Graduate School in Science - Molecular Catalysis and Surface Chemistry

THE OBJECTIVES

The full-time MSc study in molecular catalysis and surface chemistry entails a 2 years specialization program offered by the Faculty of Chemistry for foreign students. It aim is to produce specialist in catalytic chemistry with the emphasis on i) applied aspects of catalysis and related materials chemistry, or ii) more fundamental investigations of surface reactions dynamics and kinetics. The key point of the program is to provide the student with a critical mass of general theoretical and experimental background complemented by more profound specialization in the chosen topic.

THE ADMISSION REQUIREMENTS

The Candidates must have, or expect to gain before entry, at least a BSc, or equivalent in Chemistry or related disciplines.

THE PROGRAM AND ORGANIZATION OF THE STUDIES

The MOLCAT program covers principal aspects of modern catalysis and surface chemistry, wherein the complementary experimental and theoretical approach is integrated with dedicated material synthesis. Within this broad framework, students will focus the research on one selected, narrowly defined topic. This constitutes the major field of the student. From the second semester on each student has an individual tutor from the department senior staff who provides guidance, consultation and organization of the program in the major field and the rest of her/his study and other activities.

The academic year is divided into two semesters; each including a 15-week program of lectures, seminars and practicals (about 20 hours per week). The seminars corroborate the lectures and are devoted to more in-depth analysis of the most important topics and case studies.

In addition to the weekly routine of lectures and tutorials covering the work, which will be examined in the final examinations, there are additional micro-projects that must be undertaken as part of the degree. In the first year student must produce two elaborated essays (one per semester) in the given topic related to the studies (one theoretically and one experimentally oriented).

In order to complete the full MSc program, students must acquire 60 ECTS points (equivalent to Masters Credits) each year, giving a total of 120 ECTS credits. At the first year the emphasis is placed on development of the experimental and theoretical background. The second year is more research oriented and the MOLCAT student select a research group and undertakes a two semester full-time research project. The results of this project is the submission of MSc Thesis, which are reviewed and followed by an oral examination (defence).

The layout of the MOLCAT program

1st year

course	course format	hours/ week	hours/ year	crediting basis	credits
General School Seminar	seminar	2	30	participation	4
Catalysis	lecture, seminar	2 2	30 30	examination test	3 3
Solid State Chemistry	lecture	2	30	test	3
Surface and Interfacial Chemistry	lecture, seminar	1 1	15 15	examination test	1.5 1.5
Kinetics and Thermodynamics of Catalytic reactions	lecture seminar	2 2	30 30	examination test	3 3
Experimental methods in Catalysis and Surface Chemistry	lecture, laboratory	2 10	30 150	examination reports	3 15
Powder diffraction and Phase analysis	lecture	2	30	examination	3
Catalytic materials and their preparation methods	seminar, practicals	2 5	30 30	test report	3 3
microproject	tutorial	2	60	2 extended essays	6
2 optional lectures*	lecture	2x2	60	test	6

2nd year

course	course format	hours/ week	hours/ year	crediting basis	credits
General School Seminar	seminar	2	60	participation	4
Quantum Chemical Modeling of Catalytic Reactions	lecture, practicals	2 2	30 30	Examination report	3 3
MSc seminar	seminar	1.5	20	participation	2
MSc project	experimental or computer modeling	16	480	thesis defense	48

* they can be selected from the list of assembled lectures from all specializations of JAGSS

General School Seminar – with participation of students and tutors of all JAGSS specializations.
Seminar Format: *two hours per week in four semesters*.
Short Description: The Seminar aims at improving interdisciplinary background and better integration of the JAGSS students.

Catalysis
Course Format: *two hours of lecture and two hours of classes per week in the fall semester*.
Short Description: Basic notions and definitions, description levels of catalytic phenomena, kinetic and molecular picture, time and space scales. Catalytic cycles - thermodynamic and kinetic analysis. Energetic diagrams and analysis of simple and complex catalytic cycles (identification of elementary steps, kinetic coupling, thermodynamic and kinetic reaction products), structure-reactivity relationships. Microscopic picture of heterogeneous catalysis, adsorption, diffusion, surface reaction, Langmuir-Hinshelwood and Eley-Riedl mechanisms, oscillatory processes. Dynamics of surface reactions, elementary processes, potential energy surfaces, analysis of molecular pathways of surface reactions. Description of simple and complex catalytic processes, transport limitations.

Powder diffraction and Phase analysis
Course Format: *two hours of lecture per week in the spring semester*
Short Description: Degree, range and kind of order in the crystalline and pseudocrystalline phases. Real structures, crystallinity, size of crystallites. Examination of defects and strains in crystals. Introduction to X-ray

phase analysis, investigation of chemical reactions and phase transitions. New research techniques in the chemistry of materials and catalysts. Instrumentation and accuracy (use of external and internal standards). Creation of experimental databases, reference databases for qualitative analysis.

Quantum Chemical Molecular Modeling of Catalytic Reactions
Course Format: *two hours of lecture and two hours of practicals per week in the fall semester*.
Short Description: The course provides an overview of modern computation methods, typical schemes and calculation approaches specific for application of quantum chemistry in catalysis. Students are familiarized with practical use of molecular modeling software and visualization programs.

Introduction to Surface and Interfacial Chemistry
Course Format: *one hour of lecture and one hour of seminar per week in the fall semester*.
Description: This course is intended to introduce students to the concepts and techniques involved in the study of chemical processes at surfaces. Special emphasis will be placed on the chemistry of catalytic surfaces and gas/solid, gas/liquid interfaces. Topics to be covered include thermodynamics and kinetics of surfaces; crystal and electronic structures of clean surfaces; adsorption and desorption; surface kinetics and dynamics including diffusion; growth and etching; surface reaction models. Electrical properties of surfaces and interfaces, isoelectric point, ionic exchange capacity, work function, charge transfer, field and surface ionization, electron emission will also be covered.

Catalytic materials and their preparation methods
Course Format: *two hours of lecture and five hours of practicals per week in the fall semester*.
Short Description: Classification heterogeneous catalysts following their structure and application, metals and alloys, oxide, sulfide, carbide and nitride catalysts, zeolites, clays and related materials. Survey of the structure and the most characteristic properties of zeolites, isomorphic substitution, acid and basic sites, application of zeolites as sorbents and supports. Principal preparation methods of the catalyst. Solid state reactions and transformations. Sol-gel processes, hydrothermal synthesis and molecular imprinting. Supported catalysts; characterization of the carrier and active phases, mixed oxide materials, nanostructured and hybrid systems. Principal functionalization methods. Significance of pore structure and specific surface area. Catalysts for model investigations and industrial catalysts.
Practicals: Synthesis of four selected types of new catalytic materials (zeolites, silicalites and their analogues; bifunctional catalysts, synthetic and mineral mesoporous catalysts; polymetallic catalysts) and investigations of influence of the composition, structure and texture on physicochemical and catalytic properties.
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Experimental Methods in Catalysis and Surface Chemistry
Course Format: *two hours of lecture and five hours of practicals per week in the spring semester*
Short Description: Survey of modern experimental methods, interaction of electromagnetic radiation with the matter- Probst diagram, basic types of measurements, application of molecular probes. Imaging and microscopy: SEM, TEM/AEM and EPMA (examination of sample morphology and point composition), AFM and STM (surface atomic microscopy). Determination of phase and elemental composition- XRD/ED, XRF, XRE (global composition, crystallinity, grain size). Surface analysis: sorption methods (specific surface area, porosity, pore distribution). XPS/UPS, AES, SIMS techniques (examination of surface composition, valence and coordination states). Investigation of molecular structure of active sites, adsorbed molecules and reaction intermediates: UV-VIS-NIR (electronic structure, coordination, valence states), IR/RS, DRIFT (identification of surface species, reaction mechanism), EXAFS, SEXAFS, XANES, NEXAFS (co-ordination and bond lengths in amorphous systems), MAS NMR, EPR and Mossbauer spectroscopy (investigation of active canters, adsorbed species, surface reaction mechanisms, radical processes).
Laboratory: Students are introduced to practical aspects of phase analysis, catalysts morphology, surface area and porosity measurements, elemental microanalysis, spectroscopic characterization of catalysts bulk and surface, identification of active sites and their reactivity monitoring. Characterization of catalysts with temperature programmed methods. Stationary and transient kinetic and catalytic test studies. The laboratory consists of a series of small supervised projects concluded by written reports.

Solid State Chemistry
Course Format: *two hours of lecture per week in the fall semester*
Short Description: Classification of solids: crystalline, porous and highly divided substances. Structure and morphology of solids. Chemical, structural and morphological defects (classification and Kroger-Vink notation, thermodynamics of defects). Transport properties and diffusion. Electronic structure (band theory and chemical bonding, Bloch functions, Fermi level and surfaces, DOS, local and cluster models, Hubbard and Anderson approach. donor and acceptor levels, electronic and chemical properties, chemical doping, *p-n* junctions.

Electric, magnetic and optical properties of solids. Interfacial phenomena. Heterogeneous solid state reactions in ionic solids, metals, amorphous materials.

Thermodynamics and Kinetics of Catalytic Processes

Course Format: *two hours of lecture and two hours of seminar per week in the spring semester*
Short Description Thermodynamic analysis of catalytic processes and modeling. Analysis and prediction of rates of reactions in flow and non-flow conditions involving homogeneous and heterogeneous systems, fundamental kinetic models, stationary and transient kinetic studies, mass and heat transfer. Experimental laboratory reactors, industrial reactors and process engineering.

MSc Seminar

Students present and discuss current results obtained in the course of their MSc project

Facilities and Related Opportunities

The Faculty is well equipped to carry out modern chemical research and education in catalysis and surface chemistry. The principal instrumentation includes powder Philips X'Pert and X'Pert PRO automated diffractometers with low and high temperature and chemical reactor attachments, Bruker 500 MHz NMR (with solid state facility) and ELEXYS CW X-band EPR spectrometers, infrared (Bruker 48PC and EQUINUX with liquid helium cryostat), Raman (Biorad FT 40) and UV-Vis (Shimadzu) spectrophotometers, numerous gas and liquid chromatographs, a VSW ESCA instrument, a Micromeritics ASAP 2010 gas sorption station, a Mettler Toledo scanning calorimeter and Balzer TGA/MS analyzer, and various other specialized equipment for the characterization of catalysts and the investigation of reactions.