

chemistry environment physics catalysis energy healthcare molecules nanomaterials



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- 🕞 Ústav fyzikální chemie J. Heyrovského AV ČR

Heyrovský Institute of Physical Chemistry of the CAS, a public research institution, develops the scientific legacy of the Nobel Prize winner, Professor Jaroslav Heyrovský, in the fields related to physical chemistry. Over 200 scientists, ranging from promising young researchers to world-renowned top experts, are engaged in systematic basic and applied research. The theoretical knowledge and experimentally acquired knowledge of the physical chemical processes occurring in molecules and atoms are of importance for industrial catalysis, energy production and storage, health care and the environment.

Introduction

The Institute operates the **Heyrovský Technology Transfer Centre,** which promotes cooperation between the Institute and the commercial sector in order to link the research and technological potential of the Institute with the needs of the commercial sphere.

Biophysical Chemistry

Biophysical Chemistry department implements two basic research lines employing fluorescence spectroscopy and microscopy ("Biospectroscopy"), and electrochemical methods ("Bioelectrochemistry"). Supported by computational approaches, both research lines aim at a common goal: to understand the structure, functionality and dynamics of biologically relevant systems at a molecular and atomistic level. These systems of interest lie within the context of the current topics related to neurodegenerative diseases, cell signalling, immune response, gene therapy and enzymology.



- 1 Measurements on a fluorescence microscope
- 2 High resolution fluorescence microscope







4 An image of a white blood cell viewed under a fluorescence microscope

We focus on:

- the development of new methods of fluorescence spectroscopy, microscopy and electrochemistry,
- > molecular processes in human cells,
- > charge transfer through model interfaces,
- > electron transfer in proteins,
- > sub-diffraction manipulation of light by plasmonic nanoparticles.

Department participate in many research projects on national and international level such as the ONEM project developing a novel combination of optical and electron microscopy with partner institutions from Wien and Leiden University. The department's research is well accepted by the scientific community and has led to several awards (J. Heyrovský medal, Otto Wichterle award, Academic Award - Praemium Academiae, Lumina quaeruntur, Josef Hlávka award among others).



Dynamics of Molecules and Clusters





1 Construction of a new beam apparatus for research of the elementary processes in liquids





2 Lasers in the laboratory with CLUB and AIM apparatus

3 Laser chemistry on the AIM apparatus

Our studies of electron attachment to molecules and clusters have an influence on nanofabrication and the development of high voltage switching devices, where we have even been collaborating with the industry. But the electron attachment to molecules in cluster environments is relevant to biophysics as well, e.g., to such seemingly remote areas as cancer treatment and (post)radiation chemistry. These are just a few examples where our department's fundamental research contributes to understanding at the molecular level processes that are of global practical importance.

Experimentally, we implement various techniques of UV and IR laser spectroscopies, different mass spectrometric techniques, ion imaging and electron spectroscopy, DNAorigami etc. The speciality of our department within our institute are our home-built experimental setups, which we constantly modify and develop new experimental techniques.

Electrochemical Materials

department focuses on the preparation and characterization of electrochemically active materials with a special emphasis on nanomaterials based on elemental carbon, semiconducting oxides, and inorganic 2D crystals. The main topics of our research include, in particular, the development of new electrode materials and electrolytes for rechargeable Li-ion, Na-ion, Li-sulphur batteries, or others based on transition metal ions. We also develop new materials for dye-sensitized and perovskite solar cells, which can be used, for example, as omnipresent transparent panels in the near future, and thereby considerably contributing to the balancing of energy production in our society.

For the preparation of photoelectrodes for applications in the energy production as well as environmental fields, we use advanced methods enabling controlled deposition of





- 1 Development of new materials for rechargeable batteries
- 2 Advanced research of processes of energy storage and conversion
- **3** Testing the activity of innovative photocatalysts for water decontamination



thin layers of thickness lower than 1 nanometre and also their complete characterization ranging from structure to quantifying the efficiency of solar-to-electrical energy conversion. We also aim to develop environmentally friendly applications for the improvement of polluted water in our country as well as in developing countries, for water purification plants etc. For these purposes, we study photocatalytic materials, mostly based on metal oxides, which are able to decompose even hard-to-degrade organic contaminants to CO_2 and mineral acids.

With the aid of state-of-the-art spectroscopic and microscopic techniques that we simultaneously develop and improve, we also study physico-chemical processes in gaseous nanobubbles at the solid-liquid interface, in nuclear reactors at the surface of cladding tubes, or in two-dimensional materials. We cooperate with partners in industrial and academic sectors, for example, with HE3DA company which develops batteries for stationary energy storage, or with top institutions like EPF-Lausanne in Switzerland or Manchester University in United Kingdom, where we closely collaborate with, among others, the Nobel Prize in Physics laureate Prof. K. Novoselov.

Electrochemistry at the Nanoscale

The Department of Electrochemistry at the Nanoscale focuses its research activities on electroactive molecular systems from the perspective of nanoscale dimensions. We aim to understand charge transfer processes and related phenomena at the molecular level. The systems that we study have been designed for various applications including molecular electronics, energy conversion and storage, development of electrochemical sensors for pesticides, heavy metals and atmospheric pollutants, as well as catalysts for their removal from the environment.

We also investigate structure-property-reactivity relationships and reaction mechanisms in biologically relevant substances including hormones, antioxidants and drugs. Members of the Department are also involved in the advancement of the







- 1 Electrochemical flow-through cell for sensing pollutants
- 2 Impedance spectroscopy measurements of industrially relevant compounds
- **3** Scanning probe microscope for measuring of the conductivity of single molecules





electrochemical instrumentation, including impedance and pulse sensing techniques, in-situ spectroelectrochemistry, nanoscale imaging of surfaces and reaction interfaces and single molecule conductivity and thermopower measurements. In addition we explore the capabilities of 3D printing in the manufacture of microfluidic electrochemical sensing and catalytic platforms.

Our results are regularly published in top journals in the fields of electrochemistry, physical chemistry, analytical chemistry and environmental chemistry and are recognized by the international community. Our research is supported by grant projects including those focusing on charge transport in single molecule electronic components, electrocatalytic reduction of carbon dioxide or the development of electrochemical (bio) sensors based on novel electrode materials.



Chemistry of lons in Gaseous Phase

Department of Chemistry of lons in Gaseous Phase studies reactions between ionized and neutral molecules. The results obtained provide insights into the processes occurring at the atomic level and are also crucial for understanding the processes in the atmosphere and for analytical mass spectrometry, which can be used in many other fields.

One of the department's laboratories is dedicated to researching new methods for the sensitive analysis of trace substances in the air. Mass spectrometry is used here to determine molecular structures, identify unknown compounds and quantify known substances in a gaseous sample.





- 1 Double-focusing mass spectrometer ZAB2-SEQ
- **2** Development of a new drift tube mass spectrometry method
- 3 Low pressure plasma as a source of ions
- **4** Laboratory version of the HANKA space instrument for online analysis of micrometeorites



Another area of scientific activity of the department is space research. We design and build laboratory prototypes of high-resolution space mass spectrometers, which are used to develop new instruments for future space missions. We also use mass spectrometry methods to experimentally study chemical reactions in the ionospheres of the planets and moons of the solar system. This includes studies of fastcharged particles interacting with neutral molecules using a specially modified sector mass spectrometer.

The research results are used in medicine, biology, forensics and food science. The department is also part of international scientific teams preparing future space missions to explore the solar system and the possible exploitation of its mineral wealth by future.





Molecular Electrochemistry and Catalysis

department focuses on fundamental research in unraveling the relationships between the structure, geometry, electron distribution, redox properties and reactivity of organic, inorganic, organometallic and complex molecules, including their synthesis.

We aim at interconnecting the outputs of fundamental studies with the design and synthesis of new molecules suitable for diverse applications (catalysis, chemical transformations, chemosensors, medicinal chemistry, etc.).

Areas of interest:

- > design, synthesis, and reactivity of new molecules,
- > electrochemical research of redox processes,
- catalysis,
- > physical-chemical properties,
- combination of photochemistry and electrochemistry UV-vis and EPR spectroscopy,
- > quantum chemical calculations for prediction and interpretation.





1.0 × 10

- 1 Crystals of an organometallic titanium compound in an oxygen- and water-free environment
- 2 Experimental equipment for electrochemical measurements on different electrodes
- **3** Spectro-electrochemical cell for simultaneous measurement of UV-vis and EPR spectra during electrochemical generation of radicals
- 4 pH dependence of aza-macrocycle copper complex cyclic voltammetry
- 5 Polymerization autoclave containing precipitated polyethylene after a test run with a new catalyst

pH 7.38 pH 7.98 pH 8.68 pH 9.63

pH 10.80 pH 11.88



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Special attention is given to molecules with multiple redox centres, where their mutual interactions, intramolecular electron transfer, distribution of electron density and extent of delocalization are experimentally studied. Besides the macrocyclic compounds with the expected application as specific receptors and molecules for singlet fission (conversion of solar energy), the molecules of main interest involve transition metal complexes bearing organic ligands designed for homogeneous catalysis and medicinal applications. The experimental facilities and equipment include a synthetic laboratory capable of handling highly air- and moisture-sensitive materials, NMR, EPR, MS and UV-vis/IR spectrometers, full electrochemical equipment and their in-situ combinations with the above-mentioned methods for studies of radical intermediates to elucidate reaction mechanisms.



Nanocatalysis

Department of Nanocatalysis focuses on the design of materials on the subnanometer to nanometer scale for fundamental studies of a wide spectrum of catalytic processes. Key features of the developed materials are their exact chemical composition and defined structure, with these parameters controlled down to the atomic scale.

Synthesis of the nanocatalysts is:

By size-selected deposition in vacuum, when metal clusters with exact number of atoms of one or two metals are deposited on technologically relevant supports, with particle sizes randing from a single atom to few nanometers in size. In this process, first a beam consisting of atomic clusters of various sizes and compositions is created, from which clusters of desired mass are filtered out using a mass spectrometer. Next, these clusters are deposited on catalytically relevant supports. The clusters fabricated possess highly precise chemical composition and their size and composition can be varied with atomic precision. The effect of atomic composition of the clusters on their catalytic performance along with the suitability of the support are investigated in heterogenous reactions such as CO₂,



- 1 Laboratory for the fabrication of clusters with precisely controlled size and atomically precise composition
- **2** Schematic illustration of clusters at action
- **3** Apparatus for the testing of nanocatalysts



- 4 Hybrid nanostructured iron-oxide based catalysts with integrate copper nanoparticle in efficient conversion of CO₂ into useful chemicals
- **5** X-ray absorption spectrum of a single nickel nanoparticleof approx. 80 nm in size used in methane conversion, collected at a synchrotron
- 6 Ru_{1-x}Ti_xO₂ nanocrystal of a size of about 50 nm
- 7 Schematic of the structure of Ru_{1-x}Ti_xO₂ derived from synchrotron X-ray data



conversion, CO oxidation, or for the highly selective oxidation of hydrocarbons. In collaborations with international partners electrocatalytic water splitting and CO₂ conversion, or oxygen reduction in Li-O₂ batteries is studied.

- Chemical synthesis of hybrid catalysts with sizes between a few and tens of nanometers. These catalysts are prepared by advanced synthetic methods and are highly efficient in the conversion of green-house gases CO₂ and methane or in the selective transformations of higher hydrocarbons.
- Chemical preparation of nanorystalline particles. The synthesis of nanocrystalline electrocatalysts is based on theoretical predictions of suitable active sites which promote desired activity of the developed materials in reactions for energy storage in alternative fuels such as hydrogen or fuels gained form the reduction of CO₂. The synthesis of these model nanocrystalline materials takes place by using cryogenic, solvothermal and precipitation methods. The function of the prepared materials is then tested under catalytically relevant conditions. The materials are characterized by X-rays with the goal to establish general structure-function relationship between their catalytic properties and structure.

Low-dimensional Systems

research focuses on 1 and 2D materials such as graphene, metal chalcogenides, carbon nanotubes and related materials. We have established an extensive infrastructure to comprehend the material processing from synthesis, to modification, to analysis, and finally advancing to device fabrication.

The research project stems from the evaluation of basic principles, gaining control over the material's properties to thrive with applications in the fabrication of sensors, transistors and microelectronics.



1 Inspection of sensors and electrical paths on lithography

2 Integration into function blocks



- **3** Characterisation Spectroscopic inspection of the device
- **4** Transistor: An example of a MoS₂-based MOS-FET transistor
- **5** SEM image of fractal SERS substrate for analysis of biological samples



The department is further divided into several specialized subgroups, each providing essential insight into their respective field or aspect, which altogether enables them to conduct research in its complexity.



MM Spectroscopy

Theo Department of Spectroscopy is the leading Czech centre for applied and basic research in spectroscopic techniques. Our research activities include developing sensitive sensors for gas and air analysis, investigating new high-tech materials for use in high-power light sources, characterising new materials, generating reactive species on surfaces and developing new analytical techniques in the field of forensic sciences.

We also focus on other current topics in contemporary science: we are addressing unanswered questions about the chemical evolution of the Earth and the identification and quantification of prebiotic processes that may lead to the origin of life on Earth-like planets such as Mars or even distant exoplanets. We investigate fundamental processes in plasmas generated by large lasers or flame processes.



- 1 Preparation of an experiment on the transformation of planetary atmospheres through the effects of an asteroid impact. Will it someday be possible to use space telescopes to determine how early planets, battered by shooting stars, evolved?
- 2 The Ariel Space Telescope will provide answers to many fascinating questions about exoplanets. Laboratory experiments in our department are essential to understanding the observations that Ariel will make.
- **3** In the high-resolution spectroscopy lab, we study the fundamental characteristics of molecules and atoms. Without this data, it is impossible to study the mechanisms of chemical reactions, new materials, or to decipher the composition of shooting stars or distant exoplanets.



- 4 The high-resolution spectrometer is specially adapted for the detection of unstable chemicals in plasma. Its measurements allow the observation of events lasting only millionths of a second in electric discharges or laser sparks. The technical solution in our laboratory is unique in the world. After dismantling the same instrument at Okayama University, our continuously scanning time-resolved Fourier interferometer is now the only one of its kind in the world.
- **5** We study the plasma of meteors, shooting stars, with simulations using one of the largest lasers in the world. In the interaction chamber, a sample of the rare Pallasite, an iron meteorite with grains of olivine from the interior of a long-extinct asteroid, is being prepared for a laser strike.
- **6** Unstable radicals, ions and atoms are detected by timeresolved spectroscopy using electric and laser sparks in gaseous media.
- 7 Research in our laboratory has motivated the preparation of a purely Czech CubeSat SLAVIA mission to study meteor plasma and interplanetary dust in Earth orbit after 2027.

Our department cooperates closely with world-leading research institutions (e.g. Sorbonne or Cambridge University) as well as major domestic universities and research institutes. Our partners are also private entities with a significant share in research and innovation as well as government institutions.

Scientists and students of the Department of Spectroscopy have received a number of academic awards (e.g. Werner von Siemens Prize, Czech Head, Learned Society, Wichterle Premium). Currently, our department coordinates the involvement in important space missions, such as the Ariel Space Telescope, the EnVision probe to Venus or the Czech CubeSat SLAVIA. The department also works on the development of technical equipment for these missions.





Structure and Dynamics in Catalysis

atalysis is the basis of today's chemical production and accounts for about 20% of the world's gross domestic product. At the same time, it is used to eliminate pollutants from chemical processes and other sources, e.g., exhaust gases. The inevitable transformation of chemical production, production of new materials into the ecologically sustainable one, and the utilization of new resources require new catalysts and catalytic processes.

For the preparation of new, highly active, and selective catalysts from laboratory to the levels needed for pilot operations, we employ active sites stabilized in microporous 3D aluminosilicate or carbon matrices. The first step is the synthesis of matrices with targeted properties. Then, the introduction of active sites defined at the atomic level designed



using quantum chemical calculations follows. The structure of the active sites is verified using several techniques, including scanning and transmission electron microscopy, temperatureprogrammed reactions, and multi-spectroscopic analysis, which combine solid phase multinuclear NMR spectroscopy, diffuse-reflection UV-Vis-NIR spectroscopy, laser-induced kinetic emission spectroscopy, Mössbauer spectroscopy, and







- **1** Synthesis of zeolite-based catalysts
- 2 On behalf of awarded team, Mgr. J. Dedecek, SCs., DSs. collected the Czech Intellect award in the Invention category (2020)
- **3** Operando FTIR analysis of the structure of active sites
- 4 Siting of divalent cations in zeolite TNU-9
- 5 Mechanism of dioxygen splitting over binuclear Fe(II) site



infrared spectroscopy. Most of these techniques are used in-situ to study the reactivity of prepared catalysts, also at the atomic level. The final stage of catalyst development is to test its activity using reaction kinetic tests, where the resulting products are monitored using gas chromatography and mass spectroscopy.

Attention is focused on applying acid-catalysed reactions for the transformation of hydrocarbons for more efficient petrochemical production and on redox processes using active sites based on transition metals for the elimination of NO/ NO_x , the greenhouse N₂O gas and the selective oxidation of methane to methanol. We were awarded the Czech Intellect award 2020 for developing this reaction.

Theoretical Chemistry



development and applications of the quantum chemistry methods have more than sixty years tradition in the J. Heyrovský Institute of Physical Chemistry. At the present time the research at the department of Theoretical Chemistry can be seen to be headed in several basic directions.

Strongly correlated systems

Molecular systems with a strong electron correlation constitute one of the challenges of contemporary quantum chemistry. Therefore, we are engaged in the development and applications of modern methods for a more accurate description of such systems, based on multireference and externally corrected coupled clusters (CC), density matrix renormalization group (DMRG), and post-DMRG methods.



- 1 Molecular resonance analysis by RAC
- 2 In our laboratory you can find computing clusters
- **3** Lectures at Czech universities



Structure of surfaces, clusters, zeolites and nanostructures

Zeolites are microporous, crystalline aluminosilicate materials. Together with cluster surfaces they offer an external and internal surface area for the catalysis of chemical reactions. Our research focuses on the structure of active centers and we were part of the team that was awarded the Czech Intellect prize in 2020.

Electron-molecule collisions

The study of electron-molecule interactions is necessary for understanding processes in the upper levels of planetary atmospheres, for the development of technologies in the semiconductor industry, and for research and treatment of cancer in medicine. Our research is focused on the development of methods for elastic and inelastic collisions.







Non-adiabatic molecular dynamics for photochemistry

Modelling of photochemical processes requires combining the dynamics of atomic nuclei with transitions between electronic states of the molecule. We thus develop and apply methods of molecular dynamics with non-adiabatic and spin-orbit couplings, recently also with the support of machine learning techniques.

Quantum Computers

Algorithms of quantum computing are based on the phenomena of quantum mechanics. We are concerned with quantum algorithms for quantum chemistry tasks, such as the search for the energy of the molecular ground state.

Computational Chemistry

our work we are inspired by nature, natural phenomena, transformations that are constantly taking place in and around us. Like other chemists, we are interested in how such processes take place, what drives them and how such transformations can be mimicked, made more efficient for our purposes, or, on the contrary, reduced if they do not take place properly, e.g. as a result of disease. This involves the design of new substances with suitable properties.

Instead of chemical flasks and apparatuses, our tools for work are computers and the laws of quantum, molecular and statistical mechanics and molecular dynamics, which we use to analyse complex (bio)chemical systems and their functions. This is at different structural levels - from the microworld to the electron. In this sense, we seek to understand how healthy and



- 1 Atomistic description of cell cytoplasm
- **2** Peptide interacting with the cell membrane







- **3** Zoom into the active site of the enzyme
- 4 Change in the electronic structure and energy of the active site of an enzyme during its reduction or oxidation
- 5 The active site of the enzyme with metal ions and the mechanism of the catalytic cycle



damaged lipid membranes behave on the cell surface, how enzymes function in the cellular (aqueous) and non-aqueous environment, and what and how the dynamics and stability of these enzymes can be regulated. In enzymes, we are also particularly interested in their reactive centres, their electronic structure, what influences this electronic structure and what is its influence on the high reactivity and selectivity so typical of enzyme catalysis. From the theoretical models that we study and that we confront with experimental facts, we deduce important structure-function relationships and generalize the physicochemical principles that govern the systems we study. We seek to apply these principles to the design of compounds that have the potential to cure disease or effectively catalyse reactions of societal importance.

Center for Innovations in the Field of Nanomaterials and Nanotechnologies

Theo research of the Center for Innovations in the field of nanomaterials and nanotechnologies (Nanocenter) is aimed at the development of novel methods for protecting the environment and the complex conservation of artifacts of major cultural hereditary importance. The uniqueness of our approach consists in a very close connection of advanced academic research and its application in novel technologies. This focus is based on extensive expertise in the field of nanotechnology, photochemical and photocatalytic transformations. A comprehensive integrated scientific team connects scientists from the various fields of science, which enables complex solutions to relevant problems with significant societal impact.





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- 1 Application of cleaning gels on a fragment of a medieval panel painting from the Moravian Gallery, Brno
- **2** Photocatalytic apparatus
- **3** Sample of the composite photocatalyst
- 4 The study of the mechanical properties of materials at the micro- and nanoscale using the Nanoindenter



Our research focuses on:

- Air depollution: comprehensive photocatalytic technologies for the degradation of $NO_{x^1}O_3$, VOCs, dust particles, etc. Water depollution: novel photocatalytic technologies for the removal of emerging aqueous pollutants such as antibiotics, drugs or organic dyes.
- Culture heritage protection: procedures and materials for the comprehensive conservation and preventive protection of historic monuments based on the research in the field of materials science and nanotechnology in general and in their use for the restoration of historical artifacts in particular. Scale-up: technological aspects essential for real production,
- suitability and ease of application.
- Methodology development: realistic transfer of laboratory data to the real-world conditions.
- Developed technologies evaluation: overall environmental impact, covering the potential toxicity of functional nanomaterials themselves and the products of the photocatalytic pollutant transformation.
- **Scientific awards:** Transfera Technology Day 2021, 2nd place in the final round

Education Centre

Institute is an academic workplace that is dedicated to the education of young men and women interested in science coming from universities, secondary and primary schools in a longterm and systematic way throughout the year. The number of educational programmes introducing science and research to the target groups exceeds one hundred annually.

University students are involved in our scientific and research activities as part of their bachelor and master theses. They often continue their involvement in science as PhD students and become collaborators with scientists in their projects. The target group of primary and secondary school children receives a varied mix of programmes including workshops or practical measurements in laboratories, lectures, excursions, clubs and internships in scientific teams, summer schools and weekend chemistry courses.



- **1** Chemical theater inspires wonder and enthusiasm for chemistry
- **2** The legacy of Jaroslav Heyrovský and polarography has been commemorated to the general public since 2009 with the travelling exhibition The Story of a Drop



- **3** The only way to engage a student in chemistry is through experiments, which is the basis of our educational programmes for all ages
- **4** A chemistry workshop, where we test theories through experiments
- **5** Students gain new knowledge and new friends at the summer school



Other key events in the outreach of science and research aimed at the general public include the varied programme of the September International Researchers' Night, exhibitions at the Science Fair and events as part of the Week of the Czech Academy of Sciences festival. You can meet our scientists in the science café programme, in our travelling exhibitions (e.g. Story of a Drop or Touch the (exo)planets) or in the media.

Each year, up to fifty of our scientists, professionals and students are involved in delivering a diverse mix of programmes. Coordination of the programmes is provided by the Education Section. In this way, we work with more than 100 schools across the country. The events are largely financially supported by grants from the Ministry of Education, for example.









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