UNIVERSITY of MISKOLC
Faculty of Materials Science and Engineering

AntalKerpely Doctoral School of Materials Science & Technology

Application of Theoretical Chemistry Methods for Industrial Processes

Béla Viskolcz

COURSE DESCRIPTION

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Application of Theoretical Chemistry Methods for Industrial Processes

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Lecturer

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Recommendation

The lecture is proposed for all students of the AntalKerpelyDoctoralSchool, especially in the field of Chemical Processes and Technologies.

Language

Hungarian or English.

Scope

The aim of the course is to give a background for the students to understanding the industrial processes using theoretical chemistry as a tool which can be an application to discover the industrial processes in chemical reactors. Using modern computational chemistry methods can be useable to find out the possible side processes and their mechanism. The students to be able to help improve the industrial processes and to make a proposal.

Methodology

The course is held in contact lectures and hands-on trainings. At first, the general description of the physical chemistry background and the overview of the mechanismsthereafter the theoretical methods and their applicability will be reviewed.

Topics

The concept of elementary reactions, reaction mechanisms, reaction networks of the elementary reactions and their interpretation.

Characteristics of the Potential surfacesof the elementary reactions, potential energy surface of partial and full reaction mechanism: properties and calculations.

Calculations of the mechanism for simple chemical industrial process.
Catalysts effect on the reaction mechanism: efficacy and selectivity. Overview of computational methods for surfaces and catalysis.

Determination of individual oxidation and reduction processes: calculation of complete product spectrum. Intermediates and pathways probability, understanding of by-products formation.

Planning and design of complex kinetic models. Finding and mapping databases. Building process of Specific database. Create a sample database related of the students' research fields.

Industrial applicability of group additivity rules. Check the consistency using the additivity rules of own data sets.

References

1. Ferenc Ruff, Imre G. Csizmadia: Organic Reactions: Equilibria, Kinetics and Mechanism, Amsterdam, Elsevier 1994.
2. Christopher J. Cramer: E*ssentials of ComputationalChemistry: Theories and Models* (2nd Edition), Wiley, 2004.
3. Mc Quarrie: Physicalchemistry a molecularapproach *University Science Books, Sausalito, California, 1997.*
4. + If a student intends to applyany method linked to this course for her/hisdoctoral research, then she/he will be able to request specific articles.

Exam

Oral exam.

Complex exam questions

1. Potential energy surfaces of reaction mechanism and elementary reactions. Advantages, disadvantages and limitations of computational methods. Theory versus industrial, experimental observations and literature
2. Reaction Networks and their interpretation and applicability of optimization of industrial processes.
3. Interpretation of elementary processes occurring catalysts, their effect on reaction mechanism. Catalysts surface properties and catalytic activity.
4. Creation of database using theoretical methods, validation and consistency checks
5. Mechanisms based on theoretical calculations: accuracy, advantages and limitations of their applicability in practice. Predictions for industry processes.