GHENT UNIVERSITY

Course Specifications

Valid as from the academic year 2024-2025

Molecular Modelling of Industrial Processes (E071341)

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

Credits 6.0 **Study time 180 h**

Course offerings and teaching methods in academic year 2024-2025

A (semester 2)	English	Gent	seminar
			lecture

Lecturers in academic year 2024-2025

Van Speybroeck, Veronique	TW17	lecturer-in-charge
Cnudde, Pieter	TW17	co-lecturer

Offered in the following programmes in 2024-2025	**crdts**	**offering**
Bridging Programme Master of Science in Chemical Engineering	6	A
Master of Science in Bioscience Engineering: Chemistry and Bioprocess Technology	6	A
Master of Science in Chemical Engineering	6	A

Teaching languages

English

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 studied together with various reaction mechanisms in a variety of molecular environments. Furthermore an introduction is given to techniques that allow to simulate industrially relevant catalysts and materials under operando conditions and on longer length and time scales. To this end molecular dynamics methods, machine learning potentials that allow to represent the potential energy surface in a more efficient way are also introduced.

Contents

- Molecular Modeling versus experimental observations for adsorption, diffusion, kinetics in nanostructured materials.
- Sequence of a molecular modeling exercise : accurate representation of the

molecular structure of realistic materials, potential energy surface, phase space sampling (molecular dynamics, Monte Carlo), derivation of thermodynamic and kinetic properties.
- 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
- Molecular Orbital theory, derivation of the chemical bonding based on symmetry concepts
- External and internal degrees of freedom of the molecule. Ab initio determination of thermodynamic quantities such as enthalpy, entropy
- Ab initio description of the kinetics and thermodynamics of chemical reactions
- Techniques to represent realistic materials and catalysts such as machine learning potentials, methods to represent the external surface of the catalyst, advanced sampling techniques and link with spectroscopic signals.
- Dynamic models to describe diffusion, adsorption and kinetics in industrial catalysts
- Applications in the field of zeolite catalysis, industrially important separations over nanostructured materials, metal catalyzed processes.

Initial competences

Moleculaire structuur en statistische fysica, organic chemistry, 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 50 nm. Understanding of many-body techniques to model molecular systems and intra- and inter molecular interactions.

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 kinetic and thermodynamic properties. Have a good understanding of the molecular modeling tools to model realistic materials and catalysts for industrial applications.

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

Seminar, Lecture

Extra information on the teaching methods

The lectures consist of theory courses and courses where actual research topics are discussed in the area of molecular modeling of industrially relevant catalysts and materials. 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,CP2K... During these sessions, the students work on a laptop and the calculations themselves are performed on the High Performance Computerinfrastructure of the UGent. Very intensive coaching is given to allow hands-on assistance.

Study material

Type: Slides

Name: Slides and additional research papers
Indicative price: Free or paid by faculty
Optional: no
Available on Ufora : Yes
Online Available : Yes
Available in the Library : No
Available through Student Association : No

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
Review papers :Challenges in modeling dynamic processes in realistic nanostructured materials at operating conditions,Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences 2023, 381, 20220239; https://royalsocietypublishing.org/doi/abs/10.1098/rsta.2022.0239;V. Van Speybroeck, M. Bocus, P. Cnudde, L. Vanduyfhuys, ACS Catal. 2023, 13, 17, 11455–11493; https://pubs.acs.org/doi/10.1021/acscatal.3c01945

Course content-related study coaching

Assessment moments

end-of-term assessment

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

Oral assessment open-book

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

Oral assessment open-book

Examination methods in case of permanent assessment

Possibilities of retake in case of permanent assessment

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