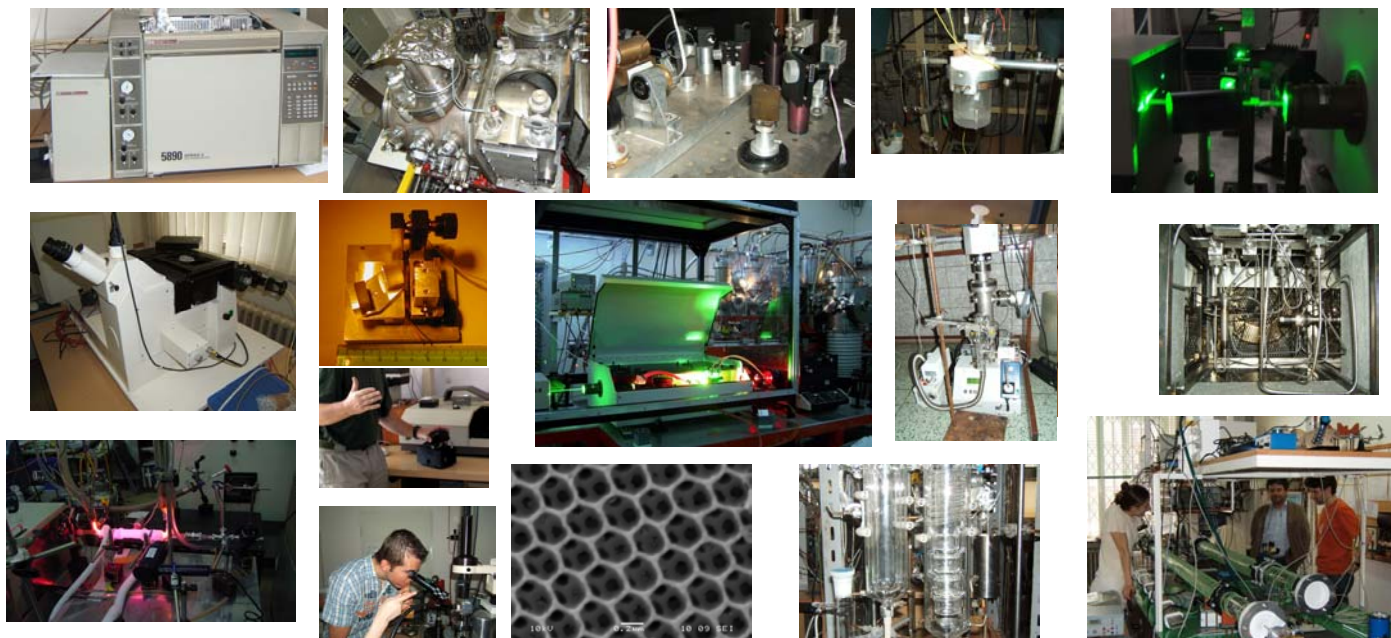
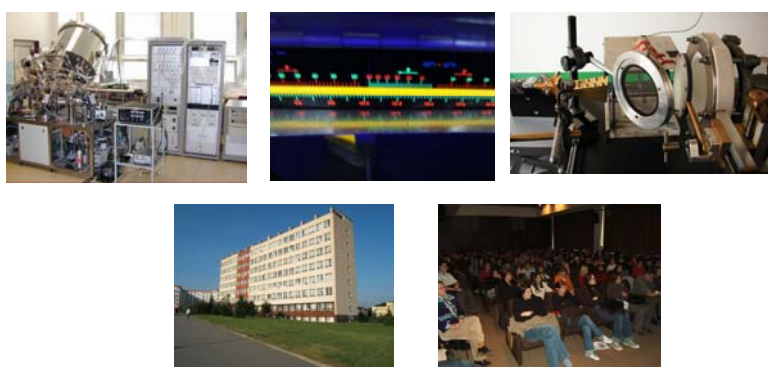


J. Heyrovský Institute of Physical Chemistry Academy of Sciences of the Czech Republic



ANNUAL REPORT 2005



Academy of Sciences of the Czech Republic
J. Heyrovský Institute of Physical Chemistry

Annual Report 2005

Director:

Prof. RNDr. Petr Čásky, DrSc.

Vice-director:

Prof. Ing. Vladimír Mareček, DrSc.

Scientific Secretary:

Ing. Květoslava Stejskalová, CSc.

Scientific Council Chairman:

Doc. Dr.rer.nat. Martin Hof

Economic and Technical Manager:

Ing. Vladimír Levit

Address: Dolejškova 3, 182 23 Prague 8, Czech Republic
Telephone (secretariat): (+420) 2 8658 3014; (+420) 2 6605 2011; (+420) 2 6605 3265

Fax: (+420) 2 8658 2307

E-mail: director@jh-inst.cas.cz

Internet address: <http://www.jh-inst.cas.cz>

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1. BASIC INFORMATION

1.1. Scope of Activities

In 2005, the Institute continued to carry out fundamental research in a range of branches of physical chemistry, electrochemistry and chemical physics. Fundamental research was the Institute's main objective, but some applied aspects were also pursued.

Furthermore, the Institute continued to be deeply involved in training of both undergraduate and graduate students, in supervision of their Ph.D. and Diploma theses, and in teaching at universities. The Institute also served as Marie Curie Training Site of European Commission in synthesis of porous materials for adsorption applications ("Intelligent design of nanoporous sorbents"). In addition, it functioned as a member of IHP Research Training Networks of European Commission in electron and positron induced chemistry.

1.2. Most Important Events in 2005

- 15th Brdička Memorial Lecture was held on June 23 by prof. Avelino Corma Canos (Instituto de Tecnología Química, Valencia);
- Student Seminar was held in castle Třešň (June 27-29, 2005);
- Since September 1, 2005, the organization structure of the scientific departments of the institute has been changed: two new departments have been established - Department of Theoretical Chemistry and Department of Biophysical Chemistry; and Department of Catalysis has been divided into Department of Catalysis I and Department of Catalysis II.
- Department of Catalysis together with the Czech Zeolite Group organized the 3rd International FEZA Conference on Zeolites under the auspices of the Federation of European Zeolite Associations (Prague, August 23-26, 2005) with more than 400 participants from over the world. The Conference was preceded by the 1st FEZA School on Zeolites (Prague, August 20-21, 2005) with 100 participants. The proceedings of both events have been published in cooperation with Elsevier Publishing House in the series Studies in Surface Science and Catalysis (Vol. 157 and Vol. 158).
- Two new laboratories of the institute (*Laboratory of clusters in molecular beams* and *Laboratory of Fourier transform high resolution spectroscopy*) have been opened in the Department of Physical Chemistry.

2. FINANCES

2.1. Non-investment Means

Non-investment financial resources of the Institute in 2005 amounted to 134.153 million CZK (Table 2.1.)

Table 2.1. Breakdown of the non-investment funds of the Institute in 2005 (in thousand CZK; 1 USD ~ 24 CZK)

Source	Income	
	thousand CZK	per cent
State budget	84 693	63.1
Domestic research grants	35 000	26.0
Foreign research grants	6 847	5.2
Contracts	1 183	0.9
Licences	200	0.1
Others	6 230	4.6
Total	134 153	100.0

2.2. Investment Means

Besides 0.195 million CZK for building maintenance, 22.850 million CZK were available in 2005 from the budget and research grants for purchase of major instrumentation and computer technique. These means were spent for acquisition of equipment including the following major items:

- Excimer laser (XeCl) COMPEXPro 102 (Lambda Physik GmbH, Germany)
- Basic IX81 microscope added with MicroTime 200 confocal and time-resolved optical unit (PicoQuant GmbH, Germany)
- Analyzer Advanced Optima 200/Limas 11HW (ABB, Germany)
- Adsorption Apparatus ASAP2020 (Micromeritics, USA)
- Potentiostat/ galvanostat AUT 30. FRA 2.V (EcoChemie, Netherlands)

3. RESEARCH

Activities of the Institute were focused primarily on basic research in a range of areas of chemical physics, physical chemistry and electrochemistry.

The research was carried out within the framework of six departments: Theoretical chemistry, Biophysical chemistry; Chemical Physics; Catalysis I; Catalysis II; Electrochemistry.

Acronyms used:

(a):	associated contractor (project leader is affiliated with another institution)
AS CR:	Academy of Sciences of the Czech Republic
DFG:	German Research Association (Deutsche Forschungsgemeinschaft)
EC:	European Commission
GA ASCR:	Grant Agency of the Academy of Sciences of the Czech Republic
GA CR:	Grant Agency of the Czech Republic
MEYS:	Ministry of Education, Youth and Sports of the Czech Republic
MIT	Ministry of Industry and Trade of the Czech Republic

DEPARTMENT OF THEORETICAL CHEMISTRY

TOPIC 1. Development and Application of Quantum Chemical Methods

Grant projects

GA AS CR

Dynamics of excited molecular systems.

Paidarová (a), No. 100400501, 2005-2009.

Main results in 2005: Accurate ab initio calculation of potential energy surfaces (PES) for the three lowest states of He_3^+ were done by multi-reference CI method with large basis set at about 1200 nuclear configurations. This enables to build up semi-empirical models of potential energy surfaces of the He_n^+ clusters for structural, spectroscopic and dynamical studies.

State specific multireference Brillouin-Wigner coupled cluster method with triexcitations.

J. Pittner, No. IAA4040401, 2004-2007.

Main results in 2005: The Multireference BWCC method with non-iterative inclusion of triexcitations, MRBWCCSD(T), which is a multireference analogue of the widely applied CCSD(T) method, was successfully implemented. This will allow applications to chemically interesting systems of moderate size, thanks to the lower computational demands of CC methods with non-iterative triples.

GA CR

**Modelling of helium ionic clusters: structure, spectra, thermodynamics and dynamics.
I. Páidarová (a), No. 203/04/2146, 2004-2006.**

Main results in 2005: 1) The Discrete Momentum Representation (DMR) method developed at the institut for theoretical investigation of nonresonant electron-molecule collisions was extended by the implementation of the local correlation-polarization potential which enables to study processes with collision energy under 10eV. Polarizabilities and their derivatives, which are required for asymptotic polarization potential, were calculated by ab initio linear response method for CH₄.

Analytic gradient for the state-specific multireference Brillouin-Wigner coupled cluster method.

J. Pittner, No. 203/04/0425, 2004-2006.

Main results in 2005: Continuing of the implementation of the equations for the MRBWCCSD analytic gradient. The solution of MR lambda equations was finished and presently the orbital response contributions are continuing. Besides this, a study of singlet-triplet splitting in trimethylenemethane and of the reaction path for its synthesis from methylenecyclopropane, as an application of the MR BWCCSD method was performed.

MEYS

European Laboratory for Multireference Quantum Chemical Methods.

P. Čársky, MEYS (COST), No. COST OC D23/001, 2001-2005.

International Academy of Quantum Molecular Sciences.

P. Čársky, INGO project No. LA145, 2002-2005.

Computer tools for analysis of high resolution infrared spectra.

P. Pracna, project of Czech-Poland collaboration No. 2004-2005-04, 2004-2005.

EU projects

Research Training Network: Electron and positron induced chemistry (EPIC).

**P. Čársky (a), EC (IHRP, 5th Programme Training Network),
No. HPRN-CT-2003- 00179, 2002-2005.**

Electron induced processing at the molecular level (EIPAM).

P. Čársky (a), EC, No. HPRN-CT-2002-00286, 2004-2008.

DEPARTMENT OF CHEMICAL PHYSICS

TOPIC 1. Dynamics and Kinetics of Ion - Molecule Collisions.
Organic Mass Spectrometry.

Grant projects

GA AS CR

Collisions of slow polyatomic ions with surfaces: Energy transfer and chemical reactions.

Z. Herman, No. A4040405, 2004-2006.

Main results in 2005: Ion survival factors, fragmentation and chemical reactions of projectile ions $C_3H_n^+$ ($n=2-8$), $C_7H_n^{2+}$ ($n=6,7,8$) and $C_7H_n^+$ ($n=7,8$) colliding with room-temperature and heated carbon (HOPG) surfaces were determined in ion-surface scattering experiments. Results for dications and cations $C_7H_n^{2+/+}$ were compared; the ion survival probability for dications was found to be about twice as high as that one for cations. The main chemical reaction observed was hydrogen ion transfer and formation of protonated projectile ions in reactions of the projectile with the surface material.

Unimolecular reactions kinetics of the gas phase radicals.

M. Polášek, No. 400400502, 2005-2007.

Main results in 2005: Unimolecular chemistry of O-alkylated nitroalkane cations in the gas phase was studied by tandem mass spectrometry and ab initio calculations. These ions will be used as precursors for preparation of alkyl radical adducts to nitro-compounds. Radicals corresponding to hydrogen atom adducts to 1-methylcytosine were generated from N-3 and C-5 protonated 1-methylcytosine cations and characterized by neutralization reionization mass spectrometry. These radicals were found to be stable on microsecond time scale.

Reaction of molecular dications CHX^{++} ($X= F, Cl, Br, OH, SH, NH_2$): Theoretical and experimental investigation.

J. Roithová, No. B4040302, 2003-2005.

Main results in 2005: The investigations concentrated on formulation of general dependencies of CHX_2^+ reactivities and stabilities in dependence of the substituent X were done. The key study "Competition of proton- and electron transfers in gas-phase reactions of hydrogen-containing dications CHX_2^+ ($X = F, Cl, Br, I$) with atoms, non-polar and polar molecules" brought several novel findings. Preference for proton transfer vs. electron transfer in reactions of hydrogen-containing dications with polar molecules is the most interesting result with important implications for chemistry in superacidic media. In addition, other dications were studied in order to get a general view of their stability in relation to the way of their generation and internal energy content.

GA CR

Study of elementary processes in low-temperature and technologically oriented plasma and development of relevant diagnostic methods.

P. Španěl (a), No. 202/03/0827, 2003-2005.

Main results in 2005: Reliable quantitative data were obtained on the processes of formation and loss of complex ions containing an organic core and several water ligands. Systematic description of the diffusion losses of these ions in flow tubes enabled significant increase of

accuracy of selected ion flow tube mass spectrometry method of determination of trace gas concentrations.

EU projects

Atomic and molecular data for plasma modelling.

Z. Herman (a), IAEA Co-ordination Project, No. 13488/RO, 2005-2008.

Atomic physics, data for edge plasmas & plasma - wall interactions.

Z. Herman (a), EURATOM, No. EURATOM-IPP-CR, 2000-2005.

European Planetology Network.

Z. Herman (a), EC 6th Programme, EuroPlaNet No. RICA-001637, 2005-2008.

TOPIC 2. Chemistry of Surfaces, Interfaces and Thin Films (Photoelectron Spectroscopy).
Surface Interactions on Metals.

Grant projects

GA CR

Characterization of doped photosensitive titania with optimized properties.

Z. Bastl (a), No. 104/04/0467, 2004-2006.

Main results in 2005: XPS study of N-doped and F-doped TiO₂ powders was carried out in order to explain differences in their photo catalytic properties. Oxide films were grown by oxygen ion beam irradiation of Ti and V metals. The population of individual oxidation states of metal present in the films, their depth distribution and thermal stability were examined by angle-resolved XPS.

Laser ablative and non-ablative treatment of polymers; approach to novel polymeric structures.

Z. Bastl (a), No. 104/04/2028, 2004-2006.

Main results in 2005: Nanocomposites produced by IR laser ethylene-sensitized heating of gaseous iron pentacarbonyl and hexamethyldisiloxane and their thermal behavior were studied by photoelectron spectroscopy methods. Nanocomposites produced were shown to consist of nanosized iron particles covered by polycarbosilane shell, which become superficially oxidized due to incomplete protection by surrounding polymer. These nanocomposites can be promising precursors for nanostructured magnetic ceramics.

Reactivity of s,p-/d- Bimetallic Nanostructures.

J. Pišek (a), No. 202/05/0244, 2005-2007.

Main results in 2005: Elementary surface processes such as growth, thermal stability and chemical reactivity (tested by adsorption of CO or C₂H₄) was studied by surface science techniques (FEM, TPD, PES) on model systems. Strong influence of chemical state of support on Pd layer growth was proved on Pd/W and Pd/WO_x/W systems. Thermal aging of these systems revealed a decrease of adsorption activity caused by encapsulation of Pd layer by W₂⁺ (or W₄⁺) species.

TOPIC 3. Molecular Spectroscopy and Photochemistry.

Grant projects**AS CR****From a computer controlled spectroscopic experiment to an international database for remote detection of molecules.****Š. Urban, No. ET400400410, 2004-2008.**

Main results in 2005: A special software for the spectrometer control, data acquisition and monitoring of measurements was developed. Detailed analysis of the high resolution acetonitrile spectra provided the first determination of the pressure dependencies of the rotational, centrifugal distortion, and hyperfine constants. Detailed studies of high resolution rotational-hyperfine spectra of the three chloromethane and two CH₂Br isotopologues.

GA AS CR**Fast tunable MID-IR and IR laser diode spectrometer based on non-linear optical effects.****S. Civiš, No. A4040104, 2001-2005.**

Main results in 2005: The study was targeted on the development of new type of GaSb-based semiconductor laser operating in continuous-wave mode at room temperature and above. The lasers were optimized using absorption high resolution methods for which the new high resolution Fourier Transform infrared IFS Bruker 120 spectrometer has been used. Simultaneously with the study of the laser's features the new detection techniques has been developed. A study of the infrared spectra of the CH₄, CO, CO₂, NH₃ and N₂O, acetylene and ethane gases has been carried out in all available spectral ranges (2100, 3100, 4300, 6500 cm⁻¹). The spectra of automobile exhaust gases at various motor temperatures were measured qualitatively and quantitatively.

Microwave spectroscopy of nitrogen and halogen atmospheric components with significant hyperfine structure of rotational levels.**Š. Urban, No. 400400504, 2005-2009.**

Main results in 2005: The new Prague microwave set-up was completed and opened for scientific studies. Several experimental studies of rotational-hyperfine spectra of atmospherically important molecules (acetonitrile, chloromethane, bromomethane) were started. The special experimental layout for hyperfine studies of radicals was fixed and the first hyperfine spectra of the FCO₂ radical was measured in Prague.

New laser-based hybrid technologies for thin layer deposition.**Z. Zelinger (a), No. A1010110, 2001-2005.**

Main results in 2005: High resolution spectroscopy of halogenated radicals in the laser plume and additional discharge plasma – the chloromethyl radical, CH₂Cl, the bromomethyl radical, CH₂Br – experimental evidence of paramagnetism of measured radicals, spectroscopic identification of measured lines, new molecular constants for the bromomethyl radical and substantial improvement of molecular constants for chloromethyl radical.

GA CR

Design and characterization of new photosensitizers and investigation of their interaction with target biological macromolecules.

P. Kubát (a), No. 203/04/0426, 2004-2006.

Main results in 2005: Interaction of porphyrin-type sensitizers (meso-tetraphenylporphyrins and lanthanide texaphyrins) with species of biological interests (PAMAM dendrimers, cyclodextrins and nucleotides) was studied by laser kinetic spectroscopy and by other spectroscopic techniques. Porphyrins intercalated into photochemically stable and well-defined inorganic hosts (hydrotalcites, clays) were found to generate singlet oxygen. Generation of singlet oxygen assigns these materials for photo-disinfection.

MEYS

Infrared and sub-millimeter wave spectroscopy of molecular ions - contribution to the analyses of data from the Herschel observatory of ESA.

Z. Zelinger, BARRANDE project No. 2004-037, 2004-2005.

The role of the upper troposphere and lower stratosphere in global change.

Z. Zelinger, COST project No. OC 723, 2003-2006.

Assessing and managing of nitrogen fluxes in the atmosphere-biosphere system in Europe

Z. Zelinger, COST project No. OC 729, 2005-2010.

Infrared and sub-millimeter wave spectroscopy of molecular ions - contribution to the analyses of data from the Herschel observatory of ESA.

Z. Zelinger, KONTAKT project No. 766, 2005-2006.

DEPARTMENT OF BIOPHYSICAL CHEMISTRY

TOPIC 1. Fluorescence Spectroscopy

Grant projects

GA AS CR

Solvent relaxation in phospholipids bilayers: physical understanding and biophysical applications.

M. Hof, No. A4040405, 2005-2007.

Main results in 2005: Two applications of the solvent relaxation technique, which was originally developed for biosciences at the JHIPC, were investigated: a) determination of the influence of the curvature on the water structure in the headgroup region of phospholipid bilayer; b) investigation of the pH-dependent hydration of poly(oxyethylene) shells in polystyrene-block-poly(2-vinylpyridine)-block-poly(oxyethylene) micelles in aqueous solutions.

GA CR

Understanding, control, and preparation of self-assembling biomembrane systems at interfaces.

M. Hof, No. 203/05/2308, 2005-2007.

Main results in 2005: First experimental realization of Time-Resolved Fluorescence Correlation Spectroscopy (TR-TCS) and its first application in membrane research was carried out. Comparison of the z-scan approach for characterization of lipid diffusion within bilayers (originally developed in the JHIPC) with multi foci FCS. Characterization of potential controlled adsorption and lateral mobility of lipid molecules onto polycrystalline gold.

TOPIC 2. Molecular structures at liquid|liquid interfaces

Grant projects

GA CR

Polymerization of adsorbed layers at the liquid/liquid interface.

V. Mareček, No. 203/03/0822, 2003-2005.

Main results in 2005: It was shown that desorption of the surface active agents (substituted cyclodextrin, phospholipids) embedded in the formed polymer layer can lead to the formation of pores which make the ion transfer feasible. A new method for obtaining silicate layers on the liquid interface was worked out and feasibility of the layer doping with other ions was proved. In cooperation with the university in Atlanta the NMR method was successfully used for the detection of different solvatomers of Li ion in nitrobenzene saturated with water and for monitoring of their transfer reactions.

TOPIC 3. Biosensors

Grant projects

MEYS

Characterization of cancer-related metalloproteins and their interaction with DNA.

I. Šestáková (a), COST project No. D21.002, 2002-2005.

Main results in 2005: In connection with reactions of metal ions exchange, rabbit liver metallothioneins with bound Cd(II) or Zn (II) were studied in the presence of additional Cd²⁺ or Zn²⁺ ions in solution. Using voltammetry or chronopotentiometry on hanging mercury drop electrode, inert or labile behavior of complexes can be distinguished. Constant Current Chronopotentiometric Stripping Analysis with adsorptive accumulation and application of high negative stripping current enables to follow substitution of bound Zn (II) for cadmium and no changes of originally bound Cd(II) in metallothionein molecule. With the application of low current (100 to 20 nA), progressive formation of reorganized complex exhibiting labile behavior is observed for both types of metallothioneins.

MIT**Research and development of a new type of electrochemical biosensor for the detection of nucleotide sequences in DNA and of genotoxic agents in the environment.****T. Navrátil (a), No. 1H-PK/42, 2004-2007.**

Main results in 2005: Electrocatalytical behavior of osmium modified oligonucleotides and of osmium modified DNA on solid amalgam electrodes was described and its application was proposed for construction of DNA hybridization sensors. The conducting ink films, prepared from different types of carbon and other materials, extend the potential working ranges of traditional working electrodes and present cheaper, renewable alternative to disposable electrodes. Design of metabolic pathways of degradation of supplemented creatine leading to the formation of thiodiglycolic acid under influence of some vitamins and thiolic compounds was realized.

DEPARTMENT OF CATALYSIS I**TOPIC 1. Synthesis and Reactivity of Catalytic Materials**Grant projects**AS CR****Development of program environment for mathematic simulations and predictions in catalysis and electrocatalysis.****Z. Sobalík, No. 1ET400400413, 2004-2008.**

Main results in 2005: Relevant experimental data for modeling of catalysis and electrocatalysis processes were collected. Program for description of aggregation of three dimensional clusters controlled by diffusion and providing a method for analysis of their formation has been developed and successfully tested. Procedure for input of the experimental data on metallo zeolites for mathematical modeling using QMPOT program was accomplished. This procedure provides for combined calculation of the DFT level with a parallel "embedding" of the relevant zeolite structure.

GA AS CR**Control of negative charge distribution in skeleton of high-silica zeolites.****J. Dědeček, No. 4040308, 2003-2006.**

Main results in 2005: a) Model describing mechanism of the control of aluminum local density in silicon rich zeolites was suggested and significant effect of the Al local density on the activity/selectivity of zeolite based catalysts was demonstrated.

b) New method based on $^{6,7}\text{Li}$ MAS NMR enabling monitoring of Al siting in individual the framework T sites was developed. The Al distribution in framework T sites is non-random and is controlled by the conditions of zeolite synthesis.

GA CR**Effect of gaseous additives and gas phase reactions on the course of catalytic redox reactions.****D. Kaucký, No. 104/04/D124, 2002-2005.**

Main results in 2005: The effects of additives on industrially important processes of NO and N₂O transformations to N₂ and O₂ were broadly screened. The approaches for promoting the catalysts performance by additives were improved. Also, the results contributed considerably to the understanding of the mechanism and dynamic behavior of the reactions of interest.

Nanostructured inorganic materials based on molecular sieves for sensor application.**J. Dědeček, No. 203/05/2309, 2005-2007.**

Main results in 2005: The interaction of transition metal ion centers in aluminosilicate molecular sieves with guest molecules was studied under high-temperature operando conditions by the combination of UV-Vis and FTIR spectroscopy. At lower temperatures, fast formation of metal-ligand complexes predominates and is followed by significant hysteresis in the resuscitation of original spectroscopic parameters while at high temperatures, changes in the valence state of bare cationic centers are observed.

Catalytic ammoxidation of propane.**B. Wichterlová, No. 104/03/1120, 2003-2005.**

Main results in 2005: It has been shown that N₂O as a co-reactant to molecular oxygen enhances selective oxidation of low paraffins if CoFe-zeolites are used as catalysts. N₂O is decomposed with formation of atomic oxygen over Fe species and oxidizes propane to alcohol, which is immediately dehydrated to olefin. Co ions oxidize propane to propene and CO_x as well as by-products formed in oxidation by atomic oxygen. The results might be promising for application of end-pipe gases containing N₂O, e.g., from adipic acid units, for selective oxidation of paraffins.

Organized materials for highly selective catalytic and separation processes.**B. Wichterlová, No. 203/03/H140, 2003-2006.**

Main results in 2005: The project supports education and training of PhD students in the field of heterogeneous and homogeneous catalysis from the viewpoint of the catalyst structure and reaction performance on a molecular level. The project ranges from structural studies of catalysts at ex-situ conditions up to the real conditions of the catalytic reactions. In parallel dynamics of catalytic and separation processes is studied.

MIT**Application of residual and waste aluminosilicates for production of building materials on the basis of inorganic polymers.****Z. Sobalík (a), No. FI-IM/079/IMPULS, 2004-2006.**

Main results in 2005: The basic difference between the ageing process of internal and external layers in the geopolymers and their further changes with time of maturing of the material has been evidenced. The process of transformation of the geopolymer during acidic treatments has shown its partial dealumination, and at the same time zeolitization of the remaining material. The resulting material displayed some level of mesoporosity

MEYS

European Federation of Catalysis Societies.

Z. Sobalík, No. INGO LA169, 2003-2005.

Organic synthesis of zeolites: Activation of CO₂ and of organic carbonates for fine chemicals.

Z. Sobalík, No. COST D29/0013/04, 2004-2006.

International Association of Catalytic Societies.

B. Wichterlová, No. INGO LA 170, 2003-2005.

EU project

Integrated design of catalytic nanomaterials for a sustainable production.

B. Wichterlová (a),), EC (6th Programme), No. NMP3-CT-2005-011730/ IDECAT, 2005-2010.

TOPIC 2. Interactions and Mobility of Molecules in Microporous Systems

Grant projects

AS CR

Ceramic materials with hierarchical porous structure for membrane separation technologies.

M. Kočířík (a), No. 1QS 401 250 509, 2005-2008.

Main results in 2005: A series of porous filtration elements with uniform pore structure was manufactured from α -alumina and the technological parameters (milling time of the starting grains and firing temperature) were optimized with respect to mechanical stability of the material and material permeability for permanent gases. Optimum milling time was found to be 2 hours and optimum firing temperature of green compacts was 1300°C.

GA AS CR

Coupling of diffusion flows in porous membranes and catalysts as studied by permeation and NMR techniques.

M. Kočířík, No.400400501, 2005-2007.

Main results in 2005: A strong coupling of diffusion flow of ethylene with those of C₄ to C₅ hydrocarbons in HZSM-5 crystals was observed at temperatures below 200°C. This coupling was found to be due to immobilization of higher hydrocarbon species and attainment the percolation threshold in the system of zeolite channels. The attainment of percolation threshold was found to control the temperature onset of catalytic bed production. Besides theoretical values of percolation thresholds were determined for channel system in MFI zeolites type using topological equivalence of MFI channel system with diamond lattice.

GA CR

Growth of nanofiltration layers from colloidal solutions. Effect of electrochemical properties of colloidal solutions on kinetics of the layers.**L. Brabec, No. 203/05/0846, 2005-2007.**

Main results in 2005: Hydrothermally synthesized polycrystalline self-supported layers of silicalite-1 as well as its large crystals-twins were studied by mild etching with HF acid. Etching patterns evidence the amorphous interface film between crystals in the case of layers and forming of pyramidal crystal parts in the case of large prismatic crystal twins. These twins were tested by nanoindentation resulting to values of their microhardness and modulus of elasticity. Starting electroforetic experiments were performed with well defined SiO₂ colloidal solutions on a disc electrode to find suitable conditions for deposition of continual SiO₂ film.

Polymer-based membrane composites for separation of small molecules.**M. Kočířík (a), No. 104/03/0680, 2003-2005.**

Main results in 2005: Polyimide-polysiloxane membranes were synthesized with different content of zeolitic inclusions. It was found by SEM that adhesion of polymer layer to the zeolitic inclusions was considerably enhanced by the presence of polysiloxane. The nitrogen permeation tests showed that membranes were free of macroscopic defects. The application of the technique of iodine indicator showed that intracrystalline space of zeolitic inclusions was not blocked by solvents used in the process of membrane preparation.

Nanostructured materials – texture from physical adsorption.**M. Kočířík (a), No. 104/04/096, 2004-2006.**

Main results in 2005: A technique to estimate transport related structure parameters of porous bodies was developed based on combination of nonstationary permeation of single component permanent gases in the region of enhanced excess pressure (up to 8 bar) and nonstationary counter diffusion measurements of binary species in semi-open Wicke-Kallebach cell. This measuring techniques together with developed software to solve mathematical model of mass transport in the porous system appears to be promising for estimation of all three transport related structure parameters of DGM (Dusty Gas model).

Contribution of non-zeolitic pores to the separating function of composite membranes containing zeolites.**O. Prokopová, No. 104/03/D183, 2003-2006.**

Main results in 2005: Earlier knowledge on tubular membrane synthesis with ZSM-5 separation layer has been supplemented. Set of experimental data showed large membrane quality variability on synthesis parameters (support quality, TPAOH concentration, hydrothermal temperature program, calcination). It has been continued in mathematical analysis of template removal kinetics.

Porous catalysts and membrane supports: A relationship between mass transport and textural properties.**A. Zikánová (a), No. 203/05/0347, 2005-2007.**

Main results in 2005: A technique was developed to construct digital images of macrosections of α -alumina porous bodies. The technique is based on impregnation of the porous system with a polymer species and fine grinding of the sections in distinct material depths. The SEM images with sufficient material contrast were prepared using material imaging in the regime of backscattered electrons. The application of standard mathematical techniques of image analysis provided the necessary stochastic characteristics of porous material. This accomplished the key step in stochastic reconstruction of porous system.

MEYS

Development of zeolitic membranes for separation and capture of CO₂.
O.Prokopová, No. BARRANDE 2005-06-046-1, 2005-2006.

TOPIC 3. Sol – Gel Microstructured Materials

Grant project

AS CR

New crystalline TiO₂ materials with hierarchical pore structure.
J. Rathouský, AS CR-DAAD (Germany) project, 2005-2006.

Hybrid inorganic-organic composite materials with controlled texture properties.
J. Rathouský, AS CR-CNRS (France) project, 2005-2006.

EU project

Transparent nanocomposite electrodes based on thin films of mesoporous oxides with anchored electroactive sites.

J. Rathouský, DFG, No. 436-TSE 113/46/0-1, 2005-2006.

Main results in 2005: Mesoporous silica thin films were shown to be an appropriate matrix for immobilization of discrete electroactive moieties (polyoxometalate, hexacyanoferrate, ferrocene) yielding uniform transparent thin film electrodes with defined texture and enhanced electrochemical activity. The whole bulk volume of the modified silica films is electrochemically accessible. The electron exchange between the adjacent redox centers (electron hopping) is proposed as possible charge propagation pathway through the insulating silica matrix.

DEPARTMENT OF CATALYSIS II

TOPIC 1. Molecular sieve chemistry and catalysis

Grant projects

AS CR

Synthesis of mesoporous zeolites for catalytic application.
J. Čejka, AS CR-KOSEF (Korea) project, 2005-2007.

Intelligent design of nanosorbents for gas storage.
J. Čejka, AS CR-CNRS (France) project, 2005-2006.

GA AS CR**Transition metal oxides supported on mesoporous molecular sieves for olefin metathesis reactions.****J. Čejka, No. 4040411, 2004-2007.**

Main results in 2005: New types of heterogeneous catalysts for metathesis of linear olefins were developed. These catalysts based on molybdenum oxide on siliceous mesoporous molecular sieves (MCM-41, MCM-48 and SBA-15) or rhenium oxide on organized mesoporous alumina operate at mild reaction conditions and exhibit much higher activities compared with traditional catalysts.

Tailoring the zeolite properties for catalytic applications.**G. Košová, No. B4040402, 2004-2006.**

Main results in 2005: Main effort has been centered on the optimizing of the reaction conditions of the synthesis of zeolites MCM-58 and MCM-68 and on the understanding of the location of aluminum in the aluminosilicates framework. Based on the MAS NMR spectra of synthesized zeolites it seems that distribution of aluminum can be substantially changed due to the synthesis parameters or reactant types applied.

GA CR**Synthesis of fine chemicals via heterogeneous catalysis.****J. Čejka, No. 203/03/0804, 2003-2005.**

Main results in 2005: Optimization of the catalyst formulation of zeolite Beta for acylation of toluene with isobutyric acid derivatives and acylation of isobutyl benzene with acetic anhydride was carried out. It was found that zeolite Beta due to its three-dimensional large pore channel structure represents the optimum reaction volume for performing these acylation reactions. Combination of acidic form of zeolite Beta with Beta modified with Pd led to the preparation of the bi-functional catalyst being able to simultaneously acylate toluene with isobutyric anhydride and to hydrogenate isopropylphenyl ketone formed by acylation reaction to isobutyl toluene.

New micro/mesoporous composite catalysts for transformations of aromatic hydrocarbons.**J. Čejka, No. 203/05/0197, 2005-2007.**

Main results in 2005: Optimization of the synthesis of mesoporous zeolite ZSM-5 with controlled volume of mesoporous was carried out using carbon particles of defined size. It was shown that the maximum of the size of mesopores corresponds nicely to the size of particles used. Nitrogen adsorption isotherms were applied to describe in a detail the inner volume and pore size distribution of pores in these materials.

Bifunctional heterogeneous catalysts for palladium-catalyzed coupling reactions.**J. Čejka, No. 104/05/0192, 2005-2007.**

Main results in 2005: Mesoporous molecular sieves MCM-41 and MCM-48 were modified with Pd to prepare highly active catalysts for C-C coupling reactions. The reaction of cis-2-buten-1,4-diol with 2-aminoethanol to form N-(2-hydroxyethyl)pyrrole was tested over these catalysts. The main objective is currently focused on the decrease in the leaching of active sites during the reaction.

MIT**Development of special types of oxidation catalysts for tailored synthesis of fragrances.****J. Čejka (a), No. FT-TA/040/TANDEM, 2004-2007.**

Main results in 2005: New type of oxidation catalyst based on conventional silica modified by Sn was prepared and tested in oxidation of cyclic ketones to corresponding lactones using hydrogen peroxide as oxidating agent. These catalysts were found to catalyze this so-called Baeyer-Villiger oxidation at mild conditions with high conversions, selectivities to lactone almost 100 % and with a high efficiency to hydrogen peroxide used.

Development of progressive types of alumina for special applications.

J. Čejka (a), No. FT-TA/042/TANDEM, 2004-2007.

Main results in 2005: Synthesis of organized mesoporous aluminas were focused on the utilization of a cheap source of alumina (aluminum chlorohydrate) and optimizing the synthesis procedure in aqueous medium. Ionic liquids were applied as structure-directing agents for this synthesis. Organized mesoporous aluminas with surface areas between 250-300 m²/g and pore dimensions of about 3.8-3.9 nm were prepared and characterized.

MEYS

Czech zeolite group.

J. Čejka, No. INGO LA 144, 2002-2005.

FEZA conference.

J. Čejka, No. INGO LA 255, 2005-2005.

EU projects

Intelligent design of nanoporous sorbents.

J. Čejka (a), EC (6th Programme), No. MRTN-CT-2004-005503/INDENS, 2005-2008.

TOPIC 2. Organometallic Catalysis

Grant projects

GA AS CR

Synthesis of cationic titanocene complexes and their reactivity towards olefins and acetylenes.

M. Horáček, No. B4040403, 2004-2006.

Main results in 2005: Cationic titanocene complexes functionalized by benzyl groups were prepared by reactions of tris(pentafluorophenyl)borane (B(C₆F₅)₃), with the titanocene derivatives containing two vicinal methylene groups. The obtained cationic complexes were investigated by X-ray single crystal analysis and spectroscopic methods, and their activity towards linear dimerization of alkynes was examined. Half-sandwich titanium complexes CpTiR₃ R = Me, O-tBu were prepared and their reactivity towards B(C₆F₅)₃ was investigated in polymerization reactions. Unexpected results were obtained in the case of compound with one tert-butoxy group which gives during the reaction with borane unknown products catalyzing polymerization of tetrahydrofuran.

GA CR

Mesoporous hybrid catalysts for preparation of specialty polymers.

H. Balcar, No. 203/05/2194, 2005-2007.

Main results in 2005: New hybrid catalysts producing polyphenylacetylenes and polyalkenylenes free of catalyst residues were prepared by anchoring [Rh(diene)acac]

complexes on MCM-41 and Schrock carbene complexes $\text{Mo}(=\text{CHCMe}_2\text{Ph})(=\text{N}-2,6\text{-i-Pr}_2\text{C}_6\text{H}_3)(\text{OR})_2$, [OR = OCMe₃ or OCMe(CF₃)₂] on MCM-41, MCM-48 and SBA-15 mesoporous molecular sieves.

Functionalization of cyclopentadienyl ligands in Ti and Zr complexes by silanes. Utilization of Si-H bonds in synthesis and catalyst anchoring.

M. Horáček, No. 104/05/0474, 2005-2007.

Main results in 2005: The Si-H bonds were introduced into tetramethylated cyclopentadienyl ligand and the corresponding titanocene or zirconocene monochloride complexes were prepared. Their oxidation by AgCl yielded the pertaining titanocene or zirconocene dichloride complexes. The reduction of dichloride complexes by magnesium resulted in the generation of low-valent titanocene or zirconocene complexes stabilized by bis(trimethylsilyl)ethyne. The high reactivity of the Si-H bond leads to formation of ansa-titanocene or zirconocene complexes containing bridging tetramethyldisilylene group and abstraction of hydrogen during the reduction. These new organometallic complexes were reacted with terminal alkynes to examine their catalytic activity in dimerization and trimerization reactions.

MIT

New hybrid catalysts for metathesis of olefins and preparation of specialty polymers.

H. Balcar, project of Czech-Belgium collaboration No. 2004-2005-07, 2004-2005.

DEPARTMENT OF ELECTROCHEMISTRY

TOPIC 1. Electrochemistry of Liquid Interfaces and Membranes

Grant projects

GA AS CR

Electroanalysis on metal nanoparticles deposited on the supported liquid.

Z. Samec, GA AS CR, No. 4040407, 2004-2007.

Main results in 2005: Most significant results included an observation of the random nucleation and growth of Pt nanoparticles at the polarised liquid-liquid interface, and the first evidence of electrocatalysis of the interfacial oxygen reduction by Pt nanoparticles.

GA CR

Electrochemistry in biomedically important polyions at the interface of two immiscible electrolyte solutions with applications in drug analysis.

Z. Samec, No. 203/04/0424, 2004-2006.

Main results in 2005: Amperometry using a polymer coated GC electrode was optimized for a determination of heparin in untreated human blood plasma samples at biomedically relevant concentrations.

Microfluidic analysis system for monitoring of amino acids in biological fluids.

J. Langmaier (a), No. 203/04/0519, 2004-2006.

Main results in 2005: Standard amino acids were derivatized with phenylisothiocyanate (PITC) to form stable chemically detectable PITC-derivatives. The PITC-derivatives were

electrochemically investigated in acid, basic and neutral media on gold, platinum and glassy carbon electrodes in order to develop simple and universal protocol for amino acids detection applicable in analysis coupled with separation techniques. Most of studied derivatives were found to undergo analytically exploitable two electron oxidation.

EU projects

Nanostructures for energy and chemical production.

Z. Samec (a), EC (6th Programme), No. NMP3-Ct-2004-505906/NENA, 2004-2007.

TOPIC 2. Electrocatalysis

Grant projects

GA AS CR

Charge transfer in organized supramolecular systems of fullerenes.

L. Kavan, No. 4040306, 2003-2006.

Main results in 2005: The electrochemical reduction processes in highly organized fullerene films were elucidated. The clusters, 20—50 nm in size are formed spontaneously as a result of irreversible cathodic reactions in aqueous electrolyte solution. Similar nanostructuring proceeds also in ionic liquids, where the electrochemical reduction is, however, partly reversible. The polymerization of fullerenes is accompanied by their partial hydrogenation in aqueous medium.

***In-situ* gravimetric investigation of ion transfer and adsorption at the interface of two immiscible liquids.**

P. Krtil, No. B4040305, 2003-2005.

Main results in 2005: A new design of thin layer arrangement for EQCM study of ion transfer across ITIES was developed. The new design uses cross-linking of polypeptide based polyelectrolytes as an anchor for the aqueous phase. The viability of the design was demonstrated on a simple ion and combined electron ion transfer across water|1,2-dichloroethane interface.

GA CR

The exploitation of alkali alkynides for the electrochemical and chemical preparation of long-chain oligoynes and carbon nanotubes.

J. Hlavatý, No. 203/03/0825, 2003-2005.

Main results in 2005: But-2-yn-1-ol (2-butyne-1-ol) was prepared as a new substance in 37% yield like a valuable precursor for oligoyne synthesis.

Template mesoscopic TiO₂ for electrodes and photocatalysts.

L. Kavan, No. 203/03/0824, 2003-2005.

Main results in 2005: Highly efficient mesoporous TiO₂ layer for their application in solar cells was demonstrated. The film was grown via layer-by-layer deposition, and characterized by a novel methodology based on the adsorption of n-pentane. The 1 μm-thick mesoporous film, made by the superposition of 3 layers, showed enhanced solar conversion efficiency by about 50 % compared to that of traditional films of the same thickness made from randomly oriented anatase nanocrystals.

Low temperature synthesis of electrochemically active phases in the Li-Ti-O, Li-Mn-O and Li-Fe-Mn-O systems; their electrochemical characterization.

P. Krtil, GA CR, No. 203/03/0823, 2003-2005.

Main results in 2005: The role of the solvent polarity on the structure of solvothermally synthesized Li-Ti-O spinels was elucidated. The solvents with high dielectric constant direct the structure of prepared cubic phases towards structures with Ti disorder between 16c and 16d positions; with decreasing solvent polarity one obtains structures closer to ordered spinels. The role of the defect distribution within the particles of the insertion materials was demonstrated on sol-gel prepared RuO₂ and Li-Mn-O spinels. The materials with localized defect show lower tendency to phase transitions upon insertion/extraction of Li.

MIT

Photocatalytic surfaces with selfcleaning properties. Development of technology for preparation of new materials with surfaces exhibiting selfcleaning and disinfection effects based on photocatalysis utilizing energy of light.

J. Jirkovský (a), MIT, No. FD-K3/086/FOPOS, 2003-2005.

Main results in 2005: Consortium of six partners aimed at the development of novel surface materials exhibiting self-cleaning and antibacterial properties based on the photocatalytic action utilizing solar irradiation. Among other results, recipes for silicate paints for external use containing the photoactive titanium dioxide have been worked out. The synthesis of the photoactive component is purposely based on the technology of titanium white used by the Czech producer Precheza Přerov. The necessary testing methods for the photoactivity of powder photocatalysts as well as photocatalytic coatings have been developed and introduced in the laboratory at the Heyrovský Institute.

MEYS

Research centre for nanotechnologies and materials for nanoelectronics.

L. Kavan (a), Centrum LC510, 2005-2009.

Main results in 2005: Formulation of the so called resonance rule, which rationalizes the diameter and chirality selective Raman spectroelectrochemical response of single walled carbon nanotubes. This rule explains the spectroelectrochemistry of semiconducting single walled carbon nanotubes in a self consistent way. The application of our resonance rule to double walled carbon nanotubes points at fundamental confusion in the literature, as far as the chirality assignment of inner tubes is concerned.

Research centre for nanosurface engineering

J. Jirkovský (a), Centrum No. 1M0577-NANOPIN, 2005-2009.

Main results in 2005: Collaboration of five partners comprises fundamental research of unique photocatalytic properties of photoactive materials based on nanocrystalline titanium dioxide as well as applied research of their practical utilization in the field of self-cleaning and antibacterial coatings, photocatalytic purification of water and air, organic synthesis and solar energy conversion. Among other topics, aging of colloidal solutions of quantum sized particles of titanium dioxide have been thoroughly investigated. Gradual increase of the mean size and decrease of the specific surface area of the nanoparticles is accompanied by an increase of their photoactivity and changes of their other physico-chemical properties.

Nanoelectric oxidic semiconductor for optoelectronic application.

L. Kavan, No. COST 1P05 OC069, 2005-2008.

Adsorption Properties of Titanium Dioxide in Relation to Photocatalysis.

J. Jirkovský (a), KONTAKT No. 2005-22, 2005-2006.

EU projects

Innovative multi-purpose thin-film UV reactor.

L. Kavan (a), EC (5th Programme), EVK1-CT-2002-300258/UVREC, 2003-2005.

Molecular orientation, low band gap materials and new hybrid device concepts for the improvement of plastic solar cells.

L. Kavan (a), EC (6th Programme), No. SES6-Ct-2003-502783/MOLYCELL, 2004-2006.

Nanocrystalline Heterosupermolecular Materials for Optoelectronic Applications.

L. Kavan (a), EC (6th Programme), No. NMP3-CT-2005-516982/HETEROMOLMAT, 2005-2008.

TOPIC 3. Organic and Organometallic Electrochemistry

Grant projects

AS CR

Metalloorganic Oligophenylvinylens.

S. Záliš, AS CR- University Stuttgart project (DFG grant), 2005-2007.

GA AS CR

Electronic properties, structure and reactivity of the azine group $C=N-N=C$ and mechanism of biologically important azines degradation.

J. Ludvík, No. 4040304, 2003-2005.

Main results in 2005: The complex mechanism of reduction of acyclic azine grouping ($>C=N-N=C<$) in aqueous media has been formulated in detail for various pH ranges. The six-electron degradation proceeds in sequence of three two-electron steps: azine \rightarrow hydrazone \rightarrow imine \rightarrow amine. The electron transfer processes are complicated by simultaneous hydrolysis of azines, hydrazones and imines leading to carbonyl compounds as secondary products. Decreased electron delocalization (aromaticity) of various types of azines due to the N-N single bond has been discussed.

Redox reactions of free radicals, reactivity in presence of host molecules.

L. Pospíšil, No. 400400505, 2005-2008.

Main results in 2005: Nitroaromatic radicals generated in aprotic solvents undergo further reduction. We found the first example of the double layer influence on a redox process involving an organic anion radical. Large amount of precise data on the double layer structure in acetonitrile was analysed and the Frumkin correction was discussed. We found also the first example of an oscillating system, which involves a radical.

GA CR

Preparation, reactivity and electrochemistry of new aminocarbene complexes of chromium and iron.

J. Ludvík (a), No. 203/04/0487, 2004-2006.

Main results in 2005: Series of chelated and unchelated aminocarbene complexes of chromium and tungsten are important syntones in organic chemistry and promising catalysts. Using electrochemically followed intramolecular electron interactions the oxidation and reduction centers were localized, the role of the type and structure of ligands and influence of substitution and central atom on redox properties, electron delocalization and reactivity were elucidated.

Electron transfer in supramolecular complexes, large molecules with more active centers and in organized structures.

L. Pospíšil, No. 203/03/0821, 2003-2005.

Main results in 2005: Research dealt with characterization of host-guest complexes, which include redox active compounds as guests and cyclodextrins as host molecules. We solved problems to which extent redox properties are retained even inside a cavity of oligosaccharides (cyclodextrins). In the case of an organometallic complex we achieved the suppression of undesirable termination reactions. Inclusion in other case leads to preferential dechlorination of pesticides yielding chloride ions and prevents formation of chloroanilines. Other topic solved a problem of labeling bovin serum albumine with multiple organometallic redox centers for applications in clinical analysis.

MEYS

Sonoelectrochemistry - physical mechanisms and applications in molecular electrochemistry.

J. Klíma, No. COST 1P05OC074, 2005-2008.

Chemical and electrochemical properties of oximes – antidotes against nervous gases.

J. Ludvík, No. KONTAKT 1P05ME785, 2005-2008.

Electrochemistry of nano-structures at heterogeneous interfaces: Formation, properties and electron transfer reactions.

L. Pospíšil, No. COST 1P04 OCD 15.10, 2004-2006.

Organometallic and metallo-organic building blocks for photonic materials.

A. Vlček, No. COST 1P04 OCD14.20, 2004-2007.

Optically and electronically controlled states of metal-based molecular systems. Experiment and theory.

A. Vlček, No. COST 1P05 OC068, 2005-2008.

4. PUBLICATION AND POPULARIZATION ACTIVITIES

4.1. Synopsis of Papers Published in 2005

Members of the Institute are authors or co-authors of 214 research papers which appeared in 2005 in reviewed periodicals, proceedings of conferences, and monographs.

In addition, 12 popularization papers in professional publications appeared. Contributions in non-professional journals and newspapers are not included.

Table 4.1. Publications issued in 2005

Type of publication	Number
Research papers in periodicals	152
Contributions in conference materials	37
Contributions in monographs	13
Popularization papers	12

Members of the department of theoretical chemistry, chemical physics, biophysical chemistry, catalysis I, catalysis II and electrochemistry were authors or co-authors of 14, 62, 34, 30, 25 and 57 of the issued publications, respectively.

In 117, 42 and 55 publications authors from institutions abroad, universities in the Czech Republic, and other institutions in the Czech Republic, respectively, participated. Authors of 60 publications were exclusively members of the Institute.

Members of the Institute are given with their full names in the following list of published papers.

4.2. Research Papers in Periodicals

1. Kardahakis S., Pittner Jiří, Čársky Petr, Mavridis A.
Multireference configuration interaction and coupled-cluster calculations on the $X^3\Sigma^-$, $a^1\Delta$, and $b^1\Sigma^+$ states of the NF molecule.
International Journal of Quantum Chemistry. 104 (4), 458-467 (2005).
2. Kerkines I. S. K., Čársky Petr, Mavridis A.
A multireference coupled-cluster potential energy surface of diazomethane, CH_2N_2 .
Journal of Physical Chemistry. A. 109 (44), 10148-10152 (2005).
3. Pittner Jiří, Demel Ondřej
Towards the multireference Brillouin-Wigner coupled-clusters method with iterative connected triples: MR BWCCSDT-alpha approximation.
Journal of Chemical Physics. 122 (18), 181101-181106 (2005).
4. Pittner Jiří, Li X., Paldus J.
Multi-reference Brillouin-Wigner coupled-cluster method with a general model space.
Molecular Physics. 103 (15-16), 2239-2245 (2005).
5. Teberekidis V.I., Kerkines I.S.K., Tspis C.A., Čársky Petr, Mavridis A.
Ground states of BeC and MgC: A comparative multireference Brillouin-Wigner coupled cluster and configuration interaction study.
International Journal of Quantum Chemistry. 102 (5), 762-774 (2005).
6. Pick Štěpán, Demangeat C.
Density-functional study of oxidation at the Mn-Co interface.
Surface Science. 584 (2-3), 146-152 (2005).
7. Fišer J., Polák Rudolf
Electron affinities of BN, NO and NF: Coupled cluster and multireference configuration interaction calculations.
Collection of Czechoslovak Chemical Communications. 70 (7), 923-940 (2005).
8. Paidarová Ivana, Durand P.
Effective couplings between quantum resonances: application to the resonant dissociation of the $^6\text{Li } ^7\text{Li}$ molecule.
Czechoslovak Journal of Physics. 55 (2) 203-216 (2005).
9. Paidarová Ivana, Sauer S. P. A.
Calculations of dipole and quadrupole polarizability radial functions for LiH and HF: A comparison of different linear response methods.
Advances in Quantum Chemistry. 48, 185-208 (2005).
10. Srnec Martin, Zahradník Rudolf
Diatomics AB (A = Be, Mg; B=O, S) and oligomers thereof: A theoretical study.
Chemical Physics Letters. 407 (4-6), 283-288 (2005).

11. Zahradník Rudolf, Smec Martin, Havlas Zdeněk
Electronic spectra of conjugated polyynes, cumulenes and related systems: A theoretical study.
Collection of Czechoslovak Chemical Communications. 70, 559-578 (2005).
12. Zahradník Rudolf, Šroubková Libuše
Formation and physical characteristics of van der Waals molecules, cations, and anions: Estimates of complete basis set values.
International Journal of Quantum Chemistry. 104 (1), 52-63 (2005).
13. Herman Zdeněk
Studies of hydrocarbon ion collisions with carbon surfaces in the Association EURATOM-IPP.CR.
EFDA Fusion Newsletter. 3, 7-7 (2005).
14. Jašík Juraj, Žabka Ján, Feketeová L., Ipolyi I., Märk T. D., Herman Zdeněk
Collisions of slow polyatomic ions with surfaces: Dissociation and chemical reactions of $C_2H_2^+$, $C_2H_3^+$, $C_2H_4^+$, $C_2H_5^+$, and their deuterated variants $C_2D_2^+$ and $C_2D_4^+$ on room-temperature and heated carbon surfaces.
Journal of Physical Chemistry. A. 109 (45), 10208-10215 (2005).
15. Tepnual T., Feketeová L., Grill V., Scheier P., Herman Zdeněk, Märk T. D.
Surface collisions of formic acid cations $HCOOH^+$ and $DCOOD^+$ with a hydrocarbon-covered stainless steel surface.
International Journal of Mass Spectrometry. 244 (2-3), 164-170 (2005).
16. Devlin J. P., Fárník Michal, Suhm M. A., Buch V.
Comparative FTIR spectroscopy of HX adsorbed on solid water: Ragout-jet water clusters vs ice nanocrystal arrays.
Journal of Physical Chemistry. A. 109 (6), 955-958 (2005).
17. Fárník Michal, Nahler N. H., Buck U., Slavíček P., Jungwirth P.
Photodissociation of HBr on the surface of Ar-n clusters at 193 nm.
Chemical Physics. 315 (1-2), 161-170 (2005).
18. Fárník Michal, Toennies J. P.
Ion-molecule reactions in 4He droplets: Flying nano-cryo-reactors.
Journal of Chemical Physics. 122 (1), 014307 (2005).
19. Roithová Jana, Schröder D., Schwarz H.
Decomposition of neutral, singly, and doubly protonated benzoquinone in the gas phase.
Chemistry - A European Journal. 11 (13), 628-638 (2005).
20. Roithová Jana, Schröder D., Schwarz H.
Unimolecular fragmentation of CH_3NH_2 : Towards a mechanistic description of HCN formation.
European Journal of Organic Chemistry. 15, 3304-3313 (2005).

21. Schraml J., Tkadlecová M., Pataridis S., Soukupová L., Blechta V., Roithová Jana, Exner O.
Ring-Substituted Benzohydroxamic Acids: ¹H, ¹³C and ¹⁵N NMR Spectra and NHOH Proton Exchange.
Magnetic Resonance in Chemistry. 43 (7), 535-542 (2005).
22. Marešová V., Hampl J., Chundela Z., Zrcek F., Polášek Miroslav, Chadt J.
The identification of a chlorinated MDMA.
Journal of Analytical Toxicology. 29 (5), 353-358 (2005).
23. Yao Ch., Cuadrado-Peinado M. L., Polášek Miroslav, Tureček F.
Specific generation of 1-methylcytosine radicals in the gas phase.
Angewandte Chemie. International Edition in English. 44 (41), 6708-6711 (2005).
24. Polášek Miroslav, Kaczorowska Malgorzata, Hrušák Jan
Iso-nitrous acid radical cation in the gas phase: first experimental evidence.
Chemical Physics Letters. 402 (1-3), 138-142 (2005).
25. Yao Ch., Cuadrado-Peinado M. L., Polášek Miroslav, Tureček F.
Gas-phase tautomers of protonated 1-methylcytosine. Preparation, energetics, and dissociation mechanisms.
Journal of Mass Spectrometry. 40, 1417-1428 (2005).
26. Asghar R. B., Diskin A. M., Španěl Patrik, Smith D., Davis S. J.
Influence of convection on the diffusive transport and sieving of water and small solutes across the peritoneal membrane.
Journal of the American Society of Nephrology. 16 (2), 437-443 (2005).
27. Dryahina Kseniya, Španěl Patrik
A convenient method for calculation of ionic diffusion coefficients for accurate selected ion flow tube mass spectrometry, SIFT-MS.
International Journal of Mass Spectrometry. 244 (2-3), 148-154 (2005).
28. Smith D., Španěl Patrik
Selected ion flow tube mass spectrometry (SIFT-MS) for on-line trace gas analysis.
Mass Spectrometry Reviews. 24 , 661-700 (2005).
29. Smith D., Španěl Patrik
Selected ion flow tube mass spectrometry (sift-MS) for on-line trace gas analysis.
Mass Spectrometry Reviews. 24 (5), 661-700 (2005).
30. Španěl Patrik, Wang T., Smith D.
Coordinated FA-MS and SIFT-MS analyses of breath following ingestion of D₂O and ethanol; total body water, dispersal kinetics and ethanol metabolism.
Physiological Measurement. 26 (4), 447-457 (2005).
31. Engel B., Španěl Patrik, Smith D., Diskin A. M., Davis S. J.
Longitudinal measurements of total body water and body composition in healthy volunteers by online breath deuterium measurement and other near-subject methods.
International Journal of Body Composition Research. 2 (3), 99-106 (2005).

32. Baše T., Bastl Zdeněk, Plzák Z., Grygar T., Plešek J., Carr M.J., Malina V., Šubrt J., Boháček J., Večerníková E., Kříž O.
Carboranethiol-modified gold surfaces. A study and comparison of modified cluster and flat surfaces
Langmuir 21(17), 7776-7785 (2005).
33. Dřínek V., Vacek K., Yuzhakov G., Bastl Zdeněk
Interaction between the Silyl and Silylen Centres in the Deposits Prepared by Pulsed Laser Ablation of Silicon Monoxide and Ammonia, Methylamine and Dimethylamine.
Applied Physics A-Materials Science and Processing. 81 (5), 1019-1023 (2005).
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IR laser ablative desulfurization of poly (1,4-phenylene sulfide).
Journal of Analytical and Applied Pyrolysis. 73 (1), 145-149 (2005).
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Thermal Behaviour of Polyoxocarbosilane Shells in Fe-based (core) – Polyoxocarbosilane (Shell) Nanocomposites.
Thermochimica Acta. 439 (1-2), 80-85 (2005).
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Electrocatalytic properties of polypyrrole films prepared with platinate(II) counter-ions.
Synthetic Metals. 155, 501-508 (2005).
37. Melegy A. A., Ismael I. S., Bastl Zdeněk
A comparative study of the adsorbed Pb(II), Cd (II) and Zn (II) on smectite, kaolinite and illite using XPS.
Erzmetall. 58, 283-290 (2005).
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N₂ Laser-induced Formation of Copolymeric Ultrafine Particles in a Gaseous Tetraethenylgermane - Carbon Disulfide Mixture.
Journal of Photochemistry and Photobiology. A - Chemistry Section. 171 (1), 21-26 (2005).
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Solution Photolysis of Ferrocene into Fe-Based Nanoparticles.
Journal of Photochemistry and Photobiology. A - Chemistry Section. 171, 251-256 (2005).
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IR Laser Production of Nano-Structured Polyborocarbosiloxane Powders with Si-O-B Bonds.
Solid State Sciences. 59, 123-131 (2005).
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Infrared Laser Synthesis and Properties of Magnetic Nano-Iron-Polyoxocarbosilane Composites. *Applied Organometallic Chemistry*. 205 (19), 1015-1021 (2005).

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4.4. Contributions in Monographs

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4.5. Popularization Papers

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Chemical Physics in the J. Heyrovský Institute of Physical Chemistry of the Academy of Sciences of the Czech Republic (inCzech).
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2. Záliš Stanislav, Šebera, Jakub, Vlček Antonín Jr.
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Čs. čas. fyz. 55, 6, p. 588-591 (2005).
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Ion chemistry in gas phase and in collisions with surfaces(inCzech).
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4. Fárník Michal
Experiments with clusters in the molecular beams (inCzech).
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5. Votava Ondřej
Experimental studies of free radicals and other unstable molecules (inCzech).
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7. Plšek Jan, Knor Zlatko
Surface physics and chemistry at the atomic scale (inCzech).
Čs. čas. fyz. 55, 6, p. 611-614 (2005).
8. Janda Pavel, Pelouchová Hana
Scanning probe microscopy and its application for characterization of phenomena on solid/liquid interface (inCzech).
Čs. čas. fyz. 55, 6, p. 614-617 (2005).
9. Hof Martin, Benda Aleš, Sýkora Jan
Fluorescence correlation spectroscopy and its new applications in the biological science (inCzech).
Čs. čas. fyz. 55, 6, p. 617-620 (2005).
10. Bastl Zdeněk
Study of thin layers and solid surfaces by electron spectroscopy methods (inCzech)..
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11. Zahradník Rudolf
Mutual approach between/among natural science (inCzech).
Čs. čas. fyz. 55, 5, 639-642 (2005).
12. Těšínská E., Dolejšek Zdeněk, Heyrovský Michael, Rotter M.
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4.6. Further Major Activities in the Popularization of Science

- a) A broadcast relation of Purkyně Fellow Dr. Michal Fárník on the chemistry of clusters in molecular beams in Program "Science and Technique" in Czech Radio (December 7, 2005).
- b) Interview of Dr. Roman Čurík, laureate O. Wichterle prize 2005, in "Studio 24" in Czech television (June 22, 2005).
- c) Relation "Fast electrons" (theoretical chemistry) in the program Czech Head in Czech television (December 16, 2005)
- d) Visit of 10 students of the Prague Institute of chemical technology (May 2, 2005).
- e) Open Door Days for the public on November 10 and 11, 2005 (165 visitors).
- f) "Miraculous world of molecules" - cycle of 7 popularization lectures on chemical physics for 172 secondary school students (November 10, 2005).
- g) Informative seminar for 35 secondary school teachers given by 5 scientist on new methods and techniques in chemical physics and electrochemistry (April 27, 2005).
- h) Festive presentation of awards to the winners of competitions for secondary school students in professional disciplines on December 21, 2005.

5. LECTURES AND SEMINARS

Lectures and seminars organized in the Institute included

- annual Brdička Lecture,
- annual Student Seminar,
- institute seminars,
- seminars of individual departments.

5.1. Brdička Lecture

The Institute has organized since 1991 annually a festive lecture to commemorate Professor Rudolf Brdička (1906-1970), the founder and director of one of the constituent parts of the present Institute. Invited speakers have been outstanding internationally recognized scientists active in some field related to the research currently pursued in the Institute.

The 15th Brdička Lecture entitled

“Supramolecular Entities Based on Molecular Sieves for Catalysis and Synthesis of New Materials ”

was delivered on 23 June 2005 by Prof. Dr. **Avelino Corma Canos** of Instituto de Tecnología Química, Valencia.

5.2. Annual Student Seminar

The annual seminar of Ph.D. students and advanced undergraduates working on their diploma theses under supervision of researchers from our institute took place in Třešť from 27 to 29 June. Contributions were presented by 18 Ph.D. students and 5 undergraduates. Each student was awarded by a financial premium according to the performance shown.

5.3. Institute Seminars

Eight Institute seminars were presented in 2005, four of them held by members of the Institute, two by speakers from other domestic institutions and two from abroad.

20.01.	R. Zahradník <i>Heyrovský Institute</i>	Outlook of theory in chemistry, about the way to infinity and why MgO is (probably) red
17.02.	K. Bouzek <i>Prague Institute of Chemical Technology</i>	Electrochemistry in environmental protection – real alternative?
10.03.	O. Votava <i>Heyrovský Institute</i>	Spectroscopy of unstable particles in supersonic expansion
14.04.	V. Pačes <i>Institute of molecular genetics of AS CR</i>	New approaches to the origin of life
05.05.	J. Roithová <i>Heyrovský Institute</i>	Chemistry in gas phase (Tasks of physical organic chemistry solved by mass spectrometry combined with computational chemistry)
06.10.	B. Speiser <i>University in Tübingen</i>	Molecular electrochemistry in small dimensions - combinatorial microelectrochemistry and redox-active silica nanoparticles
22.11.	J. Vacek <i>Institute of organic chemistry and biochemistry AS CR and University of Boulder</i>	Molecular dynamics of large systems: From biomolecules to nanostructured materials
	J. Chocholoušová <i>Institute of organic chemistry and biochemistry AS CR and Michigan State University</i>	
01.12.	M. Kočířík <i>Heyrovský Institute</i>	Journey to reactors with membrane separation function

5.4. Seminars of Individual Departments

54 seminars were held in the individual departments by members of the Institute and by hosted speakers both from domestic and foreign institutions.

Table 5.1. Synopsis of Departmental Seminars

Department	Seminars given by			Total
	internal speakers	hosted speakers from CR from abroad		
Theoretical Chemistry, Chemical Physics, Biophysical Chemistry	6	0	14	20
Catalysis I and II	16	1	6	23
Electrochemistry	10	0	1	12

**DEPARTMENT OF THEORETICAL CHEMISTRY; CHEMICAL PHYSICS;
BIOPHYSICAL CHEMISTRY**

Internal speakers

04.04.	Jana Roithová	Redox-active ligands: from fundamental aspects to biorelevant studies
02.05.	Štěpán Urban	Doppler limited and sub-Doppler millimetre wave spectroscopy in Prague
10.11.	T. Navrátil	DNA damage detected by electrochemical methods
08.12.	T. Král	DNA condensation studied by single molecule fluorescence
13.12.	J.Roithová	New approaches to polyaromatic hydrocarbons in interstellar space
	M.Fárník	Experiments with clusters in molecular beams

Hosted speakers

25.02.	D. Field <i>Aarhus University, Denmark</i>	Low energy electron-molecule collisions
11.04.	M. Saniga <i>Astronomical Institute, Slovak Academy of Sciences</i>	A Geometrical Chart of Mental Space-Time
18.04.	D. Schröder <i>Technical University of Berlin</i>	How to activate 'inert' molecules? Reactivity-tuning by ligands effect

16.05.	H. Kang <i>Seoul National University, South Korea</i>	Reactive scattering of low-energy Cs ⁺ ions from surfaces and applications to surface and ice chemistry
23.05.	K. H. Hoffmann <i>Technical University Chemnitz</i>	Recent developments in finite time thermodynamics
26.05.	J. Kohno <i>Genesis Research Institute Tokyo, Japan</i>	Isolation of liquid molecules into gas phase: laser ablation of liquid beam and liquid droplet
26.05.	H. Willner <i>Bergische Universität, Wuppertal</i>	Reactive intermediates in the atmospheric depletion of CFC replacements
02.06.	F.E. Harris <i>University of Utah</i>	New life for old few-body systems
06.06.	I. Hertel <i>Max Born Institute for Nonlinear optics and short pulse spectroscopy, Berlin</i>	Laser induced, ultrafast physics and chemistry in large finite molecular systems
09.09.	H. Ohtaki <i>Ritsumeikan University, Kusatsu, Japan</i>	Preferential solvation of ions in mixed solvents
14.09.	U. Buck <i>Max-Planck-Institute, Goettingen</i>	Size selective spectroscopy of hydrogen bonded system
10.10.	S. P.A. Sauer <i>University of Copenhagen, Denmark and Max-Planck-Institut für Kohlenforschung, Germany</i>	Ab Initio calculations of NMR spin-spin coupling constants using the SOPPA method
20.10.	R. Richter <i>University of Heidelberg</i>	The formation of supported lipid bilayers – a study combining AFM and QMC-D
21.11.	F. Tureček <i>University of Seattle, Washington USA</i>	Soft and reactive landing of biomolecular ions: Preparative mass spectrometry

DEPARTMENT OF CATALYSIS I AND II

Internal speakers

1.01.	L. Čapek	Metallozeolites for selective reduction of NO to nitrogen for diesel engines
18.01.	M. Kočířík A. Zikánová	Semi-open Wicke-Kallenbach diffusion cell and possibilities of its application in investigations of membranes, adsorbents and catalysts

08.03.	J. Čejka	New trends in synthesis of molecular sieves
22.03.	B. Wichterlová	EU Project – NO _x reduction on oxidic and zeolitic catalysts for diesel exhalates abatement
05.04.	P. Hrabánek	Synthesis and characterization of zeolitic membranes – PhD study
26.04.	L. Lukešová	Reactivity of silyl-substituted titanocenes – PhD study
10.05.	J. Rathouský	Modified mesoporous films
17.05.	A. Zukal	Mesoporous TiO ₂ films: synthesis and characterization
24.05.	P. Sazama	Reduction of NO _x by hydrocarbons over Ag-zeolites and Ag-alumina – PhD study
31.05.	K. Kovandová-Juristová	Preparation and characterization of inorganic membranes – PhD study
14.06.	K. Novoveská	Oxidative dehydrogenation and ammoxidation of low paraffins over metallozeolites
18.10	J. Dědeček	Progress in MAS NMR of zeolites
01.11.	A. Zukal	Investigation of micro and mesoporosity in composites
22.11.	L. Brabec	Topological study of crystals of Silicalite-1
13.12.	D. Kaucký K. Jíša	Non-stationary effects in N ₂ O decomposition over Fe-zeolites

Hosted speakers

11.05.	R. Moris <i>University of St. Adrews, Scotlandu</i>	Ionic liquid and medical materials: New synthesis methodologies and applications of zeolites
19.05.	P. Meunier <i>University of Bourgogne, Dijon</i>	Ferrocenic phosphines: fascinating new results in NMR spectroscopy and catalysis
23.09.	R. Schoonheydt <i>Catholic University Leuven, Belgium</i>	Probing the basicity of zeolites: Theory and experiment
26.09.	Mladen Eic <i>University of New Brunswick, Canada</i>	Diffusion of selected hydrocarbons in bi-porous mesostructured silica SBA-15
05.10.	N. Seaton <i>University of Edinburgh, GB</i>	Molecular simulation and the design of nanoporous materials

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|--------|----------------------------------|---|
| 06.12. | J. Merna
<i>VUT Brno</i> | Alkene polymerizations catalyzed by di-imine complexes of nickel |
| 08.12. | S. Miachon
<i>CNRS France</i> | Nanocomposite MFI-alumina membranes. Preparation, characterization and transport properties |

DEPARTMENT OF ELECTROCHEMISTRY**Internal speakers**

- | | | |
|--------|------------|---|
| 28.01. | S.Záliš | DFT models of metallic clusters and their interactions with organic molecules |
| 11.01. | L.Pospíšil | Redox processes of complex cyclodextrins |
| 25.02. | J.Ludvík | Electron delocalization in carbene complexes |
| 25.03. | P.Krtíl | Application of DEMS for identification of the products of electrolysis |
| 08.04. | Z.Samec | Electrochemical processes on metallic clusters located on HOPG |
| 22.04. | J.Hlavatý | Electrochemical oxidation of butynediols |
| 13.05. | J. Klíma | Problem of distribution of ultrasonic intensity in sonochemistry and sonoelectrochemistry |
| 20.05. | V. Mareček | Progress in electrochemistry of surface layers on liquid interface |
| 04.11. | Z. Samec | Metal extraction on polarized liquid interfaces |
| 16.05. | M. Gál | Pharmaceutical supports and electrochemistry |

Hosted speakers

- | | | |
|--------|---|---|
| 02.05. | F. G. Batanica
<i>NTNU Trondheim</i> | Electrochemistry of carotenoids in the form of self-assembled monolayer at gold surface |
|--------|---|---|

6. INTERNATIONAL CONTACTS

6.1. Synopsis

The Institute was collaborating with several dozens of foreign universities and research institutions within the framework of multilateral research networks and bilateral agreements (Chap. 3).

Members of the Institute 117 joint papers jointly with authors from institutions abroad (Chap. 4).

The Institute functioned as Marie Curie Training Site of EC in synthesis of porous materials for adsorption applications (*INDENS*); and as a member of Research Training Networks of EC concerning electron and positron induced chemistry (*EPIC*)

Visitors from abroad gave 24 lectures and seminars in the Institute (Chap. 5). The Institute organized 8 international conferences (Sect. 6.3). Members of the Institute acted in editorial or advisory boards of scientific periodicals and in international scientific organizations and bodies (Chap. 8).

6.2. Working Stays

Of several tens of visitors from abroad, 18 spent 30 days or more at the Institute working on joint projects (Table 6.1.).

Table 6.1. Working stays of researchers from abroad in 2005 (30 days or longer)

Name	Country	Lenght (days)	Host	Department
<u><i>Theoretical Chemistry</i></u>				
V. Brems	Germany	365	P. Čársky	
J. Michl	U.S.A.	30	P. Čársky	
M. Tarana	Slovakia	61	P. Čársky	
<u><i>Chemical Physics</i></u>				
J. Dmytrzyk	Poland	78	Z. Bastl	
J. Polyak	Ukraine	122	Z. Bastl	
V. Poterya	Ukraine	39	M. Fárník	
A. Pysanenko	Ukradne	365	Z. Herman	
S. Vanhersecke	France	43	Z. Zelinger	
<u><i>Biophysical Chemistry</i></u>				
T. Borowik	Poland	30	M. Hof	
P. Jurkiewicz	Poland	164	M. Hof	
T. Kral	Poland	162	M. Hof	
M. Przbylo	Poland	30	M. Hof	
<u><i>Catalysis I</i></u>				
D. Rohlfing- Fattakhova	Russia	42	J. Rathouský	
A. Wegrzynowicz	Poland	32	M. Kočířík	
<u><i>Catalysis II</i></u>				
J. Pawlesa	Poland	334	J. Čejka	
<u><i>Electrochemistry</i></u>				
A. Korshunov	Russia	87	M. Heyrovský	
M. Makarova	Russia	365	P. Krtíl	
B. Ouarda	Algeria	108	J. Jirkovský	

6.3. International Scientific Meetings Arranged by the Institute

1. European Winter School on Theoretical Methods for EPIC (Electron and Positron Induced Chemistry)
Prague, 14–18 February 2005, organizers R. Čurík and V. Brems.
19 participants including 14 from abroad.
2. 25th International Seminar on Modern Electrochemical Methods
Jetřichovice, 23-26 May 2005, co-organizer T. Navrátil.
55 participants including 5 from abroad.
3. 38th Heyrovský Discussion "Electrocatalysis in nanoscale"
Trešř near Jihlava, 12 – 16 June 2005, organizers Z. Samec and P. Krtil.
38 participants including 27 from abroad.
4. 1st FEZA School on Zeolites
Prague, 21-23 August 2005, organizer J. Čejka.
102 participants including 84 from abroad.
5. 3rd International FEZA Conference
Prague, 23-26 August 2005, organizer J. Čejka.
417 participants including 389 from abroad.
6. 37th Symposium on Catalysis
Prague, 7 –8 November 2005, organizer J. Čejka.
90 participants including 18 from abroad.
7. Electrochemical Seminar Prague-Dresden
Roztoky near Křivoklát, 21-23 November 2005, organizers P. Janda and J. Ludvík.
35 participants including 16 from abroad.
8. COST D32/004/04 Working Group Meeting
Prague, 24-26 November 2005, organizers J. Klíma and J. Ludvík.
13 participants including 7 from abroad.

7. COOPERATION WITH UNIVERSITIES IN THE CZECH REPUBLIC

Acronyms used:

CU – MED	Charles University, Prague, 1 st Faculty of Medicine
CU – SCI	Charles University, Prague, Faculty of Science
CUA – AGR	Czech University of Agriculture, Prague, Faculty of Agronomy
CTU – NUC	Czech Technical University, Prague, Faculty of Nuclear Physics and Engineering
ICHT – ENG	Institute of Chemical Technology, Prague, Faculty of Chemical Engineering
ICHT – ENV	Institute of Chemical Technology, Prague, Faculty of Environmental Technology
ICHT – TEC	Institute of Chemical Technology, Prague, Faculty of Chemical Technology
MU – SCI	Masaryk University, Brno, Faculty of Science
PU – SCI	Palacký University, Olomouc, Faculty of Science
UPAR – TEC	University of Pardubice, Faculty of Chemical Technology

7.1. Lecture Courses for Undergraduates and Ph.D. Students

Synopsis:

Semester	Number of courses	Hours per semester
Summer 2005	10	219
Winter 2005	14	349
Total	24	558

Number of lecturers from the Institute: 15

Number of faculties involved: 10

**DEPARTMENT OF THEORETICAL CHEMISTRY, CHEMICAL PHYSICS
AND BIOPHYSICAL CHEMISTRY**

Lecturer	Lecture course	Faculty	Semester	Hours
S. CIVIŠ	<i>Spectroscopic analytical methods: Laser analytical spectroscopy</i>	CU - SCI	W	14
P. ČÁRSKY (WITH J. FIŠER, CU – SCI)	<i>Chemical structure</i>	CU – SCI	W	26
Z. HERMAN	<i>Theoretical reaction kinetics</i>	ICHT – TEC	S	15
M. HOF	<i>Molecular physics</i>	CTU – NUC	S	30
M. HOF	<i>Fluorescence Spectroscopy principals and biological applications</i>	CTU – NUC	S	15
M. HOF	<i>Spectroscopy</i>	PU-SCI	W	30
J. PITTNER	<i>Theoretical and computational chemistry</i>	CU – SCI	S	14
J. PITTNER	<i>Introduction to density functional method</i>	CU – SCI	W	14
Š. URBAN	<i>Selected chapters of chemical physics</i>	ICHT – ENG	W	34
Š. URBAN	<i>Molecular spectroscopy</i>	ICHT – ENG	S	34

DEPARTMENT OF CATALYSIS I AND II

Lecturer	Lecture course	Faculty	Semester	Hours
J. ČEJKA	<i>Principles and methods of heterogeneous catalysis</i>	ICHT – TEC	W	30
J. ČEJKA	<i>Zeolites and microporous inorganic materials: synthesis, structure, characterization and application</i>	ICHT – TEC	W	30

J. ČEJKA (WITH J.VOHLÍDAL)	<i>Chemical principles of industrial manufacturing</i>	CU – SCI	W	45
Z. SOBALÍK	<i>Spectroscopical characterization of heterogeneous catalysts</i>	ICHT – TEC	S	25
B.WICHTERLOVÁ	<i>Adsorption and catalysis</i>	ICHT – TEC UPAR-TEC	S	24

DEPARTMENT OF ELECTROCHEMISTRY

Lecturer	Lecture course	Faculty	Semester	Hours
L. KAVAN	<i>Selected spectral methods</i>	CU – SCI	W	28
L. KAVAN	<i>Selected spectral methods</i>	CU – SCI	S	28
J. LUDVÍK	<i>Electrochemistry</i>	ICHT – ENG	W	42
T. NAVRÁTIL	<i>Medical chemistry and electrochemistry</i>	CU – MED	W	26
L. POSPÍŠIL	<i>Physical chemistry and electrochemistry</i>	ICHT – ENV	S	16
Z. SAMEC	<i>Physical chemistry II: Electrochemistry</i>	CU – SCI	S	18
I. ŠESTÁKOVÁ	<i>Environmental and analytical chemistry (within the course "Special analytical chemistry")</i>	CUA – AGR	W	2
I. ŠESTÁKOVÁ	<i>Electroanalytical methods</i>	CUA – AGR	W	4
I. ŠESTÁKOVÁ	<i>Electrochemical methods</i>	CUA – AGR	W	24

7. 2. Training Courses for Undergraduates

Synopsis:

Semester	Number of courses	Hours per semester
		257
Summer 2005	13	
Winter 2005	8	82
Total	21	339

Number of course leaders from the Institute: 15

Number of faculties involved: 7

**DEPARTMENT OF THEORETICAL CHEMISTRY, CHEMICAL PHYSICS
AND BIOPHYSICAL CHEMISTRY**

Course leader	Training course	Faculty	Semester	Hours
Z. BASTL	<i>Electron spectroscopy</i>	CU – SCI	S	10
Z. BASTL, I. SPIROVOVÁ	<i>Photoelectron spectroscopy</i>	CU – SCI	W	5
P. KUBÁT	<i>Laser spectroscopy</i>	CU – SCI	W	10
J. PITTNER	<i>Theoretical and computational chemistry</i>	CU – SCI	S	14
J. PITTNER	<i>Structure of molecules</i>	CU – SCI	W	26
J. PITTNER	<i>Introduction to density functional method</i>	CU – SCI	W	14
Š. URBAN	<i>Selected chapters of molecular physics</i>	ICHT – ENG	W	17
Š. URBAN	<i>Molecular spectroscopy</i>	ICHT – ENG	S	17
Z. ZELINGER	<i>Spectroscopic methods for investigation of atmospheric pollution</i>	CU – SCI	S	20
J. ŽABKA	<i>Basic course of Physics</i>	ICHT – TEC	S	24
J. ŽABKA	<i>Basic course of Physics</i>	ICHT – FBT	S	24

DEPARTMENT OF CATALYSIS I AND II

Course leader	Training course	Faculty	Semester	Hours
L. BRABEC	<i>Scanning electron microscopy</i>	CTU – NUC	S	2
L. BRABEC	<i>Electron microscopy</i>	CU – SCI	W	4
K. MACH	<i>Electron spin resonance</i>	CTU – NUC	S	6
J. NOVÁKOVÁ	<i>Intermediates in catalytic reactions: Application of stable isotopes</i>	CTU – NUC	S	6
Z. SOBALÍK	<i>FTIR spectroscopy in study of catalysis</i>	CTU – NUC	S	6
B. WICHTERLOVÁ	<i>Kinetics of heterogeneous catalytic reactions</i>	CTU – NUC	S	6

DEPARTMENT OF ELECTROCHEMISTRY

Course leader	Training course	Faculty	Semester	Hours
T. NAVRÁTIL	<i>Electrochemical methods in medical chemistry and biochemistry</i>	CU – SCI	S	40
T. NAVRÁTIL	<i>Medical chemistry and biochemistry</i>	CU – MED	S	21
I. ŠESTÁKOVÁ	<i>Electrochemical methods</i>	CUA – AGR	W	2
J. LUDVÍK	<i>Electrogenerated chemiluminescence</i>	CU – SCI	W	4

7.4. Supervision of Theses

59 Ph.D. Theses and 8 Diploma Theses were supervised by members of the Institute's staff, in most cases jointly with teachers at universities.

16 undergraduates participated for different periods of time in the work of the Institute as auxiliary research assistants.

Supervised Ph.D. Theses

DEPARTMENT OF THEORETICAL CHEMISTRY, CHEMICAL PHYSICS
AND BIOPHYSICAL CHEMISTRY

Student	Faculty	Thesis title	Supervisor in the Institute	Start	Remark
P. Kania	ICT-ENG	Rotation spectroscopy of atmospherically important molecules	Š. Urban	2001	
D. Babánková	CU-SCI	Application of high-power lasers	S. Civiš	2001	
V. Horká	CU-SCI	Application of laser diodes in spectroscopy	S. Civiš	2001	Defended in 2005
J. Sýkora	CU-SCI	Solvent relaxation in biomolecules	M. Hof	2002	Defended in 2005
A. Benda	CU-SCI	Single molecule spectroscopy on biomembranes and their model systems	M. Hof	2002	
J. Humpolíčková	CU-SCI	Determination of fluorescence lifetimes in single macromolecular assemblies	M. Hof	2002	
O. Demel	CU-SCI	Development and application of the MRBWCC method with inclusion of connected triplets	J. Pittner	2002	
K. Bezpalcová	CU-MAT	Physical modelling of streaming and diffusion in urban agglomeration	Z. Zelinger	2002	
M. Novotný	CTU-NUC	Spectroscopic methods in new laser hybrid technologies	Z. Zelinger	2003	
K. Dryahina	CU-MAT	Studies of ion-molecules processes	P. Španěl	2003	
J. Šmydke	CU-MAT	Analytical gradient for the multireference Brillouin-Wigner Coupled Cluster Method	J. Pittner P. Čársky	2003	
L. Stříteská	ICT-ENG	Effect of intermolecular interactions on the molecule geometry studied by rotation spectroscopy	Š. Urban	2003	
J. Cihelka	CU-SCI	Laser spectroscopy	S. Civiš	2004	

A. Miszta	CU–SCI	Fluorescence microscopy and ellipsometry applied to model and cell membranes	M. Hof	2004
A. Olzyńska	CU–SCI	Solvent relaxation technique applied in the development of non-viral drug carriers	M. Hof	2004
J. Barucha	CU-SCI	Application of solvent relaxation in characterization of protein membrane interaction	M.Hof	2005
B. Gasinska	CU-SCI	Application of fluorescence correlation spectroscopy in development of carriers for gene therapy	M.Hof	2005
A. Zan	CU-SCI	Single molecule fluorescence spectroscopy in vitro and in vivo	M.Hof	2005
J. Brabec	CU -MAT	Development and application of CC and DFT methods	J.Pittner	2005
B. Nair Kiran	CU-SCI	Mutireference-Brillouin-Wigner-Coupled-Cluster calculation of titanocene systems	J.Pittner	2005

DEPARTMENT OF CATALYSIS I AND II

Student	Faculty	Thesis title	Supervisor in the Institute	Start	Remark
M. Boldiš	ICHT–BIO	Application of molecular sieves to isolation of fermentation products	M. Kočířik	2000	
P. Hrabánek	ICHT–TEC	Study of permeation and separation properties in coherence with application in membrane reactors	A. Zikánová	2000	Defended in 2005
M. Slabová – Staňková	ICHT–ENG	Highly ordered nanostructures of titanium dioxide	A. Zukal	2000	Terminated in 2005
V. Kreibich	ICHT–TEC	Structural chemistry of zeolite catalysts and redox catalysis	B. Wichterlová	2000	
L. Lukešová	CU–SCI	Titanocene catalysts for olefin polymeration	K. Mach	2000	Defended in 2005
P. Mokrejš	CU–SCI	Interaction of bentonites with surroundings in dependence on the bentonite history and	A. Zikánová	2000	Defended in 2005

		actual physico-chemical conditions			
H. Jirglová	ICHT-ENG	Adsorption equilibria, sorption kinetics and dynamics of polydisperse structure materials	M. Kočířik	2001	
V. Gábová	ICHT-TEC	Al distribution in aluminosilica-based high-silica molecular sieves	J. Dědeček	2001	Defended in 2005
K. Kovan- dová-Juristová	ICHT-TEC	Preparation and characterization of SiO ₂ -based microporous membrane materials for application in separation technologies and catalysis	A. Zikánová	2001	
G. Košová	ICHT-TEC	Synthesis of zeolite catalysts for selective reactions of heterocycles	J. Čejka	2001	Defended in 2005
K. Novoveská	UPAR- TEC	Selective oxidation of alkanes	B. Wichterlová	2001	
P. Prokešová	ICHT-TEC	Synthesis of zeolite – based composite materials for catalytic applications	J. Čejka	2001	Defended in 2005
O. Gonsiorová	ICHT-TEC	Synthesis and post-synthesis modifications of zeolites	B. Wichterlová	2001	
M. Schwarze	CU-SCI	Redox catalysis on molecular sieves	Z. Sobalík	2001	
P. Sazama	UPAR- TEC	Acidobasic transformations of hydrocarbons on zeolites	B. Wichterlová	2001	Defended in 2005
M. Fryčová- Šnáblová	ICHT-TEC	Polymer – loaded solvents	M. Kočířik	2002	
J. Mayerová- Klisáková	ICHT-TEC	Synthesis of zeolite catalysts for acylation reactions	J. Čejka	2002	
M. Zukalová	CU-SCI	Titanium oxide-based organized nanostructure materials	J. Rathouský	2002	
R. Hamtil	ICHT – TEC	Heterogeneous catalysts for olefin metathesis based on mesoporous molecular sieves	H. Balcar	2002	
I. Nekoksová	ICHT-TEC	Synthesis of zeolite catalysts on molecular sieves	J. Čejka	2003	
P. Topka	ICHT - TEC	Molecular sieves for olefin metathesis	J. Čejka	2003	

Z. Pavlačková	UPAR-TEC	Zeolite-based composite catalysts for transformations of aromatics	J. Čejka	2004	
K. Jíša	UPAR-TEC	Redox catalysis on zeolites in dynamical regime	Z. Sobalík	2004	
K. Nahrabec-ký	UPAR	Catalytic CO ₂ activation in chemical synthesis	Z. Sobalík	2004	Terminated in 2005
T. Trávníček	UPAR	Relation of catalytic activity of zeolites with transition metal cations	Z. Sobalík	2004	Terminated in 2005
J. Demel	CU-SCI	Immobilized palladium catalysts	J. Čejka	2005	
J. Pawlesa	ICHT-FCHT	Zeolite synthesis for adsorption applications	J. Čejka	2005	

DEPARTMENT OF ELECTROCHEMISTRY

Student	Faculty	Thesis title	Supervisor in the Institute	Start	Remark
V. Dorčák	CUA-AGR	Application of electrochemical methods to the study of plant metallothioneins and their complexes with heavy metals	I. Šestáková	1999	
J. Pícha	ICHT-TEC	Synthesis of aryl-methylketoximes and study of their properties	J. Ludvík	1999	Defended in 2005
H. Hoffmannová	ICHT-ENG	Study of electrochemically initiated intermediates	P. Krtíl	2000	Defended in 2005
D. Rozbroj	ICHT-ENG	Electrochemical study of azo-methine bonds	J. Ludvík	2001	
P. Čížková	CUA-AGR	Application of electrochemical techniques to the study of uptake and metabolism of heavy metals in plants	J. Šestáková	2001	
T. Kotrba	ICHT-ENG	Quantum chemical calculations of spectroscopic parameters of molecules	S. Záliš	2002	
J. Jirkovský	ICHT-TEC	In-situ Spectroscopic Methods used in Studies of Lithium Insertion into Oxides of Transition Metals	P. Krtíl	2003	

T. Kostlánová	CU-SCI	Solvothermal synthesis on nanocrystalline insertion hosts in Li-Ti-O systems and their electrochemical characterization	P. Krtil	2003
M. Kolář	ICHT-ENG	Pollutant degradation by means of heterogeneous catalysis	J. Jirkovský	2003
J. Šebera	CU - SCI	Quantum chemical interpretation of molecular and complex systems spectra	S. Zálíš	2003
M. Rejňák	ICHT- TEC	Electrochemical study of benzothiophene derivatives	J. Ludvík	2003
P. Mořkovská	UPAR-TEC	Redox reactions inside molecular cavities	L. Pospíšil	2003

7.5. Joint Projects and Publications

Members of the Institute's staff worked on 31 joint grant projects with universities in the Czech Republic (see Sect. 3). In 13 and 18 joint projects they acted as project leaders and associated contractors, respectively.

7.6. Membership in University Bodies

11 scientists of the Institute participated in the work of university bodies as members of Scientific Councils, Branch Councils in Ph.D. study programs, Examining Boards and Appointment Advisory Committees.

DEPARTMENT OF THEORETICAL CHEMISTRY, CHEMICAL PHYSICS AND BIOPHYSICAL CHEMISTRY

- | | |
|------------|---|
| P. Čárský: | ▪ Scientific Council of Technical University Liberec |
| Z. Herman | ▪ Branch Council for Physical Chemistry in the Ph.D. study program "Physical Chemistry" (Fac. Chem. Engng, Institute of Chem. Technol. Prague)
▪ Branch Council for Plasma Physics (Fac. Math. and Physics, Charles University Prague) |
| Š. Urban | ▪ Branch Council for Analytical Chemistry in the Ph.D. study program "Chemistry", Institute of Chem. Technol. Prague
▪ Scientific Council of Fac. Chem. Engng., Institute of Chem. Technol. Prague) |

- Examining Board for state finals (Fac. Chem. Engng, Institute of Chem. Technol. Prague)
 - Examining Board for awarding Ph.D. degrees in physical chemistry (Fac. Chem. Engng, Institute of Chem. Technol. Prague)
- M. Hof
- Branch Council for Physical Chemistry in the Mgr. and Ph.D. study programs "Physical Chemistry" (Nature Science Faculty, University Olomouc)
 - Examining Board for awarding Ph.D. degrees in physical chemistry (Nature Science Faculty, Charles University Prague)

DEPARTMENT OF CATALYSIS I AND II

- J. Čejka
- Branch Council for Organic Technology in the Ph.D. study program "Chemistry and Chemical Technology" (Institute of Chem. Technol. Prague)
- K. Mach
- Branch Council for Inorganic Chemistry in the Ph.D. study program "Inorganic Chemistry" (Fac. Science, Charles Univ.)

DEPARTMENT OF ELECTROCHEMISTRY

- L. Kavan
- Branch Council for Inorganic Chemistry in the Ph.D. study program "Inorganic Chemistry" (Fac. Science, Charles Univ.)
 - Examining Board for state finals in material chemistry (Masaryk University, Brno)
- J. Ludvík
- Examining Board for state finals (Fac. Chem. Engng, Institute of Chem. Technol. Prague)
- V. Mareček
- Scientific Council of Fac. Science, Charles Univ.
 - Branch Council for Ph.D. studies in inorganic technology (Fac. Chem. Technol., Institute of Chem. Technol. Prague)
 - Branch Council for Ph.D. studies in analytical chemistry (Fac. Chem. Engng, Institute of Chem. Technol. Prague)
 - Examining Board for state finals in physical and analytical chemistry (Fac. Science, Charles Univ.)
 - Appointment Advisory Committee (Fac. Science, Charles Univ.)
- L. Pospíšil
- Scientific Council of Fac. Environ. Protection, Institute of Chem. Technol. Prague
 - Appointment Advisory Committee (Fac. Science, Charles Univ.)
- Z. Samec
- Scientific Council of Fac. Chem. Technol., Institute of Chem. Technol. Prague
 - Branch Council for Ph.D. studies in analytical chemistry (Fac. Science, Charles Univ.)
 - Examining Board for state finals in physical chemistry (Fac. Science, Charles Univ.)

8. OTHER ACTIVITIES

8.1. Membership in Editorial or Advisory Boards of Scientific Periodicals

P. Čárský	Theor. Chim. Acta Int. J. Mol. Sci. Collect. Czech. Chem. Commun. J. Comput. Chem.
J. Čejka	Collect. Czech. Chem. Commun.
Z. Herman	Vesmír
M. Hof	J. Fluoresc.
P. Janda	Collect. Czech. Chem. Commun.
L. Kavan	Carbon
K. Mach	Organometallics
K. Micka	J. Power Sources
J. Pittner	Collect. Czech. Chem. Commun.
L. Pospíšil	Collect. Czech. Chem. Commun.
Z. Samec	Electrochim. Acta
A. Vlček	Inorg. Chim. Acta Chemtracts – Inorg.Chem. Coord. Chem. Rev.
J. Volke	Chem. Listy
B. Wichterlová	Catal. Rev. Res. Chem. Intermed.
R. Zahradník	Adv. Quantum Chem. Int. J. Quantum Chem. Chem. Listy Collect. Czech. Chem. Commun.

8.2. Officials and Elected Members of Scientific Organizations and Bodies (except universities - cf. Sect. 7.5.)

DEPARTMENT OF THEORETICAL CHEMISTRY; CHEMICAL PHYSICS;

BIOPHYSICAL CHEMISTRY

- Z. Bastl
- *J.M. Marci Spectroscopical Society* – member of the Committee and chairman of the Photoelectron Spectroscopy Section
 - *The Surface Analysis Society of Japan* – member
- P. Čárský
- *International Academy of Quantum Molecular Sciences* – member
 - *WATOC (World Association of Theoretical Organic Chemists)* – member of the Scientific Council
 - *Learned Society of CR* – member
 - *Czech Chemical Society* – member of the General Committee
 - *Ministry of Education of Slovak Republic, Commission for awarding DrSc. degrees in physical chemistry* – member
 - *American Chemical Society* - member
- Z. Herman
- *MOLEC (International Conference on Molecular Collisions)* – member of the Steering Committee
 - *Czech Chemical Society* – member of the General Committee, chairman of the Group for Chemical Physics
 - *Ministry of Education, Youth and Sports of CR, Advisory Board for funding research and development in natural sciences* – member
 - *Accreditation Committee of the Czech Government* - member of work group for chemistry
- M. Hof
- *Society of Fluorescence* – national representative and member of the Permanent Steering Committee of the Conference “Series on Methods and Applications of Fluorescence: Spectroscopy, Imaging & Probes“
 - *International Scientific Advisory Board of the Academic Center for Biotechnology of Lipid Aggregates in Wroclaw* – member
- J. Hrušák
- *Academic Council of ASCR* – member
- P. Kubát
- *Czech Society for Photobiology and Photodynamical Therapy* – member of the Committee
- J. Pittner
- *Grant Agency of the Academy of Sciences - Sub-council for physical chemistry*- member
- V. Mareček
- *Grant Agency of the Academy of Sciences* – vice-chairman
 - *Learned Society of CR* – member
 - *Ministry of Education of Slovak Republic, Commission for awarding DrSc. degrees in inorganic technology and materials* – member
 - *Academy of Sciences of CR - Commission for awarding DSc. degrees in physical chemistry*– chairman

- *The Electrochemical Society (USA)* – member
 - *International Society of Electrochemistry* – member
- P. Pracna
 - *J.M. Marci Spectroscopical Society* – auditor
- Š. Urban
 - *J.M. Marci Spectroscopical Society* – member of the Committee and chairman of the Molecular Spectroscopy Section
 - *Czech Committee for Collaboration with IIASA (Intern. Committee for Applied System Analysis) at the AS CR* – chairman
 - *IIASA* – member of the Council (chairman of the Membership Committee, member of the Executive Committee and the Program Committee)
- R. Zahradník
 - *Academy of Sciences of CR* – honorary president
 - *Learned Society of CR* – member
 - *International Academy of Quantum Molecular Sciences* – member
 - *European Academy of Arts, Science and Literature (Paris)* – member
 - *European Academy of Sciences and Arts (Salzburg)* – member
 - *Academia Europaea (London)* – member
 - *European Academy for Environmental Affairs* – member
 - *WATOC (World Association of Theoretical Organic Chemists)* – fellow
 - *Swiss Chemical Society* – honorary member
 - *Society of German Chemists* – honorary member
 - *Croatian Academy of Sciences* – corresponding member
 - *Carolinum (Societas alumnorum et amicorum Universitatis Carolinae)* – honorary member

DEPARTMENT OF CATALYSIS I AND II

- J. Čejka
 - *Grant Agency of CR, Sub-council for technical chemistry-* member
 - *Federation of European Zeolite Associations (FEZA)* – member of the Committee
 - *Czech Chemical Society, Group for Catalysis* – member of the Committee
 - *Czech Chemical Society, Czech Zeolite Group* – chairman
- M. Kočířík
 - *IUPAC Commission on Colloid and Surface Chemistry including Catalysis* – national representative
- K. Mach
 - *Royal Society of Chemistry (London)* – fellow
- Z. Sobalík
 - *Czech Chemical Society, Group for Catalysis* – vice-chairman
 - *European Federation of Catalysis Societies (EFCATS)* member of the Board for CR

- B. Wichterlová
- *International Association of Catalysis Societies* – member of the Committee
 - *Czech Chemical Society, Czech Zeolite Group* – member of the Committee
 - *Academy of sciences of CR- member of the Scientific Council*

DEPARTMENT OF ELECTROCHEMISTRY

- L. Kavan
- *Institute of Rock Structure and Mechanics AS CR* – member of the Scientific Council
 - *Czech Chemical Society, Group for Electrochemistry* – member of the Committee
 - *Czech Society for Carbon Materials* – member of the Committee
 - *COST- D35* – member of the management Committee
 - *International Society of Electrochemistry* – member
 - *The Electrochemical Society (USA)* – member
- J. Ludvík
- *Czech Chemical Society, Group for Electrochemistry* – member of the Committee
 - *The Electrochemical Society (USA)* – member
- J. Langmaier
- *The Electrochemical Society (USA)* – member
- L. Pospíšil
- *COST - D15* – member of the Management Committee
 - *ESF Unit for Physical & Engineering Sciences* – expert referee for ESF Eurocores Programme in Self-Organized Nanostructures
- Z. Samec
- *Grant Agency of the Academy of Sciences - Sub-council for physical chemistry-* member
 - *IUPAC Fellow*
 - *International Society of Electrochemistry* – member
 - *The Electrochemical Society (USA)* – member
- A. Vlček
- *European Photochemistry Association* – member of the Executive Committee, member of the Standing Committee
 - *Royal Society of Chemistry* – fellow
 - *COST Action D14 “Functional Molecular Materials”* – vice-chairman of the Management Committee
 - *COST Project D14 “Organometallic and Metallo-organic Building Blocks for Photonic Materials”* – coordinator

8.3. Appointments, Conferments

J. Čejka

Appointment to Professor of Inorganic technology at the Institute of Chemical Technology, Prague

S.Civiš

Appointment to Associate Professor of Analytical Chemistry at the Charles University, Prague

J. Ludvík

Appointment to Associate Professor of Physical Chemistry at the Institute of Chemical Technology, Prague

8.4. Awarded Prizes and Honors

Mgr. Roman Čurík, PhD.

Otto Wichterle Prize

Ing. Pavla Fojtíková - Prokešová

Prize for the 2nd place in the 2005 competition of doctoral dissertations in chemistry in CR, awarded by the French Embassy and the Company Rhodia

Mgr. Veronika Horká, PhD.

Prize for the best thesis (vibrational spectroscopy) in the competition of thesis in Spectroscopy, awarded by the J. M. Marci Spectroscopical Society

Ing. Pavel Hrabánek, PhD.

Prize for the doctoral dissertation in the competition of doctoral dissertations, awarded by the Company Unipetrol, strategic partner of Prague Institute of Chemical Technology

Ing. Kateřina Novoveská

Prize for the 1st place in the 2005 competition of doctoral dissertations in chemistry in CR, awarded by the French Embassy and the Company Rhodia

Ing. Pavel Topka

Prize of the Group for Catalysis of the Czech Chemical Society

R. Zahradník

Doctorat honoris causa Université de Montreal