



Subject card

Subject name and code	, PG_00035160						
Field of study	Engineering and Technologies of Energy Carriers						
Date of commencement of studies	February 2024		Academic year of realisation of subject		2024/2025		
Education level	second-cycle studies		Subject group		Optional subject group Subject group related to practical vocational preparation		
Mode of study	Full-time studies		Mode of delivery		at the university		
Year of study	1		Language of instruction		Polish		
Semester of study	2		ECTS credits		3.0		
Learning profile	practical profile		Assessment form		assessment		
Conducting unit	Department of Physical Chemistry -> Faculty of Chemistry						
Name and surname of lecturer (lecturers)	Subject supervisor		dr hab. inż. Maciej Śmiechowski				
	Teachers		dr hab. inż. Maciej Śmiechowski				
Lesson types and methods of instruction	Lesson type	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
	Number of study hours	15.0	0.0	30.0	0.0	0.0	45
	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	45		3.0		27.0	75
Subject objectives	The aim of the subject is to familiarize the student with the issue of molecular modeling of catalytic processes with a particular consideration of practical aspects of running computer simulations.						
Learning outcomes	Course outcome		Subject outcome		Method of verification		
	K7_W09		Student knows and understands the molecular mechanism of basic catalytic processes used in chemical technology, especially in the field of heterogeneous catalysis.		[SW1] Assessment of factual knowledge		
	K7_U05		Student can relate an experimental catalytic process with its molecular mechanism and proposes a simulation-based approach to verify its course.		[SU2] Assessment of ability to analyse information [SU3] Assessment of ability to use knowledge gained from the subject		
	K7_U07		Student analyzes studied catalytic processes with respect to molecular modifications of reactants ensuring the achievement of better efficiency or selectivity of the process.		[SU1] Assessment of task fulfilment [SU4] Assessment of ability to use methods and tools		
	K7_U06		Student selects a computational method appropriate for a posited simulation problem considering the computational complexity of the problem and the time consumption of the required calculations.		[SU2] Assessment of ability to analyse information [SU4] Assessment of ability to use methods and tools		

Subject contents	<ol style="list-style-type: none"> 1. Repetition in chemical kinetics: reaction order, reaction rate, rate constant and its determination, determination of reaction order, composite reactions, stationary state approximation, temperature dependence of rate constant, Arrhenius equation, activation energy, collision theory, transition state theory and calculation of rate constant, reactions in solutions 2. Repetition in surface science: physical and chemical adsorption, adsorption isotherms, Gibbs isotherm, adsorption from solutions, dispersed phases 3. Repetition in catalysis: catalysts and active centers, homogeneous catalysis, autocatalysis, heterogeneous catalysis (structure of catalysts, metallic catalysts, semiconductor catalysts, stages of a catalyzed reaction) 4. Overview of computational chemistry: molecular mechanics, molecular dynamics, Hartree-Fock method, Kohn-Sham equations, density functional theory, semi-empirical methods, force fields, QM/MM and ONIOM hybrid methods 5. Thermochemical calculations: geometry optimization, vibrational analysis, thermochemical properties, thermodynamics of chemical reactions, optimization to transition state, calculation of rate constant 6. Surface modeling methods: Bravais and reciprocal lattice, periodic boundary conditions, Bloch waves, Brillouin zone, band structure, Fermi level and band gap, density of states, computational problems (GW method, Hubbard model) 7. Solvation effects: polarizable continuum model (PCM), COSMO model, cluster-continuum models, molecular level solvation 8. Molecular descriptors in modeling: population analysis, electrostatic potential, localized orbitals, bond order analysis, chemical reactivity indexes (chemical potential, hardness, electrophilicity index, Fukui functions) 9. Reaction path modeling: definition of reaction coordinate, intrinsic reaction coordinate (IRC method), potential energy hypersurface, rare events dynamics, exploration of free energy hypersurface (perturbation methods, thermodynamic integration, umbrella sampling, ABF method, replica exchange, metadynamics) 10. Examples of catalytic process modeling: methanol oxidation, benzene alkylation, olefin polymerization, DeSOx and DeNOx catalysts, epoxidation and others. 11. Examples of software packages: classical molecular dynamics, quantum chemistry, ab initio molecular dynamics 											
Prerequisites and co-requisites	Knowledge of material from mathematics and physics in the range of basic academic course in 1st level studies. Basic knowledge of chemical kinetics. Suggested: introductory information in quantum chemistry or physics.											
Assessment methods and criteria	<table border="1" data-bbox="448 949 1487 1055"> <thead> <tr> <th data-bbox="448 949 794 987">Subject passing criteria</th> <th data-bbox="794 949 1141 987">Passing threshold</th> <th data-bbox="1141 949 1487 987">Percentage of the final grade</th> </tr> </thead> <tbody> <tr> <td data-bbox="448 987 794 1016">laboratory reports</td> <td data-bbox="794 987 1141 1016">50.0%</td> <td data-bbox="1141 987 1487 1016">50.0%</td> </tr> <tr> <td data-bbox="448 1016 794 1055">open-ended test in lecture material</td> <td data-bbox="794 1016 1141 1055">50.0%</td> <td data-bbox="1141 1016 1487 1055">50.0%</td> </tr> </tbody> </table>			Subject passing criteria	Passing threshold	Percentage of the final grade	laboratory reports	50.0%	50.0%	open-ended test in lecture material	50.0%	50.0%
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Recommended reading	Basic literature	<ol style="list-style-type: none"> 1. P. W. Atkins, Chemia fizyczna, PWN, Warszawa 2001. 2. K. Pigoń, Z. Ruziewicz, Chemia fizyczna 1. Podstawy fenomenologiczne, PWN, Warszawa 2005. 3. K. Pigoń, Z. Ruziewicz, Chemia fizyczna 2. Fizykochemia molekularna, PWN, Warszawa 2005. 										
	Supplementary literature	<ol style="list-style-type: none"> 1. A. Molski, Wprowadzenie do kinetyki chemicznej, WN-T, Warszawa 2001. 2. E. T. Dutkiewicz, Fizykochemia powierzchni, WN-T, Warszawa 1998. 3. L. Piela, Idee chemii kwantowej, PWN, Warszawa 2003 4. R. F. Nalewajski, Podstawy i metody chemii kwantowej. Wykłady, PWN, Warszawa 2001. 5. A. Kaczmarek-Kędziera, M. Ziegler-Borowska, D. Kędziera, Chemia obliczeniowa w laboratorium organicznym, Wydawnictwo Naukowe UMK, Toruń 2014. 										
	eResources addresses	Adresy na platformie eNauczanie: Modelowanie procesów katalitycznych - Moodle ID: 39660 https://enauzanie.pg.edu.pl/moodle/course/view.php?id=39660										
Example issues/ example questions/ tasks being completed	<ol style="list-style-type: none"> 1. Define the continuous Fukui function and its three discrete approximations. Relate the reactivity of a molecule towards different types of substitutions to the appropriate discrete functions. 2. The optimization of the geometry of a quantum chemical system has led to a stationary point. How can we distinguish whether it is a local energy minimum or a transition state? How can we predict the direction of deformation of the transition state to a stable structure? 3. Briefly describe the applications of the polarizable continuum model (PCM) in modeling molecules in solution. 4. Define the Fermi level for a solid. Based on its position, divide solids into conductors/semiconductors/insulators. 5. Describe the idea and applications of the internal reaction coordinate (IRC) method. 6. List and briefly characterize three methods of population analysis. 7. Discuss the individual rungs of the "Jacob's ladder" of electron density functionals. 8. Discuss the application of metadynamics in the exploration of the potential energy surface of a system undergoing a chemical reaction. 9. Give the text of Hohenberg-Kohn theorem II. 10. Discuss the basic elements of a typical flexible force field used in molecular mechanics. 											
Work placement	Not applicable											

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