachrach, DOI:10.1002/9781118671191, Wiley & Sons, Inc.<br>2. Essentials of Computational Chemistry: Theories and Models, Christopher J. Cramer, ISBN: 978-0-470-09182-1, Wiley & Sons, Inc.<br>3. Quantum Chemistry, 7th Edition, Ira N. Levine, ISBN-10: 0-321-80345-0, Pearson. |