**Course title:** Molecular modeling in catalysis and chemical technology – ~~selectable~~ / regular course

**Number of contact hours:** 45 hours (15h lectures, 30h computer laboratories)

**ETCS credits**: 3

**Course description:** The lecture reviews the molecular modeling methods on a background of catalysis and chemical technology. Computational methods of theoretical chemistry will be discussed: molecular mechanics, ab initio and semi-empirical methods, density functional theory, hybrid methods (QM / MM, QM / QM) and their application in modeling of large molecules and materials. Special attention will be provided on the theoretical prediction of the structure and properties substances, including reactivity. The analysis of electronic structure of materials (population and bond order analysis, Fukui indexes, density-of-state) will be presented. Examples of the use of molecular modeling in the research of systems and chemical processes, including catalytic processes, will be given. The laboratories consist of exercises on molecular modeling of selected systems: preparation of input files, running calculations using specialized software, visualization and interpretation of the results of calculations.

**Education effects** (P6S_UW, P7S_WG)**:**

- **knowledge**: student knows the most important methods in molecular modeling; knows the methods of building crystal structure of materials used in catalysis and chemical technology; is familiar with possible geometrical models used in molecular modeling

- **skills**: student is able to prepare input data and run simple calculations in the field molecular modeling as well as to interpret the results of computations; can predict the structure and properties of chemical systems

- **social**: student is able to work independently and in the group both at the laboratories and during preparation of the report; understand the advantages of molecular modeling in modern chemical technology research

**Literature:** [1 ] F. Jensen — Introduction to Computational Chemistry, , 2007, Wiley-VCH; [2 ] K. I. Ramachandran, G. Deepa, K. Namboori — Computational Chemistry and Molecular Modeling, 2008, Springer; [3 ] C. J. Cramer — Essentials of Computational Chemistry. Theories and Models, 2004, Wiley-VCH

**Assessment method:** Final test, completing the laboratories (presence and delivering of reports from each performed exercise)

**Prerequisites:** Basic knowledge in organic chemistry and technology

**Primary target group:** All specialties students

**Lecturer:** dr hab. inż. I. Czekaj, Contact person: dr hab. inż. I. Czekaj e-mail: iczekaj@chemia.pk.edu.pl