GHENT UNIVERSITY

Course Specifications

Valid as from the academic year 2015-2016

Molecular Modelling of Industrial Processes (E071341)

Course size *(nominal values; actual values may depend on programme)*

Credits 6.0 **Study time 180 h** **Contact hrs** 60.0 h

Course offerings and teaching methods in academic year 2016-2017

A (semester 2)	seminar: practical PC room classes	30.0 h
	lecture	30.0 h

Lecturers in academic year 2016-2017

Van Speybroeck, Veronique	TW17	lecturer-in-charge
De Wispelaere, Kristof	TW17	co-lecturer

Offered in the following programmes in 2016-2017	crdts	offering
Master of Science in Chemical Engineering	6	A
Master of Science in Sustainable Materials Engineering	6	A
Master of Science in Chemical Engineering	6	A
Master of Science in Bioscience Engineering: Chemistry and Bioprocess Technology	6	A

Teaching languages

Dutch

Keywords

Catalysis, chemical kinetics and thermodynamics, Density Functional Theory, Transition State Theory, Molecular Dynamics

Position of the course

Molecular modeling and simulations play a central role in the current development of industrial processes. It is an interdisciplinary research field in which physical and chemical insights are combined to understand the interactions on the nanoscale and the reactivity of individual chemical reactions. Due to the enormous increase of computational power and the development of very advanced numerical algorithms this approach is indispensable within the current field of chemical technology. Currently molecular modeling has reached the level that it enables to offer a toolset of methodologies that allow to design chemical processes and catalysts from the molecular level. Due to the complexity and the occurrence of many chemical reactions simultaneously in an industrial process, it is often very difficult to obtain insight into individual chemical reactions. In the past catalysts were often designed using a try-and-error approach. Insight at the molecular scale allows to design innovative processes in a smart way. The application area is very broad and has proven its success for the development of many green and clean processes. This course describes the various methodologies that are needed to describe the electronic structure from first principles. This knowledge allows to deduce all necessary molecular properties to simulate reactions in complex molecular environments. The chemical kinetics and thermodynamics of individual chemical reactions are studies together with various reaction mechanisms in a variety of molecular environments.

Contents

- Interactions present at the nanoscale : bonding, non-bonding, electrostatic, Van Der Waals interactions, Origin of different types of bonding (covalent, ionic, hydrogen bridges, non-bonding)
- Born-Oppenheimer approximation for molecular systems
- Techniques for the determination of the electronic structure : Independent Particle Model (IPM), Hartree-Fock concept, Post-Hartree-Fock methods, Density Functional Theory, Semi-empirical methods, Molecular mechanics.

- Basis sets : Localized Gaussian basis sets, numerical implementation of self-consistent schemes, plane-wave pseudopotential methods, implementation of DFT techniques in practical electronic structure calculations
- External and internal degrees of freedom of the molecule. Ab initio determination of thermodynamic quantities such as enthalpy, entropy
- Hybrid calculation methods : Embedding schemes for supramolecular systems. QM/MM methods to accurately describe the extended molecular environment.
- Ab initio description of the kinetics and thermodynamics of chemical reactions
- Techniques to account for the topology of industrial catalysts. Cluster models and periodic models.
- Application on reactions important for the thermal cracking of hydrocarbons, coke formation, free radical polymerization
- Application on acid catalysed conversion processes on zeolites.
- Catalytic process on metal-organic frameworks
- Metal catalyzed processes such as Fischer-Tropsch process.

Initial competences

Moleculaire structuur en statistische fysica, organic chemistry, Oppervlakfenomenen en katalyse, fysische scheikunde

Final competences

1 CONCEPTS: Chemical kinetics, activation energy, preexponential factor, transition state, reaction mechanism, reactivity, chemical structure, catalyst properties and influence on chemical kinetics. Insight into the most important interactions governing the phenomena on the nanoscale. Insight into the most important techniques and methods to treat molecular systems with dimensions going from 0.1 to 10 nm.
2 SKILLS : Determine the chemical kinetics of reactions important for various industrial processes. Determine the right molecular model system to model the reactions at a well defined model system.. Insight into the accuracy of the obtained chemical parameters.

Conditions for credit contract

Access to this course unit via a credit contract is determined after successful competences assessment

Conditions for exam contract

This course unit cannot be taken via an exam contract

Teaching methods

Lecture, seminar: practical PC room classes

Extra information on the teaching methods

The lectures consist of theory courses. On a weekly basis practical exercises are given which allow to thoroughly understand the theory. During the PC-exercises, the theory is applied on molecular system of industrial importance by means of intensive computer exercises. The most current software programs currently used in this field are applied such as Gaussian, VASP,... During these sessions, the students work in groups of two on a laptop and the calculations themselves are performed on state-of-the art computer units of the CMM. Very intensive coaching is given to allow hands-on assistance.

Learning materials and price

Syllabus together with most actual scientific articles. Course materials relevant within this research discipline.

References

W. Koch, M.C. Holthausen, A Chemist’s Guide to Density Functional Theory D. Mc Quarrie and J.D.Simon , Physical Chemistry – a molecular approach

Course content-related study coaching

Evaluation methods

end-of-term evaluation

Examination methods in case of periodic evaluation during the first examination period

Open book examination, oral examination

Examination methods in case of periodic evaluation during the second examination period

Open book examination, oral examination

Examination methods in case of permanent evaluation

Possibilities of retake in case of permanent evaluation

not applicable

Extra information on the examination methods

During examination period: : oral exam – theory with open book, written preparation.
Practical exam : Computer exercises followed by oral defence.

Calculation of the examination mark