GDAŃSK UNIVERSITY OF TECHNOLOGY

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

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, computationa 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

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%

Recommended reading

Basic literature

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

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://enauczanie.pg.edu.pl/moodle/course/view.php?id=39660

Example issues/ example questions/ tasks being completed

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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