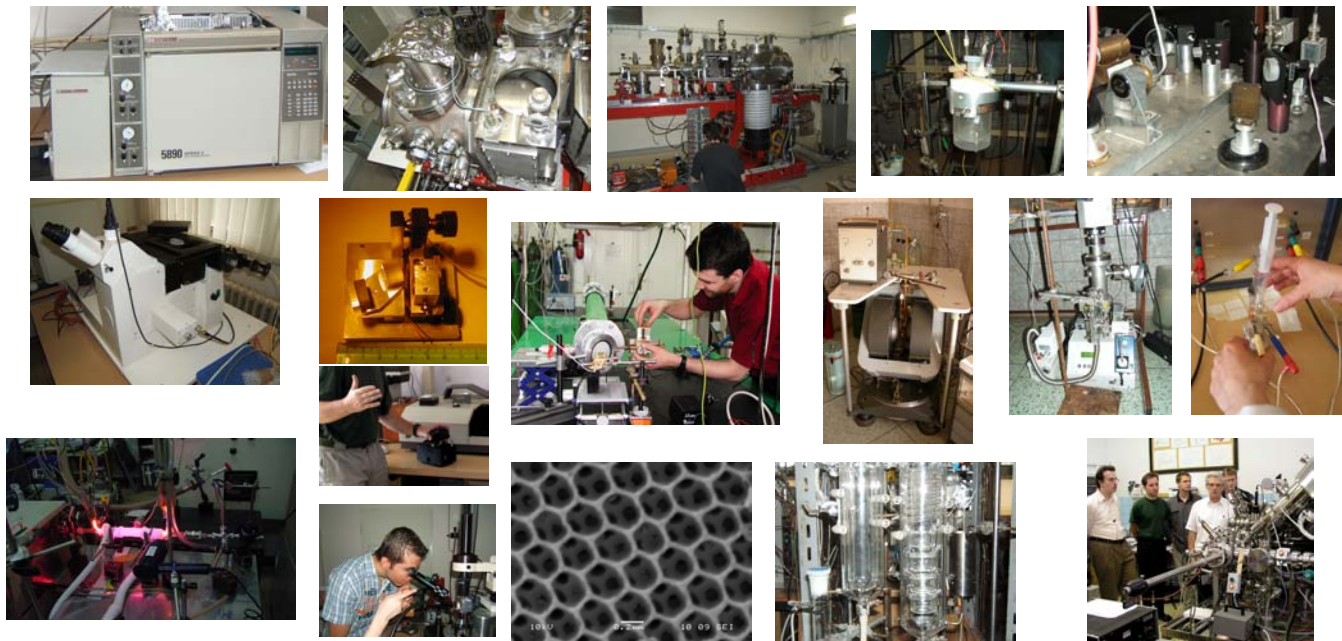


# J. Heyrovský Institute of Physical Chemistry Academy of Sciences of the Czech Republic



# ANNUAL REPORT 2004



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

# Annual Report 2004

**Director:**

Prof. RNDr. Petr Čásky, DrSc.

**Vice-director:**

Prof. Ing. Vladimír Mareček, DrSc.

**Scientific Secretary:**

RNDr. Slavoj Černý, CSc.

**Scientific Council Chairman:**

Doc. Dr.rer.nat. Martin Hof

**Economic Manager:**

Ing. Vladimír Levit

**Technical Manager:**

Ludvík Hoffmann

**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](mailto:director@jh-inst.cas.cz)

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

## CONTENTS

	page
<b>1. BASIC INFORMATION</b> .....	1
1.1. Scope of Activities	
1.2. Most Important Events in 2004	
<b>2. FINANCES</b> .....	2
2.1. Non-investment Means	
2.2. Investment Means	
<b>3. RESEARCH</b> .....	3
Research topics, grant projects, and main results in 2004	
Department of Chemical Physics	
Department of Catalysis	
Department of Electrochemistry	
<b>4. PUBLICATION ACTIVITIES AND POPULARIZATION.</b> . . .	22
4.1. Synopsis of Papers Published in 2004	
4.2. Research Papers in Periodicals	
4.3. Contributions in Conference Materials	
4.4. Contributions in Monographs	
4.5. Patents	
4.6. Popularization Papers	
4.7. Further Major Activities in the Popularization of Science	
4.8. Organization of Local Conferences	
<b>5. LECTURES AND SEMINARS</b> .....	44
5.1. Brdička Lecture	
5.2. Annual Student Seminar	
5.3. Institute Seminars	
5.4. Departmental Seminars	
<b>6. INTERNATIONAL CONTACTS</b> .....	50
6.1. Visitors from Abroad	
6.2. International Scientific Meetings Arranged by the Institute	
<b>7. COOPERATION WITH UNIVERSITIES IN THE CZECH REPUBLIC</b> .....	52
7.1. Lecture Courses for Undergraduates and Ph.D. Students	
7.2. Training Courses for Undergraduates	
7.3. Summer School for Ph.D. Students and Post-docs	
7.4. Supervision of Theses	
7.5. Joint Projects and Publications	
7.6. Membership in University Bodies	
<b>8. OTHER ACTIVITIES</b> .....	65
8.1. Membership in Editorial Boards or Advisory Boards of Scientific Periodicals	
8.2. Officials and Elected Members of Scientific Organizations and Bodies ( <i>except universities – cf. Sect. 7.6.</i> )	
8.3. Appointments, Conferments	
8.4. Awarded Prizes and Honors	

## 1. BASIC INFORMATION

### 1.1. Scope of Activities

During 2004, 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 quantum chemical methods and quantum molecular dynamics. Furthermore, it functioned as a member of IHP Research Training Networks of European Commission *i)* in generation, stability and reaction dynamics of multiply charged ions, and *ii)* in electron and positron induced chemistry.

### 1.2. Most Important Events in 2004

- Successful outcome of the evaluation of the activities, achieved results and plans of the Institute up to the year 2010 by the Evaluation Board of the Academy of Sciences of the Czech Republic.
- Election and appointment of Prof. Petr Čárský to Director of the Institute for the next four-year term effective 1 January 2005.
- Summer school "Spectroscopic methods and their application in catalysis, surface and material science, atmospheric chemistry and biodisciplines" for Ph.D. students and post-doctoral fellows from 29 August through 3 September.
- 14<sup>th</sup> Brdička Memorial Lecture held on 17 June by Nobel Prize winner Prof. Rudolph A. Marcus
- Student Seminar on 22 and 23 June in castle Třešť.

## 2. FINANCES

### 2.1. Non-investment Means

Non-investment financial resources of the Institute in 2004 amounted to 127.074 million CZK (Table 2.1.)

**Table 2.1.** Breakdown of the non-investment funds of the Institute in 2004 (in thousand CZK; 1 USD ~ 24 CZK)

Source	Income	
	thousand CZK	per cent
State budget	81 183	63.9
Domestic research grants	30 570	24.1
Foreign research grants	9 172	7.2
Contracts	2 270	1.8
Licences	200	0.2
Others	3 679	2.9
Total	127 074	100.0

### 2.2. Investment Means

Besides 0.419 million CZK for building maintenance, 20.851 million CZK were available in 2004 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:

Upgrade of Bruker Spectrometer IFS 120HR (Bruker, Germany)  
 Diffractometer Bruker D8 (Bruker AXS, USA)  
 Upgrade of Microscope NanoScope III (Veeco, USA)  
 Potentiostat AUT 30. FRA 2.V (EcoChemie, Netherlands)  
 Nulllipsisometer ELX-05 (Microphotronics, USA)  
 AvaSpec-2048FT Fast Trigger Fiber Optic Spectrometer (Avantes, Netherlands)  
 Simplified Differential Electrochemical Mass Spectrometer (DEMS) for Electrochemical Analysis (Fraunhofer ICT, Germany)

DEMS Apparatus for  
 Electrochemical Analysis



### 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 three departments: Chemical Physics; Catalysis; 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 CHEMICAL PHYSICS

#### **TOPIC 1.** Development and Application of Quantum Chemical Methods

##### Grant projects

1. European Laboratory for Multireference Quantum Chemical Methods.  
P. Čársky, MEYS (COST), No. CVOSTOC D23/001, 2001-2004.
2. Marie Curie Host Fellowship: Quantum chemical methods and quantum molecular dynamics. Development and applications.  
P. Čársky (a), EC, No. IHP-MCHT-99-1, 2001-2004.
3. Research Training Network: Electron and positron induced chemistry (EPIC).  
P. Čársky (a), EC (IHRP, 5<sup>th</sup> Programme Training Network), No. HPRN-CT-2003-00179, 2002-2005.
4. International Academy of Quantum Molecular Sciences.  
P. Čársky, MEYS (INGO), No. LA145, 2002-2005.
5. Structure and thermodynamic properties of small clusters of rare gases.  
I. Paidarová (a), GA CR, No. 203/02/1204, 2002-2004.

6. Dynamics and spectroscopy of metastable molecules: semiclassical simulations and quantum studies.  
I. Paidarová, MEYS (Barrande), No. 2003/024, 2003-2004.
7. Electron induced processing at the molecular level (EIPAM).  
P. Čársky (a), EC, No. HPRN-CT-2002-00286, 2004-2008.
8. State specific multireference Brillouin-Wigner coupled cluster method with triexcitations.  
J. Pittner, GA AS CR, No. IAA4040401, 2004-2007.
9. Analytic gradient for the state-specific multireference Brillouin-Wigner coupled cluster method.  
J. Pittner, GA CR, No. 203/04/0425, 2004-2006.
10. Modelling of helium ionic clusters: structure, spectra, thermodynamics and dynamics.  
I. Paidarová (a), GA CR, No. 203/04/2146, 2004-2006.

#### Main results in 2004

- a) Extension of the multireference BWCC quantum chemical method to the incomplete model space resulting in lower demands on computers and thereby allowing a broader application of the method. The extension represents a further step in the development of a quantum chemical method for molecular systems whose potential surfaces cannot be described by only one Slater determinant, such as biradicals or systems with a quasi-degenerate electronic state (J. Pittner).
- b) The first *ab initio* calculation allowing an interpretation of electron energy loss spectra (EELS) of molecules with more than three atoms. A theory of these spectra was missing despite the importance of the electron – molecule interactions for microelectronics, atmospheric chemistry and physics, and molecular biology (R. Čurík, P. Čársky).
- c) Extensive *ab initio* and tight-binding calculations of the spin and orbital magnetic moments for a series of small cobalt clusters embedded in a Cu(001) surface in a fully relaxed geometry. The atomic relaxations strongly reduce the magnetic anisotropy energy and the orbital magnetic moments of the embedded clusters. Magnetic properties of embedded and supported clusters were compared (Š. Pick).
- d) Quantum chemical calculation of the potential energy hypersurface and transition dipole moments of krypton ion clusters by combining semiempirical modelling (DIM) and the precision *ab initio* method. The models form a basis for the ensuing study of the ion cluster dynamics and thermodynamics (I. Paidarová).

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**TOPIC 2.** Dynamics and Kinetics of Ion - Molecule Collisions.  
Organic Mass Spectrometry

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Grant projects

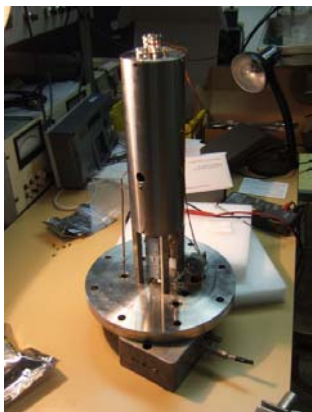
1. Generation, stability and reaction dynamics of multiply charged ions (European MCI Network).  
Z. Herman (a), EC 5<sup>th</sup> Programme, No. HPRN-CT-20000-00027, 2000-2004.
2. Atomic physics, data for edge plasmas & plasma - wall interactions.  
Z. Herman (a), EURATOM, No. EURATOM-IPP-CR, 2000-2005.
3. Theoretical and experimental investigation of dynamics of elementary processes.  
Z. Herman, MEYS (KONTAKT), No. ME561, 2002-2004.
4. Characterization of unstable molecules by mass spectrometric and theoretical methods.  
J. Hrušák, GA CR, No. 203/02/0737, 2002-2004.
5. Modeling of metallocene catalysts in the gas phase.  
M. Polášek, GA ASCR, No. B4040201, 2002-2004.
6. Recombination of  $H_3^+$ ,  $D_3^+$  and  $H_2D^+$  ions with electrons in hydrogen plasma.  
O. Votava (a), GA CR, No. 202/02/0948, 2002-2004.
7. Reaction of molecular dications  $CHX^{++}$  (X= F, Cl, Br, OH, SH,  $NH_2$ ): Theoretical and experimental investigation.  
J. Roithová, GA ASCR, No. B4040302, 2003-2005.
8. Study of elementary processes in low-temperature and technologically oriented plasma and development of relevant diagnostic methods.  
P. Španěl (a), GA CR, No. 202/03/0827, 2003-2005.
9. Collisions of slow polyatomic ions with surfaces: Energy transfer and chemical reactions.  
Z. Herman, GA AS CR, No. A4040405, 2004-2006.

Main results in 2004

- a) Investigation of surface collisions of hydrocarbon ions  $C_2H_n$  ( $n=2-5$ ) and  $C_3H_n$  ( $n=2-8$ ) of energies 15 – 50 eV with carbon surfaces and determination of ion survival probabilities, surface-induced dissociation processes, chemical reactions with the surface material, and angular and energy distribution of reaction products (Z. Herman).
- b) A combined experimental and theoretical study of DNA damage caused by electron attachment to the gas phase DNA bases cytosine and thymine (J. Hrušák).
- c) The first preparation of the cation radical of iso-nitric acid in the gas phase and experimental verification of its existence by means of mass spectrometry corroborated by quantum chemical calculations. Iso-nitric acid presumably plays an important role in combustion processes, but up to now it has not been prepared and characterized. Its cation radical may serve as a precursor in preparation of the neutral form of the acid which then might be characterized using neutralization–reionization mass spectrometry (M. Polášek).



- d) Development of SIFT-MS (Selected Ion Flow Tube - Mass Spectrometry) technique for accurate measurement of trace concentrations of HCN in humid air and breath to be used in clinical research. HCN is produced by bacteria *Pseudomonas aeruginosa* which cause serious complications in children with cystic fibrosis (P. Španěl).



A flange mounted detection quadrupole mass spectrometer is ready to be placed in the vacuum chamber after maintenance. A stack of electrostatic lenses in front of the quadrupole focuses the sample ions into the mass spectrometer (left).

Detailed view of the channel electron multiplier ion detector (right).



- e) Time resolved measurement of low ion concentrations in plasma using the highly sensitive cavity–ringdown spectroscopy (CRDS). The time dependence of CRDS signal at the  $v = 3 \leftarrow 0$  transition of  $H_3^+$  ion ( $\lambda = 1.4 \mu\text{m}$ ) was monitored during the afterglow phase of the discharge. For hydrogen concentration in plasma ranging from  $1 \times 10^{14}$  to  $8 \times 10^{14} \text{ cm}^{-3}$  the coefficient  $\alpha$  characterizing the recombination of the spectroscopically identified ion  $H_3^+$  ( $v = 0$ ) with thermal electrons was  $(1.6 \pm 0.6) \times 10^{-7} \text{ cm}^3 \text{ s}^{-1}$  (O. Votava).

### TOPIC 3. Surface Interactions on Metals

#### Grant project

1. Reactivity of bimetallic systems s,p - (Al, Sn) and transition metals (Pd, Rh): study of volume alloys and interfaces between bimetallic layers and oxides.  
Z. Knor (a), GA CR, No. 202/02/0618, 2002-2004.

#### Main results in 2004

- a) A study of the influence of the chemical nature of the support (W,  $WO_x$ ) and of the overlayer (Pd) on the electronic structure and chemisorption activity of the latter by means of synchrotrone-radiation-excited photoelectron spectroscopy (ELLETRA, Trieste). The thickness of the tungsten oxides formed in the experiments was only several monolayers and always at least three different oxides were involved. A part of tungsten remained unoxidized. Morphology, thermal stability and CO chemisorption activity of the Pd submonolayer depended on the type of the support (J. Pišek, I. Jirka).
- b) Estimation of the activation energy for desorption of CO and  $C_2H_4$  and for their oxidation to  $CO_2$  and ethylene oxide, respectively, on palladium surface supported by niobium, using thermally programmed desorption and reaction. The activation energy for  $C_2H_4$

oxidation was mildly increasing with the thickness of the Pd layer, probably due to a stronger interaction of C<sub>2</sub>H<sub>4</sub> with the larger number of defects on thicker, i.e. atomically rough surfaces (J. Plšek, Z. Knor).

- c) Work function measurements of water layers on tungsten and gold surfaces in field emission microscope indicating that water molecules adsorbed on clean tungsten were oriented towards the surface by oxygen atoms, while on gold-covered tungsten there was no preferential orientation. Heavy perturbation of the water adlayers by high electric field allowed to distinguish between the effect of the surface barrier height (work function) and its thickness. An interpretation was suggested in terms of chemical and morphological changes of the water layer due to field dissociation and solvation (J. Plšek, Z. Knor).

#### **TOPIC 4. Chemistry of Surfaces, Interfaces and Thin Films (Photoelectron Spectroscopy)**

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##### Grant projects

1. Laser photolysis and laser pyrolysis of organic and organometallic compounds for preparation of metal nanoparticles in polymer matrices.  
Z. Bastl (a), GA AS CR, No. A4072107, 2001-2004.
2. Platinum modified conducting polymers as an alternative anode material for low temperature fuel cells.  
Z. Bastl (a), GA CR, No. 104/02/0664, 2002-2004.
3. Determination of catalytic layers composition by XPS method.  
Z. Bastl (a), EC, No. ENK5-CT-2001-00572 (APOLLON), 2003-2005.
4. Characterization of doped photosensitive titania with optimised properties.  
Z. Bastl (a), GA CR, No. 104/04/0467, 2004-2006.
5. Laser ablative and non-ablative treatment of polymers; approach to novel polymeric structures.  
Z. Bastl (a), GA CR, No. 104/04/2028, 2004-2006.

##### Main results in 2004

- a) Determination of the distribution of components and of plasmon energy in bimetallic AgAu colloid nanoparticles using high-resolution photoelectron spectroscopy. The particles have an Ag core coated by the AgAu alloy with surface enriched by Ag. Such bimetallic particles find applications in optics and catalysis (Z. Bastl).
- b) Targeted modification of the ethylene-norbornen (COC) copolymer surface using oxygen and nitrogen microwave and radiofrequency plasma. A detailed spectroscopic investigation allowed to optimize the conditions for chemical functionalization of the surface and to maximize the amount of collagen immobilized on the polymer surface. Optimum modification of the surface led to a higher proliferation and differentiation of

fibroblasts. These studies were aimed at development of biocompatible composite materials for orthopaedic implants of a new generation (Z. Bastl).

- c) Photoelectron spectroscopic characterization of the electron structure and chemical composition of products of the photochemical and thermal reaction of glyoxal with trimethylpropynyl oxysilane. The results are important for tailoring the chemical composition and morphology of the products (Z. Bastl).
- d) Determination of the effect of the surface modification of polyethylene terephthalate and polyethylene naphthalate polymers by argon ions on their chemical composition and on the depth concentration profiles of thin layers of SiO<sub>2</sub> deposited onto the surface of a polyethylene terephthalate foil at various conditions. The results obtained contribute to the development of a new packing material (Z. Bastl, I. Spirovová).

## TOPIC 5. Molecular Spectroscopy and Photochemistry

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### Grant projects

1. Urban air pollution control: Model and *in situ* measurements.  
S. Civiš, MEYS (COST), No. COST 715.50, 1999-2004.
2. Fast tunable MID-IR and IR laser diode spectrometer based on non-linear optical effects.  
S. Civiš, GA ASCR, No. A4040104, 2001-2005.
3. Physical and chemical modeling of secondary pollutants production and propagation in the urban and rural areas.  
Z. Zelinger, GA ASCR, No. A3040101, 2001-2004.
4. New laser-based hybrid technologies for thin layer deposition.  
Z. Zelinger (a), GA ASCR, No. A1010110, 2001-2005.
5. Tetrapyrrole metallocomplexes: modification of nucleic acid triplex structures.  
P. Kubát (a), GA CR, No. 203/02/0420, 2002-2004.
6. The role of the upper troposphere and lower stratosphere in global change.  
Z. Zelinger, MEYS (COST), No. OC 723.001, 2003-2006.
7. Infrared and sub-millimeter wave spectroscopy of molecular ions - contribution to the analyses of data from the Herschel observatory of ESA.  
Z. Zelinger, MEYS (BARRANDE) No. 2004-037, 2004-2005.
8. Design and characterization of new photosensitisers and investigation of their interaction with target biological macromolecules.  
P. Kubát (a), GA CR, No. 203/04/0426, 2004-2006.
9. From a computer controlled spectroscopic experiment to an international database for remote detection of molecules.  
Š. Urban, GA AV ČR – INFO, No. ET400400410, 2004-2008.

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Main results in 2004

- a) Development of a theory of hyperfine nuclear interactions in molecules and its application to an interpretation of high resolution rotational – vibrational spectra of atmospheric species containing halogen and nitrogen atoms (Š. Urban).
- b) Measurement of time-resolved infrared emission spectra of the excited neutral helium dimer produced by a pulsed discharge (S. Civiš).
- c) The first observation of the rotational spectrum of the atmospherically important bromomethyl radical CH<sub>2</sub>Br (Z. Zelinger).
- d) Experimental determination of the influence of aggregation and complexation on photophysical properties of new photosensibilizers (porphyrines, sapphyrines) leading to a deeper understanding of the processes taking place in the photodynamical therapy of tumors (P. Kubát, Z. Zelinger).
- e) A comparison of the mathematical and physical models with the results of spectroscopic measurements of physical and chemical processes in atmospheric pollution (Z. Zelinger, P. Kubát).

**TOPIC 6. Phospholipids in Biological Systems (Fluorescence Spectroscopy)**

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Grant project

1. Structure and Dynamics of Complex Molecular Systems and Biomolecules. M. Hof (a), MEYS (CENTRUM), No. LN 00A032, 2000-2004.

Main result in 2004

Ellipsometric measurement of the kinetics of formation of phospholipid membranes on hydrophilic surfaces (mica, glass, silicon oxides). Chemical composition of the membrane, concentration of ions in the buffer, and lipid composition of the membrane have a decisive influence on the membrane formation and its properties (M. Hof, M. Beneš, A. Benda).

**DEPARTMENT OF CATALYSIS**

**TOPIC 1. Synthesis and Reactivity of Catalytic Materials**

Grant projects

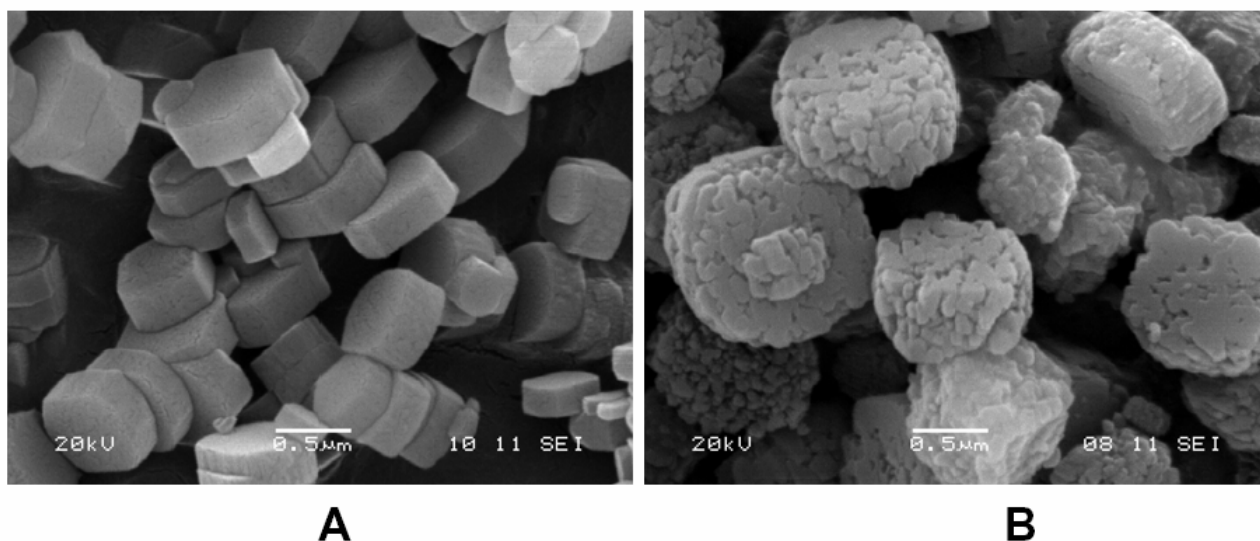
1. Structure of metal ions in oxide matrices. Relation synthesis/structure/activity/selectivity in the development of catalysts for highly selective reactions.  
B. Wichterlová, EC/COST (MEYS), No. OC D15.20/COST, 2000-2003.
2. Synthesis of molecular sieves for hydrocarbon transformation.  
B. Wichterlová, ASCR, No. S4040015, 2001-2004.
3. Redox zeolitic catalysts for nitrogen oxides abatement using process gases.  
Z. Sobalík, ASCR, No. S4040016, 2000-2004.
4. Advanced nanostructured metal/metaloxo/matrix catalysts for redox processes. Application for NO<sub>x</sub> reduction to nitrogen.  
B. Wichterlová, EC/GROWTH, No. G5RD-CT-2001-00595/AMMONORE, 2001-2004.
5. Mesoporous molecular sieves for catalytic applications.  
J. Čejka, GA CR, No. 104/02/0571, 2002-2004.
6. Effect of gaseous additives and gas phase reactions on the course of catalytic redox reactions.  
D. Kaucký, GA CR, No. 104/04/D124, 2002-2005.
7. Catalytic ammoxidation of propane.  
B. Wichterlová, GA CR, No. 104/03/1120, 2003-2005.
8. Organized materials for highly selective catalytic and separation processes.  
B. Wichterlová, GA CR, No. 203/03/H140, 2003-2005.
9. Synthesis of fine chemicals via heterogeneous catalysis.  
J. Čejka, GA CR, No. 203/03/0804, 2003-2005.
10. Control of negative charge distribution in skeleton of high-silica zeolites.  
J. Dědeček, GA ASCR, No. 4040308, 2003-2006.
11. Development of program environment for mathematic simulations and predictions in catalysis and electrocatalysis.  
Z. Sobalík, GA AS CR, No. 1ET400400413, 2004-2008.
12. Application of residual and waste aluminosilicates for production of building materials on the basis of inorganic polymers.  
Z. Sobalík (a), MIT, No. FI-IM/079/IMPULS, 2004-2006.
13. Transition metal oxides supported on mesoporous molecular sieves for olefin metathesis reactions.  
J. Čejka, GA AS CR, No. 4040411, 2004-2007.

14. Development of special types of oxidation catalysts for tailored synthesis of fragrances.  
J. Čejka (a), MIT, No. FT-TA/040/TANDEM, 2004-2007.
15. Development of progressive types of alumina for special applications.  
J. Čejka (a), MIT, No. FT-TA/042/TANDEM, 2004-2007.
16. Tailoring the zeolite properties for catalytic applications.  
G. Košová, GA AS CR, No. B4040402, 2004-2006.
17. Czech Zeolite Group.  
J. Čejka, MEYS (INGO), No. LA144, 2002-2005.
18. European Federation of Catalysis Societies.  
Z. Sobalík, MEYS (INGO), No. LA169, 2003-2005.
19. International Association of Catalytic Societies.  
B. Wichterlová, MEYS (INGO), No. LA 170, 2003-2005.

#### Main results in 2004

- a) Identification of the structure of the Cu site most active in selective reduction of NO to nitrogen located at the six-member ring at the intersection of the straight and sinusoidal channel of MFI zeolite. Population of this cationic site is controlled by the distribution of aluminum in the zeolite framework and thus by the conditions of the zeolite synthesis (B. Wichterlová, J. Dědeček).
- b) Revealing the reasons why long chain alkanes or alkenes, in contrast to low chain alkanes, lead to stable conversion in reduction of NO to nitrogen by hydrocarbons in high excess of water vapor existing in real exhaust gases. In the first step of the reaction, highly reactive long chain alkanes crack to a range of alkenes and alkanes of which the former strongly adsorb on the active Cu and protonic sites and prevent water adsorption on them (B. Wichterlová, Z. Sobalík).
- c) Development of a heterogeneous catalyst for selective reduction of nitrogen oxides by decane in an excess of oxygen and water vapor (a model of exhaust gases from diesel engines). Combination of Ag/alumina and Cu-(Fe)-ZSM 5 zeolite, both having an optimized structure, yielded a catalyst whose efficiency in NO<sub>x</sub> conversion in a broad temperature range fulfilled the limits of European Union (B. Wichterlová, Z. Sobalík, L. Čapek, J. Dědeček).
- d) Achievement of a 80 % selectivity at a 70 % conversion in the selective synthesis of isopropylketone by acylation of toluene using isobutyryl chloride or anhydride on zeolite catalysts. Zeolite Beta has an optimum reaction space and high resistance against deactivation in this reaction which represents a model of the first step in the synthesis of the medicament Ibuprofen (J. Čejka).
- e) Development of highly active and selective hybrid catalysts for metathesis of linear 1-olefins by deposition of molybdenum oxide onto mesoporous molecular sieve MCM-41 and of rhenium salts on mesoporous organized alumina. These catalysts are superior to those using conventional silica and alumina as support (J. Čejka, H. Balcar).

- f) Elucidation of the role which in MCM-22 zeolite play *i)* Mo ions and Mo carbides in methane hydrogenation; *ii)* proton and Lewis centers in oligomerization and aromatization of olefinic fragments from methane to benzene, toluene and xylenes (Z. Sobalík, B. Wichterlová).
- g) Analysis of the mechanism of pentene cracking to the demanded ethane and propene over crystalline aluminosilicates and aluminophosphates of various structures. High conversion and selectivity to low olefins can be achieved with catalysts containing intersecting channels with 10-membered rings allowing voluminous carbenium ion intermediates to be formed. The original synthesis of these catalysts is subject of patent application (B. Wichterlová, J. Čejka).



Scanning electron micrographs of ZSM-5 synthesized without (A) and with Carbon Black Pearls (B)

## TOPIC 2. Interactions and Mobility of Molecules in Microporous Systems

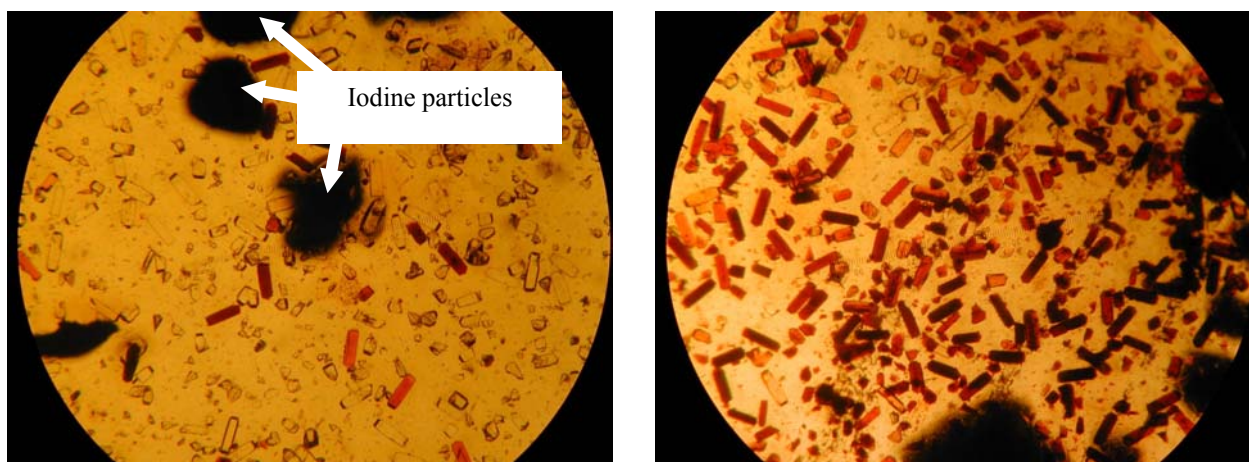
### Grant projects

1. New dealumination routes to the production of transport-optimized catalysts for crude oil conversion.  
M. Kočířík (a), EC/GROWTH, No. G5RD-CT-2001-00520/TROCAT, 2001-2004.
2. Interactions of bentonites with the environment: the effect of geological history and actual conditions; application in active waste deep repositories.  
M. Kočířík (a), GA CR, No. 104/02/1464, 2002-2004.
3. Polymer-based membrane composites for separation of small molecules.  
M. Kočířík (a), GA CR, No. 104/03/0680, 2003-2005.

4. Contribution of non-zeolitic pores to the separating function of composite membranes containing zeolites.  
O. Prokopová, GA CR, No. 104/03/D183, 2003-2005.
5. Nanostructured materials – texture from physical adsorption.  
M. Kočířík (a), GA CR, No. 104/04/096, 2004-2006.

#### Main results in 2004

- a) The first evidence of a correlation between selfdiffusion coefficients of the reactants/products of hydrocarbon cracking and the texture characteristics (size and volume of macro- and mesopores) of the used catalysts. The NMR method provides reliable values of selfdiffusion coefficients in cracking catalysts and therefore it was successfully used for optimizing their transport characteristics (M. Kočířík, A. Zikánová).
- b) Elucidation of the formation and elimination of non-zeolitic diffusion channels in zeolitic membranes. Quantification and visualization of the ratio of Knudsen diffusion through the defective pores of the total gas flow in the composite membrane silicalite-1 –  $\alpha$ -alumina and estimation of their accessibility (M. Kočířík, A. Zikánová).
- c) Development of a composite membrane from silicalite-1 and a polymer matrix. The membrane exhibits a high permeability and its selectivity for the  $H_2/CH_4$  separation attains the value of 100 (A. Zikánová, M. Kočířík).



Microphotographs of composite membrane polyimide - silicalite-1 with zeolite accessibility visualized by iodine; (A) low accessibility, (B) enhanced accessibility



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### TOPIC 3. Sol – Gel Microstructured Materials

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#### Grant project

1. Transparent thin films of mesoporous titania and mesoporous silica with embedded dye molecules as effective photocatalysts for pollutant mineralization and as optical gas sensors.  
J. Rathouský, DFG, No. WA1116/7-1, 2002-2004.

#### Main results in 2004

- a) Development of a new method for tailoring the porous structure of mesoporous alumina and other mesoporous oxides. The suitably chosen solvent determines the structure of micelles of non-ionic surfactants which act as a template and determine the texture of the organized mesoporous alumina  
(A. Zukał, J. Rathouský).
- b) Development of a flexible and effective procedure for preparation of hybride inorganic/organic films for solar elements sensibilized by dyes. The procedure involves electrodeposition of thin mesoporous films of zinc oxide modified by eosin which controls the film structure and can be subsequently replaced by another suitable dye. The resulting porous electrodes of high surface area and accessibility of the film interior for dyes show a high photoelectric efficiency  
(J. Rathouský).

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### TOPIC 4. Organometallic Catalysis

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1. Silicon-based ansa-titanocene complexes: Synthesis, properties and catalytic activities.  
K. Mach, GA CR, No. 203/02/0774, 2002-2004.
2. Catalysts for olefin metatheses and related polymerizations anchored on mesoporous molecular sieves.  
H. Balcar, GA CR, No. 203/02/0976, 2002-2004.
3. Synthesis of cationic titanocene complexes and their reactivity towards olefins and acetylenes.  
M. Horáček, GA AS CR, No. B4040403, 2004-2006.

#### Main results in 2004

- a) Synthesis of new structural types of organometallic complexes based on the substitution of silyl groups in titanocene and zirconocene complexes and in unsaturated substrates. The substitution involves new reaction mechanisms and rearrangements. The agostic interaction of proton in the yirconocene complexes with terminal acetylenes prevents or hampers their dimerization by a mechanism known with titanocene catalysts (K. Mach, M. Horáček, J. Kubišta).

- b) Experimental evidence that the length of pendant  $\omega$ -alkenylsilyl groups suitable for the cycloaddition reaction yielding cyclopentadienyl ring-tethered titanacyclopentane products at the Ti(II) centre is strongly limited to the allylsilyl group. The 3-butenylsilyl group gives the structurally characterized product arising from multiple rearrangements. The shortest vinylsilyl group gives rise to a Ti(III) *ansa*-titanocene containing allyl group in the SiC<sub>4</sub>Si bridge. Among a number of new complexes prepared in this way, acetylides are of importance for catalytic dimerization of terminal alkynes (L. Lukešová, M. Horáček, J. Kubišta, K. Mach).
- c) Modification of single-site titanium-based catalysts by substituents at the cyclopentadienyl ligands which revealed that zirconocene dichlorides with one 2,3-dimethyl-1,4-diphenylcyclopentadienyl and one cyclopentadienyl ligand form highly active catalysts for polymerization of ethene. Selected CGC catalysts modified in  $\alpha$ -position produce unprecedented ethene/styrene pseudo-random copolymers containing nearly 50 mol % of incorporated styrene (J. Pinkas, M. Horáček, K. Mach).

## DEPARTMENT OF ELECTROCHEMISTRY

### TOPIC 1. Electrochemistry of Liquid Interfaces and Membranes

#### Grant projects

1. Emulsification of liquid interfaces.  
Z. Samec, MEYS (KONTAKT), No. ME502, 2002-2004.
2. Formation of surface films from monomers adsorbed at liquid/liquid interface.  
V. Mareček, MEYS (KONTAKT), No. ME 510, 2002-2004.
3. Polymerization of adsorbed layers at the liquid/liquid interface.  
V. Mareček, GA CR, No. 203/03/0822, 2003-2005.
4. Nanostructures for energy and chemical production.  
Z. Samec (a), EC (6<sup>th</sup> Programme), No. NMP3-Ct-2004-505906/NENA, 2004-2007.
5. Electroanalysis on metal nanoparticles deposited on the supported liquid.  
Z. Samec, GA AS CR, No. 4040407, 2004-2007.
6. Electrochemistry in biomedically important polyions at the interface of two immiscible electrolyte solutions with applications in drug analysis.  
Z. Samec, GA CR, No. 203/04/0424, 2004-2006.
7. Microfluidic analysis system for monitoring of amino acids in biological fluids.  
J. Langmaier (a), GA CR, No. 203/04/0519, 2004-2006.

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Main results in 2004

- a) Clarification of the transport of medically significant polyions (heparin, protamine) across the polarized liquid/liquid interfaces. The obtained result is of importance for their determination in biological fluids (Z. Samec).
- b) Development of a new method for voltammetric determination of the rate constant of one-way homogeneous chemical reaction in a system of two immiscible liquid phases has been developed. The rate constant is simply evaluated from the value of the polarization rate at which the peak heights for the electrode reactions of an unreacted reactant and product of the chemical reaction are equal. The dependence of the rate constant on experimental conditions can be followed by comparing a single well defined value (V. Mareček, K. Holub).

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**TOPIC 2. Electrocatalysis**

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Grant projects

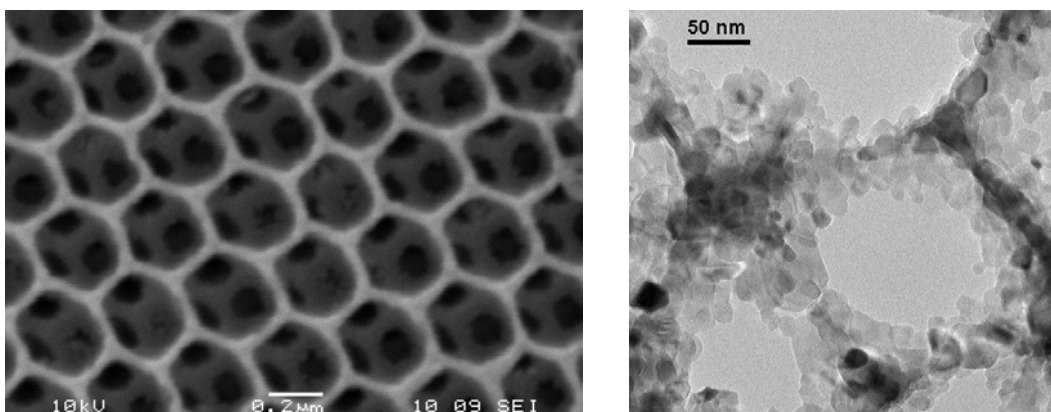
1. Synthesis and characterization of new carbon materials with polyene structure.  
L. Kavan, MEYS (KONTAKT), No. ME487, 2002-2004.
2. Soft solution based synthesis of nano-microcrystalline Li insertion materials and their electrochemical characterization.  
P. Krtil, MEYS (KONTAKT), No. ME416, 2002-2004.
3. Mineralization of organic injurants using new solar energy-based photocatalysts.  
J. Jirkovský, GA CR, No. 203/02/0983, 2002-2004.
4. Application of advanced oxidation processes for water purification utilizing solar energy combined with non-ionogenic selective sorption.  
J. Jirkovský (a), GA CR, No. 104/02/0662, 2002-2004.
5. *In-situ* study of active mass and contact layers in electrodes of the lead accumulator.  
K. Micka (a), GA CR, No. 102/02/0794, 2002-2004.
6. Template mesoscopic TiO<sub>2</sub> for electrodes and photocatalysts.  
L. Kavan, GA CR, No. 203/03/0824, 2003-2005.
7. Innovative multi-purpose thin-film UV reactor.  
L. Kavan (a), EC (5<sup>th</sup> Programme), EVK1-CT-2002-300258/UVREC, 2003-2005.
8. Charge transfer in organized supramolecular systems of fullerenes.  
L. Kavan, GA ASCR, No. 4040306, 2003-2006.
9. The exploitation of alkali alkynides for the electrochemical and chemical preparation of long-chain oligoynes and carbon nanotubes.  
J. Hlavatý, GA CR, No. 203/03/0825, 2003-2005.

10. 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.
11. *In-situ* gravimetric investigation of ion transfer and adsorption at the interface of two immiscible liquids. P. Krtil, GA AS CR, No. B4040305, 2003-2005.
12. Investigation of photoelectrochemical properties of colloid solutions of ferrioxide and titanium dioxide – a route to clarify the mechanism of natural photoprocesses and their application in photocatalytic decontamination of water utilizing solar energy. J. Jirkovský, MEYS (BARRANDE), No. 2003-20, 2003-2004.
13. Complementarity of homogeneous (Fe) and heterogeneous (TiO<sub>2</sub>) photocatalysts for pollutant removal from the aquatic compartment. J. Jirkovský (a), EC-IHP, 2003-2004.
14. 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.
15. Molecular orientation, low band gap materials and new hybrid device concepts for the improvement of plastic solar cells. L. Kavan (a), EC (6<sup>th</sup> Programme), No. SES6-Ct-2003-502783/MOLYCELL, 2004-2006.

#### Main results in 2004

- a) Development and experimental verification of a qualitative model explaining both the dependence of insertion behavior of nanocrystalline oxides on the particle size and the distribution of structural defects in the particle interior. Nanocrystalline oxides with a high localization of defects on the borderline between coherent domains are more resistant to phase changes and can be easier electrochemically charged and discharged. Therefore they are well suited for stable electrodes in Li ion batteries (P. Krtil, K. Makarova, J. Jirkovský).
- b) Elucidation of the mechanism of electrochemical Li-storage in TiO<sub>2</sub>(B) nanofibres. Its rate is not limited by solid-state diffusion of Li<sup>+</sup>. This unusual behavior is caused by ordered channel structure of the host (L. Kavan, M. Zukalová, M. Kalbáč).
- c) A new method for preparation of nanoclusters of metals active in electrocatalytic oxidation of ethylene (Au, Pd, Ni) by evaporating the active metal onto a single crystal surface of low catalytic activity (P. Janda, J. Weber, H. Pelouchová).
- d) Development of a new way of obtaining oriented quasi-isolated SWCNT, DWCNT and fullerene peapods on the Au(111) surface by friction deposition (M. Kalbáč, L. Kavan, P. Janda).

- e) Development of new doping techniques for fullerene peapods. Concerted application of electrochemical and chemical doping with  $F_2$ , K-amalgam and K-vapor brought new data about the charge-transfer in peapods. The most valuable result is our finding that potassium can be intercalated inside the peapod. In February 2005, this effect was confirmed by Iijima et al. by direct TEM imaging (L. Kavan, M. Kalbáč, M. Zúkalová).
- f) Development of new method for producing double wall carbon nanotubes from fullerene peapods. The method is based on photochemical conversion by XeCl-laser. Compared to the existing pyrolytic techniques, this procedure does not require high temperatures, and can be carried out even on plastic substrates (L. Kavan, M. Kalbáč, S. Civiš, P. Kubát).
- g) Development of a new electrochemical synthesis of anatase inverse opal with tunable stop-band. The electrodeposition allows well-defined filling of the opal template, which is attractive for fabrication of photonic crystals (L. Kavan, M. Zúkalová, M. Kalbáč).



SEM (left) and TEM (right) pictures of the inverse opal powder made from a propanolic solution of titanium (IV) tetraisopropoxide.

- h) Finding that the Raman  $G'$ -mode of double wall carbon nanotubes exhibits the optimum phonon dispersion and sensitivity to electrochemical doping. This mode has favorable properties for distinction of the inner and outer tubes already in the pristine material (L. Kavan, M. Kalbáč).
- i) Elucidation of the mechanism of total dehalogenation of low-molecular weight perfluorinated hydrocarbons by the alkali metal amalgams. Experimental data for twelve different molecules were compiled in terms of a novel mathematical model which considers explicitly the activation overvoltage. This treatment upgrades and generalizes the classical Jansta and Dousek's model of total dehalogenation of PTFE (L. Kavan, K. Micka, J. Hlavatý).
- j) Observation and explanation of a synergy effect existing in the combined homogeneous and heterogeneous photocatalytic system containing both iron(III) salt and titanium dioxide particles. This phenomenon was practically verified in the pilot plant of Compound Parabolic Collector at the Plataforma Solar de

Almería test facilities of the European Commission  
(H. Měšťánková, J. Jirkovský).

- k) Evidence of the competitive adsorption between an organic compound, as electron donor, and oxygen, as electron acceptor, on the TiO<sub>2</sub> photocatalyst surface in the course of photocatalytic degradations of organic pollutants (J. Jirkovský).
- l) Development of a pilot scale photoreactor for water disinfection and purification for an industrial partner (J. Jirkovský, V. Sváta, H. Měšťánková, M. Zukalová, L. Kavan).
- m) Demonstration that in the slow recrystallization of anatase nanoparticles during ageing of their aqueous colloidal solutions, the particle mean size increases but gradually in contrast to a considerable increase of their photocatalytic activity (M. Kolář, J. Jirkovský, M. Heyrovský).

### **TOPIC 3. Organic and Organometallic Electrochemistry**

#### Grant projects

1. Characterization of electrochemical and adsorption properties of supramolecular structures of selected pesticides.  
M. Hromadová, GA CR, No. 203/02/P082, 2002-2004.
2. Electron transfer in supramolecular complexes, large molecules with more active centers and in organized structures.  
L. Pospíšil, GA CR, No. 203/03/0821, 2003-2005.
3. Electronic properties, structure and reactivity of the azine group C=N-N=C and mechanism of biologically important azines degradation.  
J. Ludvík, GA ASCR, No. 4040304, 2003-2005.
4. Preparation, reactivity and electrochemistry of new aminocarbene complexes of chromium and iron.  
J. Ludvík (a), GA CR, No. 203/04/0487, 2004-2006.
5. Elektrochemistry of nano-structures at heterogeneous interfaces: Formation, properties and electron transfer reactions.  
L. Pospíšil, MEYS (COST), No. COST 1P04 OCD 15.10, 2004-2006.

#### Main results in 2004

- a) A new theoretical approach to the determination of ultrasound intensity in sonoelectrochemistry based on the knowledge of the absorption, propagation and inner reflection in the electrochemical cell. Application of ultrasound of high intensity in the preparative electroreduction of thiophene (J. Klíma, J. Ludvík).

- b) Experimental determination of the electron density distribution in purine and its confrontation with quantum chemical calculations (J. Ludvík).
- c) Clarification of the mechanism of photochemical substitution of carbonyl - diimine complexes  $trans(X,X)-[Ru(X)_2(CO)_2(bpy)]$  (X = Cl, Br, I) and identification of low-lying excited states and reaction intermediates on the basis of ultrafast spectroscopic measurements and quantum mechanical TD DFT calculations (S. Zálíš, A. Vlček).
- d) Experimental evidence of redox reactions of fullerene derivatives taking place in the cavity of cyclodextrins in aqueous medium (L. Pospíšil, M. Hromadová).

#### TOPIC 4. Electroanalytical Chemistry

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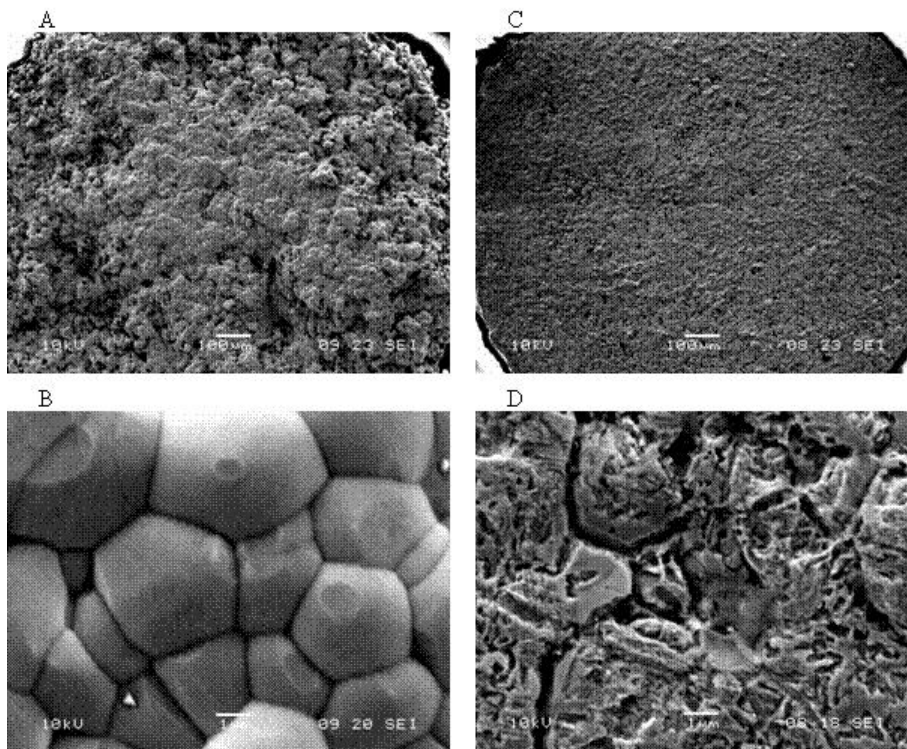
##### Grant projects

- 1. Response of plants to abiotic stress by selected heavy metals.  
I. Šestáková (a), GA CR, No. 525/02/0301, 2002-2004.
- 2. Characterization of cancer-related metalloproteins and their interaction with DNA.  
I. Šestáková (a), MEYS (COST), No. COST D21.002, 2002-2005.
- 3. 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.  
L. Novotný (a), MIT, No. 1H-PK/42, 2004-2007.

##### Main results in 2004

- a) Voltammetric determination of the effect of some victuals and the antiallergic agent ceterizine on the increased urinary excretion of thiodiglycolic acid in humans (T. Navrátil).
- b) Study of the electrochemical behavior of phytochelatin and related peptides at the hanging mercury drop electrode in the presence of cobalt(II) ions. Two types of catalytic hydrogen currents were observed due to the formation of labile complexes of cobalt with dipeptides Cys-Gly and  $\gamma$ -Glu-Cys, and of stabile complexes formed with phytochelatin PC2 and PC3. Under special conditions (pH of solution, rate of polarisation) different complexes can be distinguished and their synthesis within plant cells can be monitored (I. Šestáková).
- c) Experimental evidence that aliphatic alcoholates represent the exceptional case of species which catalyze hydrogen evolution from aqueous solutions on electrodes via oxygen atom. That is due to the optimum interfacial orientation of the catalyst in contact with the electrode: the hydrophobic aliphatic part of the alcoholate adheres to the electrode and the hydrophilic negatively charged oxygen atom protrudes into the solution and attracts protons (M. Heyrovský).
- d) Application of silver solid amalgam electrode modified with supercoiled DNA to sensitive voltammetric detection of enzymatic or chemical cleavage of DNA in solution or at the electrode (B. Yosypchuk, T. Navrátil).

- e) Characterization of the silver solid amalgam electrode by X-ray diffraction and a preliminary specification of factors influencing its use for detection of DNA hybridization or damage, and for studies of other biomolecules (L. Novotný).



Surface of silver solid amalgam electrode (SEM)

- A: unpolished surface (100 μm); B: detail of unpolished surface (1 μm)  
C: polished surface (100 μm); D: detail of polished surface (1 μm)



## 4. PUBLICATION AND POPULARIZATION ACTIVITIES

### 4.1. Synopsis of Papers Published in 2004

Members of the Institute are authors or co-authors of 224 research papers which appeared in 2004 in reviewed periodicals, proceedings of conferences, and monographs.

In addition, 7 popularization papers in professional publications appeared and 2 patents were granted.

Contributions in non-professional journals and newspapers are not included.

Table 4.1. Publications issued in 2004

Type of publication	Number
Research papers in periodicals	158
Contributions in conference materials	25
Contributions in monographs	5
Popularization papers	7
Patents	2

Members of the department of chemical physics, catalysis and electrochemistry were authors or co-authors of 78, 45 and 93 of the issued publications, respectively.

In 107, 56 and 33 publications authors from institutions abroad, universities in the Czech Republic, and other institutions in the Czech Republic, respectively, participated. Authors of 107 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. Demel Ondřej, Pittner Jiří, Čársky Petr, Hubač I.  
Multireference Brillouin-Wigner Coupled Cluster Singles and Doubles Study of the Singlet-Triplet Separation in Alkylcarbenes.  
*J. Phys. Chem. A* 108(15), 3125-3128 (2004).
2. Pittner Jiří, Gonzales Haydee Valdés, Gdanitz R. J., Čársky Petr  
The Performance of the Multireference Brillouin-Wigner Coupled Cluster Singles and Doubles Method on the Insertion of Be into H<sub>2</sub>.  
*Chem. Phys. Lett.* 386(1/3), 211-215 (2004).
3. Pittner Jiří, Hobza P.  
CCSDT and CCSD(T) Calculations on Model H-Bonded and Stacked Complexes.  
*Chem. Phys. Lett.* 390(4/6), 496-499 (2004).
4. Popovič D., David D. E., Michl J., Čurík Roman, Čársky Petr  
Joint Experimental and Theoretical Study of Vibrationally Inelastic Electron Scattering on Propane.  
*J. Chem. Phys.* 121(21), 10551-10555 (2004).
5. Zahradník Rudolf  
Interactions between Physics and Biodisciplines within the Framework of Molecular Sciences.  
*Int. J. Mol. Sci.* 5, 214-223 (2004).
6. Polák Rudolf, Fišer J.  
A Comparative icMRCI Study of some NO<sup>+</sup>, NO and NO<sup>-</sup> Electronic Ground State Properties.  
*Chem. Phys.* 303(1), 73-83 (2004).
7. Fišer J., Boublík T., Polák Rudolf  
Intermolecular Interactions in the (CO<sub>2</sub>)<sub>2</sub>, N<sub>2</sub>-CO<sub>2</sub> and CO-CO<sub>2</sub> Complexes.  
*Collect. Czech. Chem. Commun.* 69(1), 177-188 (2004).
8. Pick Štěpán, Demangeat C.  
Effect of Oxygen on the Mn-Co Ferromagnetic Coupling.  
*Catal. Today* 89, 369-374 (2004).
9. Pick Štěpán, Stepanyuk V. S., Klavsyuk A. L., Niebergall L., Hergert W., Kirschner J., Bruno P.  
Magnetism and Structure on the Atomic Scale: Small Cobalt Clusters in Cu(001).  
*Phys. Rev. B* 70, 224419.1-224419.8 (2004).

10. Kalus R., Paidarová Ivana, Hrivňák D., Gadea F. X.  
Modelling of  $Kr_n^+$  Clusters. II. Photoabsorption Spectra of Small Clusters ( $n = 2 - 5$ ).  
*Chem. Phys.* 298(1/3), 155-166 (2004).
11. Herman Zdeněk, Stamatovic A., Castleman A. W.  
Foreword.  
*Int. J. Mass Spectrom.* 233(1), 9-10 (2004).
12. Herman Zdeněk  
Surface Collisions of Small Cluster Ions at Incident Energies 10-102 eV.  
*Int. J. Mass Spectrom.* 233, 361-371 (2004).
13. Qayyum A., Herman Zdeněk, Tepnual T., Mair C., Matt-Leubner S., Scheier P., Märk T. D.  
Surface-Induced Dissociation of Polyatomic Hydrocarbon Projectile Ions with Different Initial Internal Energy Content.  
*J. Phys. Chem. A* 108(1), 1-8 (2004).
14. Alcaraz Ch., Nicolas Ch., Thissen R., Žabka Ján, Dutuit O.  
 $^{15}N^+ + CD_4$  and  $O^+ + ^{13}CO_2$  State-Selected Ion-Molecule Reactions Relevant to the Chemistry of Planetary Ionospheres.  
*J. Phys. Chem. A* 108(45), 9998-10009 (2004).
15. Denifl S., Ptasińska S., Probst M., Hrušák Jan, Scheier P., Märk T. D.  
Electron Attachment to the Gas Phase DNA Bases Cytosine and Thymine.  
*J. Phys. Chem. A* 108(31), 6562-6569 (2004).
16. Franzreb K., Hrušák Jan, Alikhani M. E., Lörinčík J., Sobers Jr. R. C., Williams P.  
Gas-Phase Diatomic Trications of  $Se_2^{3+}$ ,  $Te_2^{3+}$  and  $LaF^{3+}$ .  
*J. Chem. Phys.* 121(24), 12293-12302 (2004).
17. Dryahina Kseniya, Polášek Miroslav, Španěl Patrik  
A Selected Ion Flow Tube, SIFT, Study of the Ion Chemistry of  $H_3O^+$ ,  $NO^+$  and  $O_2^+$  Ions with Several Nitroalkanes in the Presence of Water Vapour.  
*Int. J. Mass Spectrom.* 239(1), 57-65 (2004).
18. Smith D., Španěl Patrik, Dabill D., Cocker J., Rajan B.  
On-line Analysis of Diesel Engine Exhaust Gases by Selected Ion Flow Tube Mass Spectrometry.  
*Rapid Commun. Mass Spectrom.* 18, 2830-2838 (2004).
19. Španěl Patrik, Hall E. F. H., Workman C. T., Smith D.  
A Directly Coupled Monolithic Rectangular Resonator Forming a Robust Microwave Plasma Ion Source for SIFT-MS.  
*Plasma Sources Sci. Technol.* 13(2), 282-284 (2004).
20. Wang T., Smith D., Španěl Patrik  
A Selected Ion Flow Tube, SIFT, Study of the Reactions of  $H_3O^+$ ,  $NO^+$  and  $O_2^+$  Ions with Several N- and O-containing Heterocyclic Compounds in Support of SIFT-MS.  
*Int. J. Mass Spectrom.* 237(1), 167-174 (2004).

21. Wang T., Smith D., Španěl Patrik  
Selected Ion Flow Tube, SIFT, Studies of the Reactions of  $\text{H}_3\text{O}^+$ ,  $\text{NO}^+$  and  $\text{O}_2^+$  with Compounds Released by *Pseudomonas* and Related Bacteria.  
*Int. J. Mass Spectrom.* 233(2), 245-251 (2004).
22. Schraml J., Mindl J., Roithová Jana, Blechta V., Sýkora Jan, Soukupová L., Karban J., Bártlová M., Exner O.  
Silylation of N,O-Diacylhydroxylamines: NMR Spectra and Structure of the Products.  
*Organometallics* 23(9), 2157-2161 (2004)
23. Bastl Zdeněk, Pick Štěpán  
Angle Resolved X-ray Photoelectron Spectroscopy Study of Au Deposited on Pt and Re Surfaces.  
*Surf. Sci.* 566-568, 832-836 (2004).
24. Dřínek V., Bastl Zdeněk, Šubrt J., Pola J.  
IR Laser Ablation of Silicon Monoxide in Gaseous Methanol and Hydrocarbons Deposition of Polyoxocarbosilane.  
*J. Anal. Appl. Pyrol.* 71, 431-444 (2004).
25. Godočíková E., Bastl Zdeněk, Spirovová Ilona, Baláž P.  
A Study of Mechanochemical Reduction of Lead Sulphide by Elemental Iron on the Surface by X-ray Photoelectron Spectroscopy.  
*J. Mater. Sci.* 39, 3025-3029 (2004).
26. Medvecký L., Briančin J., Bastl Zdeněk  
Influence of Electrohydropulse on Sb Doped  $\text{Ba}_{0.95}\text{Pb}_{0.05}\text{TiO}_3$  Phase.  
*Powder Metall. Prog.* 4(1), 48-56 (2004).
27. Morita H., Kumagai T., Bastl Zdeněk  
Magnetic Field Effect on Photochemical Thin Film Formation from a Gaseous Mixture of Trimethyl(2-propynyloxy)silane and Glyoxal.  
*J. Photopolym. Sci. Tech.* 17(1), 53-60 (2004).
28. Morita H., Semba K., Bastl Zdeněk, Šubrt J., Pola J.  
 $\text{N}_2$  Laser-Induced Formation of Copolymeric Ultrafine Particles in a Gaseous Tetraethenylgermane - Carbon Disulfide Mixture.  
*J. Photochem. Photobiol. A* 171(1), 21-26 (2004).
29. Ouchi A., Tsunoda T., Bastl Zdeněk, Maryško M., Vorlíček V., Boháček J., Vacek K., Pola J.  
Solution Photolysis of Ferrocene into Fe-Based Nanoparticles.  
*J. Photochem. Photobiol. A* 171, 255-260 (2004).
30. Pokorná D., Urbanová M., Bastl Zdeněk, Šubrt J., Pola J.  
Laser-Induced Gas-Phase Pyrolysis of Dimethyl Selenium: Chemical Deposition of Selenium and Poly(selenoformaldehyde).  
*J. Anal. Appl. Pyrol.* 71, 635-644 (2004).

31. Pola J., Bastl Zdeněk, Vorlíček V., Alexandrescu R., Morjan I., Dumitrache F., Sandu I., Ciupina V.  
Laser-Induced Synthesis of Iron-Iron Oxide/Methylmethoxysilicone Nanocomposite.  
*Appl. Organometal. Chem* 18, 337-342 (2004).
32. Pola J., Ouchi A., Bastl Zdeněk, Vacek K., Boháček V., Morita H.  
Nanostructured Unsaturated Carbon from Laser-Photo-Polymerization of Diacetylene.  
*Carbon* 42(12), 2521-2526 (2004).
33. Pola J., Pokorná D. Boháček J., Bastl Zdeněk, Ouchi A.  
Nano-structured Crystalline Te Films by Laser Gas-Phase Pyrolysis of Dimethyl Tellurium.  
*J. Anal. Appl. Pyrol.* 71, 739-746 (2004).
34. Srnová-Šloufová I., Vlčková B., Bastl Zdeněk, Hasslett T. L.  
Bimetallic (Ag) Au Nanoparticles Prepared by the Seed Growth Method:  
Two-Dimensional Assembling, Characterization by Energy Dispersive X-ray Analysis, X-ray Photoelectron Spectroscopy, and Surface Enhanced Raman Spectroscopy, and Proposed Mechanism of Growth.  
*Langmuir* 20(8), 3407-3415 (2004).
35. Tomovska R., Bastl Zdeněk, Pola J.  
UV Laser Chemical Vapor Deposition of Nano-Chained Copolymer from Carbon Disulfide and Ethene.  
*Macromol. Chem. Phys.* 205, 2339-2345 (2004).
36. Tomovska R., Urbanová M., Fajgar R., Bastl Zdeněk, Šubrt J., Pola J.  
UV Laser-Induced Gas-Phase Copolymerization of Carbon Disulfide and Ethene.  
*Macromol. Rapid Commun.* 25, 587-591 (2004).
37. Civiš Svatopluk, Juha L., Babánková Dagmar, Cvačka J., Frank O., Jehlička J., Králíková B., Krása J., Kubát Pavel, Muck A., Pfeifer M., Skála J., Ullschmied J.  
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The Application of Silver Amalgam Electrode in Voltammetric Determination of Cd, Pb and Cu in Reference Materials of Plant Origin (in Czech).  
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#### 4.4. Contributions in Monographs

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Selected Ion Flow Tube Mass Spectrometry (SIFT-MS) and Flowing Afterglow Mass Spectrometry (FA-MS) for the Determination of the Deuterium Abundance in the Water Vapour.  
In: *Handbook of Stable Isotope Analytical Techniques* (De Groot P. A., Ed.), pp. 88-104. Elsevier, Amsterdam 2004.
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#### 4.5. Patents

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Method to Produce Metal Selenide Thin Film.  
US Pat. No. 141:142733. Applied 3 August 2002, patented 5 August 2004.
2. Sobalík Zdeněk, Wichterlová Blanka, Markvart M., Tvarůžková Zdeňka  
Method of the Preparation of the Catalyst on Zeolite Base for Removal of Nitrogen Oxides from Waste Gasses by Reduction with Hydrocarbons (in Czech).  
CZ Pat. No. 293 917. Applied 3 May 2001, patented 23 June 2004.

#### 4.6. Popularization Papers

1. Zahradník Rudolf  
How to Tell It to Young Students? (in Czech).  
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2. Zahradník Rudolf  
Hans Hellmann: Life Story of a Scientist in the 20th Century (in Czech).  
*Chem. Listy* 98(1), 98-101 (2004).
3. Heyrovský Michael  
Jaroslav Heyrovský and Polarography  
*Resonance* (India) No.9, 51-57 (2004).

4. Heyrovský Michael  
Early Years of Cooperation between Japanese and Czech Polarographers (in Japanese).  
*Rev. Polarogr. (Japan)* 50, 314-317 (2004).
5. Heyrovský Michael  
The First Polarograph (in Czech)  
*Dějiny a současnost* No.6, 22-23 (2004).
6. Kalvoda Robert  
Polarography and Medicine (from the Viewpoint of the MEDLINE Internet Searcher) (in Czech).  
*Chem. Listy* 98(9), 831-833 (2004).
7. Heyrovská Rajalakshmi  
Gender is Nature's Creation, but Barrier is Man-Made.  
*Proc. Intern. Conf. "Women Scholars and Institutions"*, Prague, June 8-11, 2003  
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*Studies in the History of Sciences and Humanities*, 13 B, 817-821 (2004).

#### 4.7 Further Major Activities in the Popularization of Science

- a) Interview of Nobel Prize Winner Prof. R. A. Marcus, guest of the Institute, on Czech TV on June 17, 2004.
- b) Interview of Prof. Z. Herman in the journal *Česká Hlava* (Czech Head), No.1, 2004.
- c) Visit of students of the Gymnasium in Kladno, May 2004.
- d) Visit of 25 students of the J. Heyrovský Technical College for Chemistry in Ostrava, October 2004.
- e) Open Door Days for the public on November 12 and 13, 2004.
- f) Festive presentation of awards to the winners of competitions for secondary school students in professional disciplines on December 16, 2004.

#### 4.8 Organization of Local Conferences

Participation in the organization of the seminar "Modern Electrochemical Methods XXIV".  
Jetřichovice,  
3 - 6 May 2004, co-organizers T. Navrátil and L. Novotný, 40 participants from the Czech Republic.

## 5. LECTURES AND SEMINARS

Lectures and seminars organized in the Institute included

- annual Brdička Lecture,
- annual Student Seminar,
- institute seminars,
- departmental seminars.

In addition, research teams organized their internal colloquiums to discuss specific partial problems, methodical questions, progress in work, etc.

### 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 14<sup>th</sup> Brdička Lecture entitled

**“Strange Isotope Effects in Stratospheric Ozone  
and in the Earliest Minerals in the Solar System”**

was delivered on 17 June 2004 by Prof. Dr. **Rudolph A. Marcus** of California Institute of Technology, Pasadena, California.



### 5.2. Annual Student Seminar

The annual seminar of Ph.D. students and advanced undergraduates working on their diploma theses took place in Třešť from 22 to 24 June. Contributions were presented by 25 Ph.D. students and 2 undergraduates. Each student was awarded a financial premium according to the shown performance.

### 5.3. Institute Seminars

Of nine Institute seminars presented in 2004, five were held by members of the Institute and four by speakers from abroad.

05.02.	J. Schroeder <i>University Göttingen</i>	Separating different aspects of solvent effects on elementary chemical reactions
04.03.	P. Španěl <i>Heyrovský Institute</i>	SIFT MS - mass spectrometry in flow tube with selected ions
01.04.	M. Fárník <i>MPI für Strömungs- forschung, Göttingen und Universität Göttingen</i>	Dynamics of molecular clusters from the view of different spectroscopic methods
06.05.	Š. Urban <i>Heyrovský Institute</i>	Microwave high resolution spectroscopy: Theory and experiment. Results of the Joint Laboratory for High Resolution Molecular Spectroscopy of the Institute of Chemical Technology, Prague and the Heyrovský Institute
09.09.	Š. Sklenák <i>Heyrovský Institute</i>	An ONIOM study of the catalytic mechanism of yeast cytosine deaminase
14.10.	W. T. Hermens <i>University Maastricht</i>	Application of ellipsometry in the studies of protein membrane interactions
04.11.	S. Zálíš <i>Heyrovský Institute</i>	Quantum chemical modelling of optical and photochemical properties of carbonyl complexes of transition metals with mixed ligand sphere
25.11.	H. Schwarz <i>Technical University Berlin)</i>	Gas-phase catalysis by atomic and cluster metal ions: The ultimate single-site catalysts
09.12.	A. Vlček <i>Heyrovský Institute and Queen Mary's College, University of London</i>	Ultrafast dynamics of excited states. From excitation to photochemistry

#### 5.4. Departmental Seminars

60 seminars were held in 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	
Chemical Physics	3	3	13	19
Catalysis	23	0	8	31
Electrochemistry	9	0	2	11



**DEPARTMENT OF CHEMICAL PHYSICS****Internal speakers**

- 23.02. C. J. A. Bingham  
*(on leave from the University of Liverpool)* RAIRS, LEED and STM study of the adsorption of MAA, MHB and TA on Ni(110)
- 22.03. E. Devers  
*(on leave from Institut de Recherches sur la Catalyse, Villeurbanne)* Nanoparticles of platinum and platinum alloys supported over zirconia: Preparation, characterization and study of metal – support interactions
- 05.04. R. Čurik Scattering calculations on vibrational electron energy loss spectra

**Hosted speakers**

- 22.01. W. P. Reinhardt  
*University of Washington, Seattle* Quantum mechanism in the large: The Bose - Einstein condensate
- 08.03. J. Lazar  
*Institute of Scientific Instruments AS CR, Brno* Semiconductor lasers in spectroscopy and metrology
- 19.04. P. Milani  
*University of Milano* Supersonic cluster beam deposition of nanostructured films
- 26.04. B. Friedrich  
*Fritz-Haber Institut, MPG, Berlin* Manipulating molecules with nonresonant fields
- 10.05. P. Armentrout  
*University of Utah, Salt Lake City* Guided-beam studies of ion – molecule collisions
- 31.05. J. S. Francisco  
*Purdue University, Lafayette, IN* New frontier in atmospheric chemistry: Structure and reactivity of open-shell complexes
- 14.06. M. B. Mulcahy  
*University of Colorado, Boulder* Characterizing molecular sized rotors on glass and gold surfaces
- 06.09. F. Tureček  
*University of Washington, Seattle* Experimental and theoretical studies of radicals and dissociation products of DNA
- 13.09. L. Pichl  
*University of Aizu, Japan* Theoretical investigation of the electron capture in ion – molecule collisions
- 04.10. R. McCarroll  
*Université Pierre et Marie Curie, Paris* Photophysics of molecules in space

25.10.	M. Roeselová <i>Institute of Organic Chemistry and Biochemistry AS CR</i>	Processes at the water/air interface: Molecular dynamics simulations for atmospheric chemistry
08.11.	P. Jensen <i>Bergische Universität Wuppertal</i>	Modern approach to vibrational local modes
22.11.	P. Zemánek <i>Institute of Scientific Instruments AS CR, Brno</i>	Recent experiments in electron-molecule scattering
29.11.	F. Merkt <i>ETH Zurich</i>	High-resolution VUV laser spectroscopy
02.12.	P. Sherwood <i>Computational Sci &amp; Engng, Daresbury Laboratory, UK</i>	QM/MM modelling techniques for condensed phase reactions
06.12.	P. Rosmus <i>Université de Marne la Vallée, France</i>	A theoretical contribution to the ozone formation and its spectral analysis

## **DEPARTMENT OF CATALYSIS**

### **Internal speakers**

06.01.	L. Čapek	Analysis of the structure of Fe centers structure in zeolites
13.01.	A. Zukal	Morphology of mesoporous molecular sieves
20.01.	P. Sazama	State and properties of Ag in zeolites and alumina. Identification of structures at "in situ" catalytic reaction
03.02.	J. Dědeček	MAS NMR spectroscopy: Potentialities, applications, results
10.02.	O. Bortnovsky, P. Sazama	Cracking of C <sub>4</sub> and C <sub>5</sub> olefins on zeolitic catalysts
17.02.	B. Wichterlová	Aims and approaches in the projects of GA CR, GA ASCR, COST
02.03.	M. Kočířík	Aims and approaches in the project TROCAT of EU
	B. Wichterlová	Aims and approaches in the project AMMONORE of EU
09.03.	H. Drobná	<i>In situ</i> FTIR analysis of NO <sub>x</sub> selective reduction on alumina
16.03.	V. Gábová	Synthesis of zeolites with controlled Al distribution

23.03.	K. Juristová	Preparation of TiO <sub>2</sub> layers on ceramic supports
06.04.	J. Rathouský	Photocatalytic activity of hydrophobic mesoporous TiO <sub>2</sub> films
13.04.	J. Klisáková R. Hamtil	Catalysts for acylation reactions Metathesis of linear olefins catalyzed by Re <sub>2</sub> O <sub>7</sub> on organized mesoporous alumina
20.04.	K. Novoveská	<i>In situ</i> FTIR analysis of NO <sub>x</sub> selective reduction by hydrocarbons on Fe-zeolites
04.05.	H. Jirglová	Adsorption equilibria in zeolite catalysts
11.05.	M. Schwarze	Structure of Fe-zeolites for SCR-NO <sub>x</sub> .
18.05.	J. Pinkas L. Lukešová	Si migration in cyclopentadienyl complexes Si-substituted titanocene derivatives: Synthesis and reactivity
01.06.	V. Kreibich	Selective oxidation of benzene by N <sub>2</sub> O on zeolites
08.06.	I. Nekoksová P. Topka	Synthesis of Sn-MCM-41 catalyst for the Bayer-Villiger reaction Olefin metathesis
15.06.	P. Štěpánek	Reactions on zeolites in dynamical regimes
30.11.	H. Jirglová	Texture properties of the FCC catalyst and their correlation with self-diffusion coefficients of n-octane in catalyst particles
07.12.	A. Zukal	Adsorption of krypton on mesoporous solids
14.12.	D. Kaucký	Gaseous additives and kinetics of their functioning – a way to clarification of the reaction mechanism ?

**Hosted speakers**

14.01.	K. deJong <i>University of Utrecht</i>	Accessibility of active sites in mesoporous and microporous molecular sieves
31.05.	S. E. Park <i>Inha University of Korea</i>	Microwave synthesis of nanoporous materials and their catalytic application
23.06.	D. Seyferth <i>Massachusetts Institute of Technology, Cambridge, MA</i>	How organometallic chemistry began: Edward Frankland and his contemporaries

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12.07.	K. H. Theopold <i>University of Delaware, Newark</i>	Paramagnetic chromium alkyls as homogeneous olefin polymerization catalysts
05.10.	H. Toufar <i>Tricat Zeolites GmbH, Bitterfeld, Germany</i>	Special structural features of zeolites and their impact on the manufacturing process
26.10.	R. Bell <i>The Royal Institution of Great Britain</i>	Understanding the architecture of framework materials: the enumeration and evaluation of hypothetical zeolites
04.11.	L. Benco <i>University of Vienna</i>	DFT simulation of active sites in zeolites: CO adsorption on Cu-MOR
23.11.	H. Gies <i>Ruhr University, Bochum</i>	New synthesis strategies for the development of new zeolite materials in catalysis and separation

### **DEPARTMENT OF ELECTROCHEMISTRY**

#### **Internal speakers**

20.02.	L. Pospíšil	Automation of electrocapillary measurements
19.03.	Z. Samec	Catalytic oxidation of guanine derivatives on SnO <sub>2</sub> electrode. Ionization and electrode potentials
16.04.	S. Zálíš	Tautomerism of substituted chinons and chinon diimines affected by metals: Modelling of the metal–chinoproteins interaction
30.04.	Z. Samec	Effect of the membrane phase volume on the potential of an ion-selective electrode
14.05.	M. Rejňák	Reduction and dimerization of benzothiophens
28.05.	M. Kalbáč	Electrochemistry of nanostructured carbon
22.10.	B. Yosypchuk	Electrodes prepared from solid amalgams
03.12.	P. Krtíl	Effect of particle size on the insertion behaviour of nanocrystalline oxides
17.12.	J. Ludvík	Electron delocalization in carbene complexes

#### **Hosted speakers**

23.01.	D. Fermin <i>University Bern</i>	2D and 3D electrostatic assembly of metal nanoparticles on modified gold electrodes: Organization and electrochemical reactivity
19.11.	N. Serrano <i>University of Barcelona</i>	Potentiometric stripping analysis as a tool for heavy metal speciation

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## 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). The Institute continued to serve as the main coordinator of the project "Advanced nanostructured metal/metaloxo/matrix catalysts for redox processes. Application for NO<sub>x</sub> reduction to nitrogen" of the 5<sup>th</sup> EC framework programme GROWTH.

Members of the Institute published 107 joint papers jointly with authors from institutions abroad (Chap. 4).

The Institute functioned as Marie Curie Training Site of EC in quantum chemical methods and quantum molecular dynamics; and as a member of two Research Training Networks of EC concerning generation, stability and reaction dynamics of multiply charged ions, and electron and positron induced chemistry (EPIC) (Sect. 6.2).

Visitors from abroad gave 28 lectures and seminars in the Institute (Chap. 5). The Institute organized 7 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, 16 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 2004 (30 days or longer)

Name	Country	Length (days)	Host	Department
Ch. Bingham	United Kingdom	60	Z. Bastl	<u>Chemical Physics</u>
V. Brems	Germany	245	P. Čársky	
E. Devers	France	330	Z. Bastl	
P. Durand	France	50	I. Paidarová	
L. Fekete	Austria	30	Z. Herman	
P. Jurkiewicz	Poland	250	M. Hof	
T. Kral	Poland	150	M. Hof	
E. Miliordos	Greece	90	P. Čársky	
K. Nikiforov	Russia	90	Z. Knor	
B. Pezler	Poland	150	P. Čársky	
V. Temperakidis	Greece	90	P. Čársky	
W. Szczepanik	Poland	180	P. Čársky	
R. Volinsky	Israel	90	M. Hof	

				<u>Electrochemistry</u>
M. Makarova	Russia	245	P. Krtil	
B. Lajoie	France	50	J. Ludvík	
N. S. Plana	Spain	84	I. Šestáková	

### 6.3. International Scientific Meetings Arranged by the Institute

Concluding Meeting of the European Network Programme "Generation, Stability and Reaction Dynamics of Multiply-Charged Ions" (MCI-Net, 2000-2004).

Prague, 10 -11 June 2004, organizers Z. Herman and J. Hrušák. 24 participants including 18 from abroad.

37th Heyrovský Discussion "Electrochemistry on Liquid-Liquid Interfaces".

Třešť, 13-17 June 2004, organizers Z. Samec and V. Mareček. 51 participants including 40 from abroad.

Satellite Meeting on Carbon Nanostructures.

Prague, 21 July 2004, co-organizer L. Kavan. 19 participants including 10 from abroad.

19th International Conference on High Resolution Molecular Spectroscopy.

Prague, 8-12 September 2004, organizer Š. Urban. 196 participants including 182 from abroad.

7th Pannonian International Symposium on Catalysis.

Srní, 12-16 September 2004, organizer Z. Sobalík. 128 participants including 73 from abroad.

2nd Prague Seminar on Biophysics of Lipids.

Prague, 6–9 October 2004, organizer M. Hof. 26 participants including 17 from abroad.

36th Symposium on Catalysis.

Prague, 8–9 November 2004, organizer J. Čejka. 96 participants including 21 from abroad.



19th International Conference on High Resolution Molecular Spectroscopy-  
Ioannes Marcus Marci Session



37th Heyrovský Discussion "Electrochemistry  
on Liquid-Liquid Interfaces"

## 7. COOPERATION WITH UNIVERSITIES IN THE CZECH REPUBLIC

### Acronyms used:

CU – MED	Charles University, Prague, 1 <sup>st</sup> 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
TUB – CHEM	Technical University of Brno, Faculty of Chemistry
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 2004	10	180
Winter 2004	14	387
Total	24	567

Number of lecturers from the Institute: 18

Number of faculties involved: 7

**DEPARTMENT OF CHEMICAL PHYSICS**

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	22
M. HOF	<i>Spectroscopy (in English)</i>	CTU – NUC	W	30
Z. KNOR (WITH B. WICHTERLOVÁ)	<i>Adsorption and catalysis</i>	ICHT – TEC UPAR – TEC	S	20
J. PITTNER	<i>Theory of unitary group and the CI method</i>	CU – SCI	W	30
J. PITTNER	<i>Structure of molecules</i>	CU – SCI	W	26
Š. URBAN	<i>Selected chapters of chemical physics</i>	ICHT – ENG	W	34

**DEPARTMENT OF CATALYSIS**

Lecturer	Lecture course	Faculty	Semester	Hours
J. ČEJKA	<i>Principles and methods of heterogeneous catalysis</i>	ICHT – TEC	W	28
J. ČEJKA	<i>Zeolites and microporous inorganic materials: synthesis, structure, characterization and application</i>	ICHT – TEC	W	30
J. ČEJKA	<i>Chemical principles of industrial manufacturing</i>	CU – SCI	W	45
Z. SOBALÍK	<i>Spectroscopical characterization of heterogeneous catalysts</i>	ICHT – TEC	W	28
B. WICHTERLOVÁ (WITH Z. KNOR)	<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	32
V. MAREČEK	<i>Experimental methods in electrochemistry</i>	ICHT – TEC	S	7
T. NAVRÁTIL	<i>Medical chemistry and electrochemistry</i>	CU – MED	W	10
L. NOVOTNÝ	<i>General and applied electrochemistry for environmental purposes</i>	UPAR – TEC	W	26
L. NOVOTNÝ	<i>Electroanalytical chemistry</i>	UPAR – TEC	S	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	S	4

**7. 2. Training Courses for Undergraduates**

Synopsis:

Semester	Number of courses	Hours per semester
Summer 2004	10	116
Winter 2004	8	125
Total	18	241

Number of course leaders from the Institute: 16

Number of faculties involved: 7

**DEPARTMENT OF CHEMICAL PHYSICS**

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>Theory of unitary group and the CI method</i>	CU – SCI	W	14
Š. URBAN	<i>Selected chapters of molecular physics</i>	ICHT – ENG	S	17
Z. ZELINGER	<i>Spectroscopic methods for investigation of atmospheric pollution</i>	CU – SCI	S	20
J. ŽABKA	<i>Physics II: Electrostatics and electrical circuits</i>	ICHT – TEC	W	32
J. ŽABKA	<i>Physics II: Electrostatics and electrical circuits</i>	ICHT – FBT	W	32

**DEPARTMENT OF CATALYSIS**

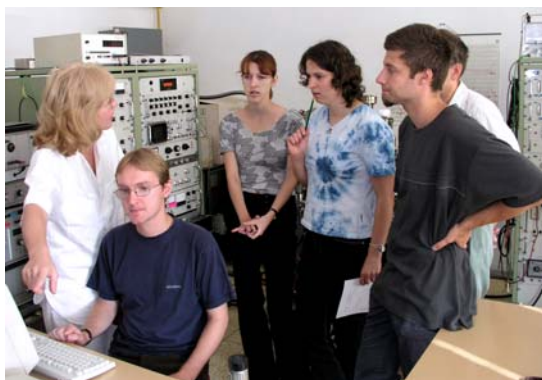
Course leader	Training course	Faculty	Semester	Hours
L. BRABEC	<i>Scanning electron microscopy</i>	CTU – NUC	S	3
L. BRABEC	<i>Electron microscopy</i>	CU – SCI	W	4
K. MACH	<i>Electron spin resonance</i>	CTU – NUC	S	6
J. NOVÁKOVÁ	<i>Intermediates in catalytic reactions: Application of stable isotopes</i>	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
A. ZIKÁNOVÁ, H. JIRGLOVÁ	<i>Reactor techniques</i>	CU – SCI	W	4

**DEPARTMENT OF ELECTROCHEMISTRY**

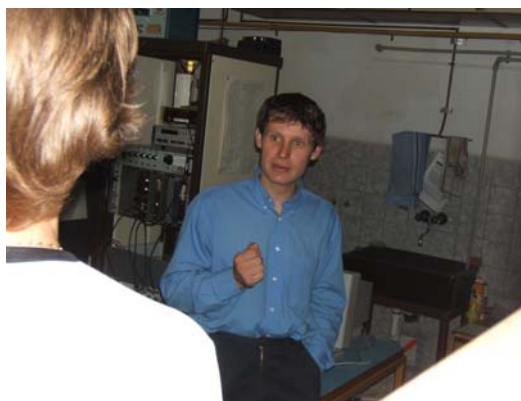
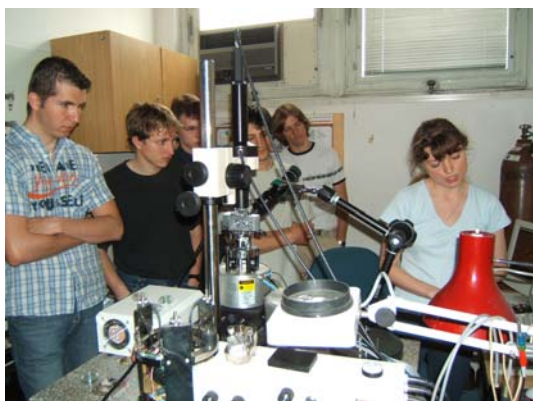
Course leader	Training course	Faculty	Semester	Hours
T. NAVRÁTIL	<i>Electrochemical methods in medical chemistry and biochemistry</i>	CU – SCI	S	18
T. NAVRÁTIL	<i>Medical chemistry and biochemistry</i>	CU – MED	W	24
I. ŠESTÁKOVÁ	<i>Electrochemical methods</i>	CUA – AGR	S	24

### 7.3. Summer School for Ph.D. Students and Post-docs

Summer school "Spectroscopic methods and their application in catalysis, surface and material science, atmospheric chemistry and biodisciplines". Prague, 29 August - 3 September 2004, organizers S. Černý and K. Stejskalová.



65 participants (Ph.D. students and post-docs of universities and research institutions in Czech Republic).



### 7.4. Supervision of Theses

62 Ph.D. Theses and 10 Diploma Theses were supervised by members of the Institute's staff, in most cases jointly with teachers at universities. On 49 Ph.D. theses worked students imbursed at least partially by the Institute. On 13 Ph.D. theses worked students imbursed by other institutes or graduates who did not have the status of Ph.D. students.

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

## Supervised Ph.D. Theses

DEPARTMENT OF CHEMICAL PHYSICS

Student	Faculty	Thesis title	Supervisor in the Institute	Start	Remark
M. Šimečková	CU-MAT	Hyperfine effects in high resolution spectra of molecules	Š. Urban	1999	Defended in 2004
M. Beneš	CU-SCI	Fluorescence correlation spectroscopy: Characterization of planar phospholipid bilayer systems for protein-membrane interactions	M. Hof	2000	Terminated in 2004
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	
J. Sýkora	CU-SCI	Solvent relaxation in biomolecules	M. Hof	2002	
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	
P. Hrubý	ICT-ENG	Energetic and electronic factors in surface phenomena on metals	Z. Knor	2003	Terminated in 2004

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

**DEPARTMENT OF CATALYSIS**

Student	Faculty	Thesis title	Supervisor in the Institute	Start	Remark
L. Čapek	UPAR-TEC	Selective catalytic reduction of NO <sub>x</sub> by hydrocarbons	B. Wichterlová	1998	Defended in 2004
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	
M. Slabová – Staňková	ICHT-ENG	Highly ordered nanostructures of titanium dioxide	A. Zukal	2000	
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	
P. Mokrejš	CU-SCI	Interaction of bentonites with surroundings in dependence on the bentonite history and actual physico-chemical conditions	A. Zikánová	2000	
J. Pinkas	CU-SCI	Low-valent titanocene – amid complexes	K. Mach	2000	Defended in 2004

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	
K. Kovan- dová-Juristová	ICHT-TEC	Preparation and characterization of SiO <sub>2</sub> -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	
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	
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	
M. Fryčová- Šnábllová	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	
P. Štěpánek	CU-SCI	Redox catalysis on zeolites in dynamical regimes	Z. Sobalík	2003	Terminated in 2004
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 <sub>2</sub> activation in chemical synthesis	Z. Sobalík	2004
T. Trávníček	UPAR	Relation of catalytic activity of zeolites with transition metal cations	Z. Sobalík	2004

**DEPARTMENT OF ELECTROCHEMISTRY**

Student	Faculty	Thesis title	Supervisor in the Institute	Start	Remark
P. Bašová	CU–SCI	Electroanalysis and electrochemistry of selected biologically active substances	L. Novotný	1996	Defended in 2004
V. Dorčák	CUA–AGR	Application of electrochemical methods to the study of plant metallothioneins and their complexes with heavy metals	I. Šestáková	1999	
J. Houser	TUB–CHEM	Potentialities of new voltammetric methods for solution of selected problems of the environment protection connected with the analysis of wastes with monomeric and polymeric matrices	L. Novotný	1999	
J. Pícha	ICHT–TEC	Synthesis of aryl-methyl-ketoximes and study of their properties	J. Ludvík	1999	
H. Hoffmannová	ICHT–ENG	Study of electrochemically initiated intermediates	P. Krtil	2000	
H. Měšťánková	ICHT–TEC	Comparative investigation of phenylurea derivatives degradation in aqueous TiO <sub>2</sub> suspensions and Fe(III) solutions	J. Jirkovský	2002	Defended in 2004
D. Rozbroj	ICHT–ENG	Electrochemical study of azo-methine bonds	J. Ludvík	2001	
R. Fadmá	UPAR–TEC	Electrochemical study of selected bioactive systems using electroanalytical sensors	L. Novotný	2001	Defended in 2004



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S. Šebková	UPAR–TEC	Electroanalysis of selected ecologically significant compounds and complexes using suitable experimental arrangement of electrodes	L. Novotný	2001	Defended in 2004
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. Krtil	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. Záliš	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	

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## 7.5. Joint Projects and Publications

Members of the Institute's staff worked on 33 joint grant projects with universities in the Czech Republic (see Sect. 3). In 21 and 12 joint projects they acted as project leaders and associated contractors, respectively.

56 joint papers were published (see Sect. 4).

## 7.6. Membership in University Bodies

12 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 CHEMICAL PHYSICS**

- P. Čársky:       ▪ 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)
- Z. Knor           ▪ Branch Council for Physics of Surfaces and Interfaces in the Ph.D. study  
program "Physics" (Fac. Mathem. and Phys., Charles Univ.)
- Branch Council for Physical Chemistry in the Ph.D. study program  
"Chemistry" (Fac. Chem. Engng, Institute of Chem. Technol. 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**

- 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.)
- 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. Novotný
- Examining Board for state finals in analytical chemistry (Fac. Chem. Technol., Univ. Pardubice)
- 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. 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. Mická	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. Microporous Mesoporous Mater. 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 CHEMICAL PHYSICS

- 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
- V. Hanuš
- *Learned Society of CR* – member
  - *European Academy of Sciences and Arts (Salzburg)* – 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
- 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

- 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
  - *Grant Agency of CR, Branch Council for Natural Sciences* – member; *Sub-council for chemistry and biochemistry* – head
  - *Czech Chemical Society, Czech Zeolite Group* – member of the Committee
  - *Academy of sciences, Commission for awarding DSc degrees*

**DEPARTMENT OF ELECTROCHEMISTRY**

- L. Kavan
- *Grant Agency of CR, Scientific Committee 203* – member
  - *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- D14* – 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
- V. Mareček
- *Grant Agency of the Academy of Sciences* – vice-chairman
  - *Ministry of Education of Slovak Republic, Commission for awarding DrSc. degrees in inorganic technology and materials* – member
  - *The Electrochemical Society (USA)* – member
  - *International Society of Electrochemistry* – member
- L. Novotný
- *Czech National Committee of IWSA (International Water Services Association)* – 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 CR, Branch Council for Chemical Sciences* – member
  - *Czech Committee for 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

Conferment of DrSc. degree by the Slovak Academy of Sciences

### **8.4. Awarded Prizes and Honors**

Ing. Libor Čapek, Ph.D.

Prize of the Ministry of Education, Youth and Sports of CR for outstanding students and Ph.D. students

RNDr. Jiří Dědeček, RNDr. Zdeněk Sobalík, CSc., Ing. Blanka Wichterlová, DrSc.

Prize of the Czech Academy of Sciences for outstanding project

Mgr. Michal Fárník, Ph.D.

J. E. Purkyně Fellowship

Mgr. Michal Horáček, CSc.

Josef Hlávka Prize

Ing. Jana Mayerová-Klisáková

Prize of the Group for Catalysis of the Czech Chemical Society

Ing. Pavla Prokešová

Prize of the Group for Catalysis of the Czech Chemical Society

Mgr. Lenka Lukešová

Prize for the 3rd place in the 2004 competition of doctoral dissertations in chemistry in CR, awarded by the French Embassy and the Company Rhodia

RNDr. Štěpán Sklenák, Ph.D.

J. E. Purkyně Fellowship