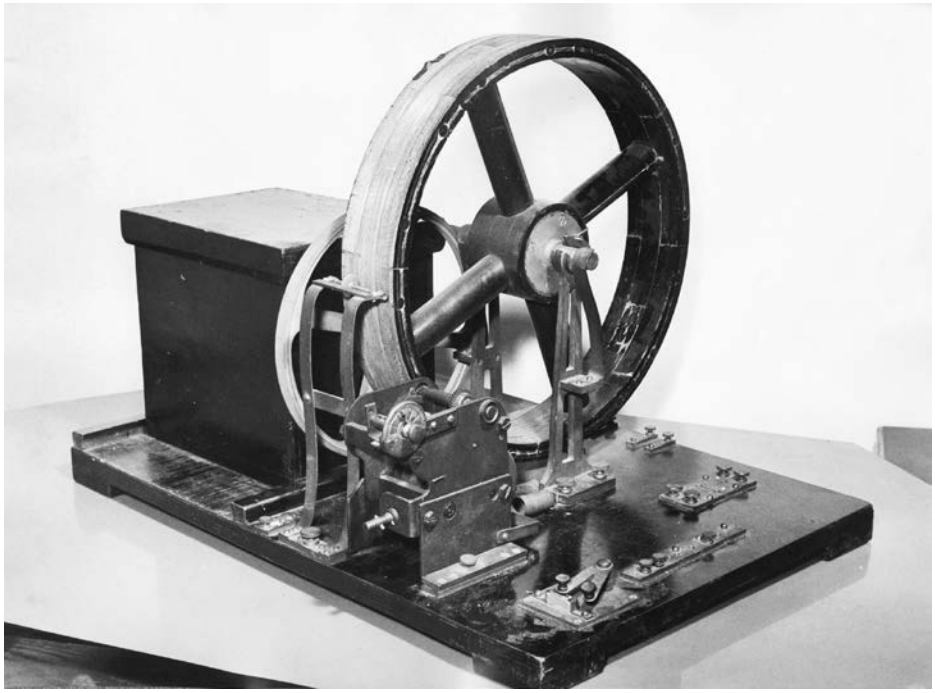
J.Heyrovský Institute
of Physical Chemistry



ANNUAL REPORT 2019

ON ACTIVITY AND ECONOMIC MANAGEMENT

J. Heyrovský Institute of Physical Chemistry

J. Heyrovský Institute of Physical Chemistry (HIPC)
of the Czech Academy of Sciences (CAS), public research institution (p.r.i.)
Identification Number: 61388955
Address: Dolejškova 2155/3, 182 23 Praha 8
Discussed by the Supervisory Board on 9th June 2020
Approved by the The Board on 24th June 2020

In Prague on 26th June 2020

Index

I. Information on bodies of the public research institution and on their activity

A) Initial members of the bodies of the institute

The director of the institution

Prof. Martin Hof, Dr. rer. nat. DSc.

appointed effective from 1st May 2017

The Board

Elected on: 23rd January 2017; members:

Chairman: prof. RNDr. Patrik Španěl, Dr. rer. nat.

Vice-chairman: prof. RNDr. Ladislav Kavan, CSc., DSc.

Internal members (HIPC)

prof. Martin Hof, Dr. rer. nat. DSc.
Mgr. Michal Horáček, Ph. D.
doc. Mgr. Jiří Pittner, Dr. rer. nat., DSc.
prof. RNDr. Zdeněk Samec, DrSc.
Mgr. Jiří Dědeček, CSc., DSc.
RNDr. Martin Ferus, Ph.D.
Mgr. Magdaléna Hromadová, Ph. D.
doc. RNDr. Ing. Martin Kalbáč, Ph. D.

External members:

prof. RNDr. Jiří Barek, CSc.
Faculty of Science, Charles University in Prague

prof. Dr. Ing. Karel Bouzek
Faculty of Chemical Technology,
University of Chemistry and Technology, Prague

prof. Mgr. Pavel Jungwirth, CSc., DSc.
Institute of Organic Chemistry and Biochemistry of the CAS

prof. Dr. RNDr. Pavel Matějka
Faculty of Chemical Technology,
University of Chemistry and Technology, Prague

prof. RNDr. Eva Tesařová, CSc.
Faculty of Science, Charles University in Prague

Supervisory Board

Chairman:	Ing. Petr Bobák, CSc., Institute of Animal Physiology and Genetics of the CAS
Vice-chairman:	RNDr. Jan Hrušák, CSc., J. Heyrovský Institute of Physical Chemistry
Members:	Ing. Zbyněk Černý, CSc. Institute of Inorganic Chemistry of the CAS
	prof. Ing. Jiří Homola, CSc., DSc. Institute of Photonics and Electronics of the CAS
	doc. Mgr. Iva Matolínová, Dr. Faculty of Mathematics and Physics, Charles University in Prague

B) Changes in the bodies of the institute

In 2019, there were no changes in the bodies of the institute.

C) Information on activity of the bodies

The director of the institute

Main management activities of the director:

a) Organization of meetings of the director's board, which took place a total of 14 times in 2019. The conclusions of the meetings are published on the internal website of HIPC.

b) Submission of the draft budget for 2019 to the Supervisory Board for comments and the The Board for approval.

c) Submission of the Annual Report on Activities and Economic Management for 2018 to the Supervisory Board for an opinion and to the The Board for approval after the auditor's verification of the closing financial statement.

d) Submission of proposals for the Otto Wichterle Award, the Josef Hlavka award and the Academic Award (Praemium Academiae).

e) Submission of proposals for actions requiring the prior consent of the Supervisory Board to this board for approval.

f) Preparation and conclusion of an amendment to the Collective Agreement with the Trade Union Organization concerning the principles and budget for drawing from the social fund in 2019.

g) Recruitment of new staff on the basis of open competition and decision on extension or reassignment of staff of the HIPC on the basis of performance evaluation.

h) Organization of the 29th R. Brdicka Memorial Lecture.

i) Appointment of a Monitoring Group for the implementation process of Human Resources Strategy for Researchers (HRS4R) in connection with the award "HR Excellence in Research Award".

j) Appointment of the commissions, including the Evaluation Commission and Commission for Ethics of Scientific Work. Furthermore, the director carried out the appointment of a scientific ombudsman, the appointment of a project group and the determination of the Criteria for the Evaluation of Scientific Work.

The Board

In 2019, meetings of the The Board took place a total of 22 times, of which 19 meetings took place in the form of voting by mail (per rollam).

8th meeting of the The Board (2nd May 2019)

- The Board approved the budget of the HIPC for 2019.

- The Board approved the minutes and resolutions of the 7th meeting of the The Board (of 6th December 2018).

- The Board approved the minutes and resolutions of the voting by mail of 17th December 2018, 31st January 2019, 7th March 2019, 25th March 2019, 28th March 2019 and 18th April 2019.

9th meeting of the The Board (20th June 2019)

- The Board approved the minutes and resolutions of the 8th meeting of the The Board (of 2nd May 2019).

- The Board approved the minutes and resolutions of the voting by mail of 27th May 2019, 5th June 2019 and 13th June 2019.

- The Board takes note of the submitted Annual Report on Activities and Economic Management for 2018, including the attached report of the independent auditor, and agrees with its wording.

- The Board agrees with the content of the letter from the Director of the HIPC to the Rector of Palacký University Olomouc expressing support for efforts to maintain a high standard of ethics of scientific work.

10th meeting of the The Board (25th November 2019)

- The Board approved the minutes and resolutions of the 9th meeting of the The Board (of 20th June 2019).

- The Board approved the minutes and resolutions of the voting by mail of 4th July 2019, 11th July 2019, 22nd August 2019, 30th August 2019, 11th September 2019, 18th September 2019, 20th September 2019, 26th September 2019, 14th October 2019, 4th November 2019, 11th November 2019, 15th November 2019 and 17th November 2019.

- The Board, based on consultation with the international advisory board, proposes to elect ombudsmen at an assembly of all university-educated staff of the institute's scientific departments convened by e-mail. The Board also proposes a term of office for the Ombudsman of 3 years with a term limit of two terms.

- The Board proposes to extend the criteria for the evaluation of scientific work to include a contribution to the creation of intellectual property and to demonstration of an independent vision of scientific work and instructs P. Španěl to propose a modified wording of the criteria until the next evaluations are announced.

The Board approved following resolutions by mail:

- The Board supported the submission of a total of 79 grant project proposals, of which 40 were submitted to the Czech Science Foundation (CSF) and 3 projects were submitted to the Ministry of Education, Youth and Sports (MEYS).

- The Board agrees with the nomination of RNDr. Viliam Kolivoška, Ph.D., MBA, Ing. Petr Kovaříček, Ph.D. and Mgr. Ing. Eva Krupičková Pluhařová, Ph.D. for the "Otto Wichterle Award".

- The Board approves the documents "RULES FOR DRAWING THE SOCIAL FUND of the J. Heyrovský Institute of Physical Chemistry of the CAS, p.r.i. for the year 2019" and "Budget for drawing the social fund for the year 2019" in the submitted wording.

- The Board recommends submitting an application for support from the Programme to support prospective human resources – Wage support of postdocs in the institutes of the CAS for the following candidates in the following order:

1.) Mgr. Monika Klusáčková, Ph.D.

2.) Mgr. Štěpánka Nováková Lachmanová, Ph.D.

3.) Ashok Chilukoti, Ph.D.

1.) Mgr. Zuzana Melníková, Ph.D.

2.) RNDr. František Vavrek, Ph.D.

- The Board recommends the appointment of a "Commission on the Ethics of Scientific Work" with following members:

Chairman: FRANK Otakar

Vice-chairwoman: DRYAHINA Kseniya

Members: ČURÍK Roman, SÝKORA Jan, TABOR Edyta, HORÁČEK Michal, MINHOVÁ MACOUNOVÁ Kateřina, FEDOR Juraj and KRUPIČKOVÁ PLUHAŘOVÁ Eva.

- The Board approves the award of the position of "significant researcher" to Dr. Karel Mach as a half-time job for a period of two years.

- The Board approves "Annex No. 1 - A schedule of wage rates and bonuses for management" of the Internal Wage Regulations of the HIPC as submitted.

- The Board approved the wording of the Guidance on Authorship in Scientific Publications.

- The Board agrees with the conclusion of the submitted Memorandum on Cooperation between the HIPC and the Police of the Czech Republic.

All the resolutions of voting by mail were approved without changes at the next possible board meeting.

Supervisory Board

In 2019, a meeting of the Supervisory Board of the J. Heyrovský Institute of Physical Chemistry of the CAS, p.r.i. took place on 31st May 2019. Six meetings by mail took place due to 24th January 2019, 28th March 2019 (two meetings), 28th June 2019, September 23rd, 2019, November 26th, 2019.

Meeting of the Supervisory Board on 31st May 2019

- The Supervisory Board discussed the Draft Budget of the HIPC for 2019.

It further suggests that the inclusion of profits in the reserve fund be discussed by mail and recommends that more detailed information be drawn up on the statement of economic contracts.

- The Supervisory Board discussed and takes note of the Annual Report on Activities and Economic Management for 2018.

- The Supervisory Board approves the Report on the Activities of the Supervisory Board for 2018.

- The Supervisory Board discussed and took note of the text of the Auditor's report on the audit of the 2018 financial statement. The auditor for the verification of the financial statements for the year 2019 according to the Audit Agreement was appointed Ing. L. Ježek.

- The Supervisory Board approves the Evaluation of the Managerial Abilities of the Director of the HIPC according to the submitted proposal.

The Supervisory Board approved the following resolution by mail:

1) The Supervisory Board agrees with the Agreement on the lease of space used for business with the company Three Bond Czech s. r. o., main office: U Slovanky 1388/5, 182 00, Praha 8 - Libeň.

The approval took place by mail No. 45 on 24th January 2019.

2) The Supervisory Board agrees with the Agreement on the lease of space used for business with Mr. Ivan Černý, Diviznová 1087, 250 82, Květnice.

The approval took place by mail No. 45 on 24th January 2019.

3) The Supervisory Board agrees with the Agreement on the lease of space used for business with Mrs. Dana Kapková, Famfulíkova 1133/14, 182 00, Praha 8- Kobylisy.

The approval took place by mail No. 47 on 28th March 2019.

4) The Supervisory Board discussed the Agreement on the lease of space used for business with the company Advanced Materials – JTJ s. r. o., Kamenné Žehrovice čp. 23, 273 01, Kladno and grants prior written consent to the conclusion of this agreement.

The approval took place by mail No. 48 on 28th March 2019.

5) The Supervisory Board agrees with the Agreement on the lease of non-residential space with Institute of Physics of the CAS, p.r.i., Na Slovance 1999/2; 182 21 - Ládví.

The approval took place by mail No. 49 on 23rd September 2019.

6) The Supervisory Board agrees with the Agreement on accommodation in a rooming house with the Institute of Plasma Physics of the CAS, p.r.i., Za Slovankou 1782/3, 182 00 Praha 8-Libeň.

The approval took place by mail No. 50 on 26th November 2019.

All members of the Supervisory Board and the The Board signed an affidavit stating that they were not aware that they or their family members were involved in juridical persons with whom the accounting unit, the J. Heyrovský Institute of Physical Chemistry of the CAS, p.r.i., concluded business contracts or other contractual relationships in accounting period from 1st January 2019 until 31st December 2019.

II. Information on changes in the founding deed

No changes were made to the founding deed in 2019.

III. Assessment of the main activity

In accordance with the valid founding deed, the HIPC carries out scientific research in the field of **physical chemistry, electrochemistry, analytical chemistry and chemical physics** and seeks the possibility of using its research results.

According to the valid founding deed as amended by the amendment of 22nd June 2010, the main activity of the HIPC is scientific research in physical chemistry, electrochemistry, analytical chemistry and chemical physics, especially research on the structure of substances and their properties, research on elementary processes of chemical reactions and processes, research of chemical and physicochemical processes in homogeneous phase and at phase interface, preparation and development of chemical compounds, materials and technologies, development of special physical and physicochemical methods and equipment and development of computer programs for quantum chemical and other theoretical calculations in the fields of the HIPC activity and for control of experiments and processing of results of the HIPC. Through its activities, the HIPC contributes to increasing the level of knowledge and education and to the use of the results of scientific research in practice. HIPC acquires, processes and disseminates scientific information, publishes scientific publications (monographs, journals, proceedings, etc.), provides scientific opinions, expert opinions and recommendations, and performs consulting and advisory activities. In

cooperation with universities, it carries out PhD programs and educates researchers. It organizes lectures, seminars and internships for students. Within the scope of its activities, HIPC develops international cooperation, including the organization of joint research with foreign partners, the recruitment and posting of interns, the exchange of scientific knowledge and the preparation of joint publications.

HIPC organizes domestic and international scientific meetings, conferences, seminars and lectures and provides research infrastructure, including providing accommodation for its employees and guests and providing catering in the cafeteria in the CAS premises "Mazanka" for employees of the Academy of Sciences of the Czech Republic. HIPC carries out projects independently and in cooperation with universities and other scientific and expert institutions.

In 2020, the HIPC continued its theoretical and experimental research in selected areas of chemical physics, electrochemistry, catalysis and related fields. Research activities take place in 12 departments and one scientific research center.

The HIPC actively supports collaboration at international level: currently, there are 88 foreign scientists in the HIPC and total number of scientists is 234.

The International Advisory Board was established as an advisory body to the director.

Its members:

prof. Timo Jacob, Ulm University, Germany

prof. Philipp Kukura, University of Oxford, United Kingdom

prof. Peter Rapta, Slovak University of Technology in Bratislava, Slovakia

prof. Dr. Jeroen Anton van Bokhoven, ETH Zürich, Switzerland

prof. Dr. Leticia Gonzales, Universitat Wien, Austria

III. 1 The most important results

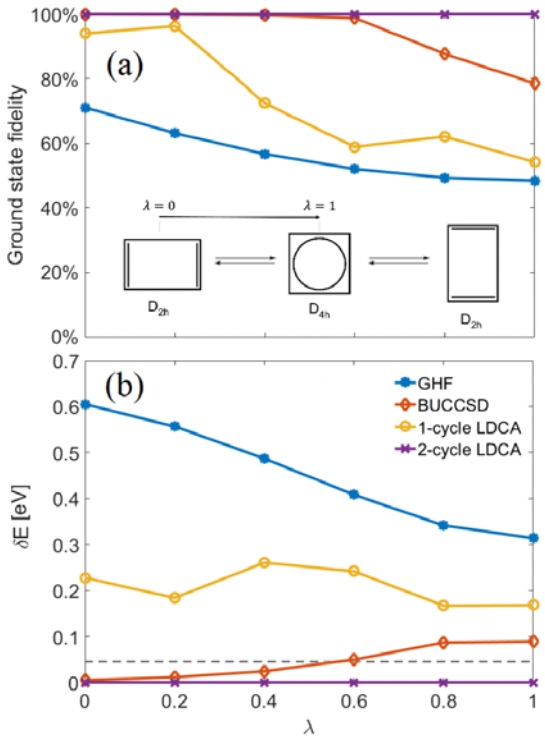
The research plan and the grants supported by the Czech Science Foundation (CSF) achieved important results that are described in this section according the departments.

Department of Theoretical Chemistry (1)

Low-depth circuit ansatz for preparing correlated fermionic states on a quantum computer

We have introduced the new circuit ansatz for preparing correlated fermionic states on a quantum register which, unlike other approaches, employs the generalized Hartree-Fock reference and is thus able to properly describe strongly correlated systems (in physics and chemistry). Moreover, by augmenting the set of available quantum gates with nearest-neighbor phase coupling, we have generated the circuit ansatz with remarkable accuracy. (in physics and chemistry). Moreover, by augmenting the set of available quantum gates with nearest-neighbor phase coupling, we have generated the circuit ansatz with remarkable accuracy.

Collaborating entity: Department of Chemistry and Chemical Biology, Harvard University, Cambridge MA, 02138



Automerization of cyclobutadiene. *The tests of accuracy of the almost linear quantum circuits (LDCA1, LDCA2) for preparation of fermionic states: the example of the automerization of cyclobutadiene.*

P. L. Dallaire-Demers, J. Romero, L. Veis, S. Sim, A. Aspuru-Guzik, Low-depth circuit ansatz for preparing correlated fermionic states on a quantum computer, Quantum Science and Technology, 2019, 4, 4, 045005

R-matrix calculations of electron collisions with a lithium atom at low energies

R-matrix calculations of the electron collisions with a lithium atom at energies below the 3s excitation threshold are presented. The ^1S^e, ^3S^e a ^1P^o phase shifts calculated in the near-threshold energy range are in excellent agreement with previous theoretical studies.

The threshold behavior of the ^3P^o phase shift is accurately analyzed along with the resonance located at the scattering energy ~60 meV. The phase shifts and cross sections calculated here show two resonances below the 3s threshold that have not been previously reported.

M. Tarana and R. Čurík, R-matrix calculations of electron collisions with a lithium atom at low energies, Phys. Rev, 2019, A 99, 012708

Department of Spectroscopy (2)

Identifiable Acetylene Features Predicted for Young Earth-like Exoplanets with Reducing Atmospheres Undergoing Heavy Bombardment

The chemical environments of young planets are assumed to be largely influenced by the impacts of bodies lingering on unstable trajectories after the dissolution of the protoplanetary disk. We provide simulated transit spectra for an Earth-like exoplanet and we predict that acetylene is as observable as other molecular features on exoplanets with reducing atmospheres that have recently gone through their own “heavy bombardments,” with prominent features at 3.05 and 12 μm.

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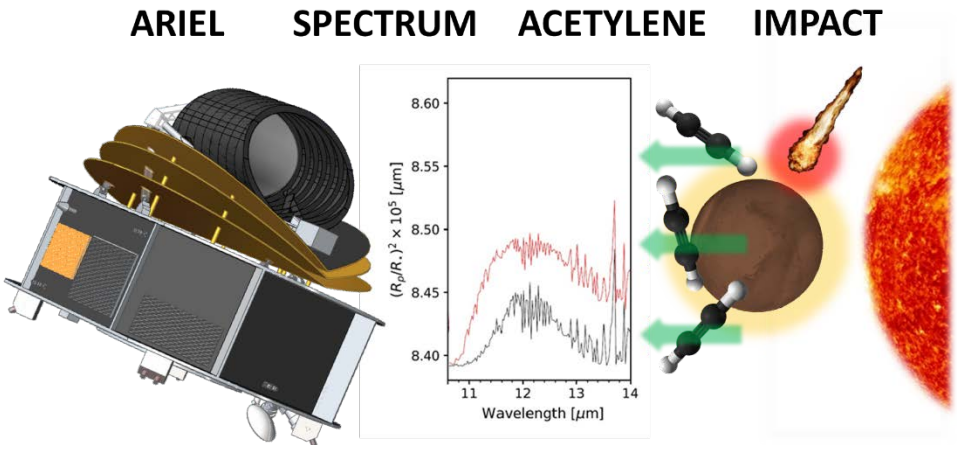


Identifiable acetylene feature after impact event observed by ARIEL satellite. *Spectra of exoplanets will be recorded by future ESA ARIEL satellite mission. Feature of acetylene produced by impact event chemistry will be observable in transition spectrum around 12 μm.*

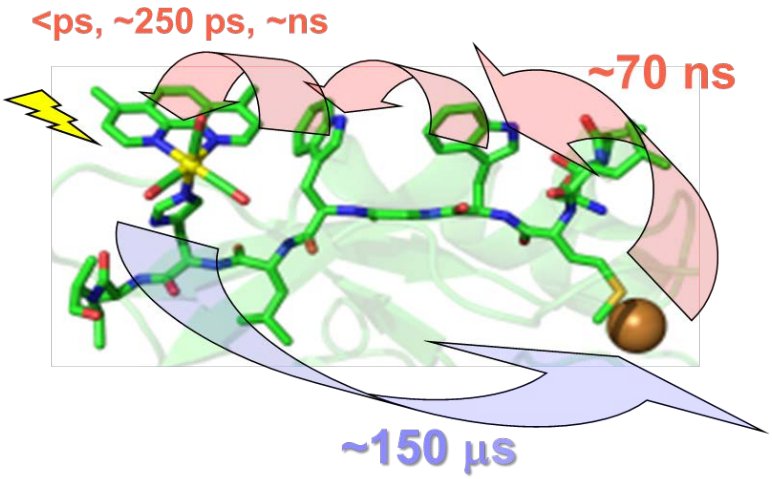
P. B. Rimmer, M. Ferus, I. P. Waldmann, A. Knížek, D. Kalvaitis, O. Ivanek, P. Kubelík, S. N. Yurchenko, T. Burian, J. Dostál, L. Juha, R. Dudžák, M. Krůs, J. Tennyson, S. Civiš, A. T. Archibald, A. Granville-Willet, Identifiable Acetylene Features Predicted for Young Earth-like Exoplanets with Reducing Atmospheres undergoing Heavy Bombardment, Astrophysical Journal, 2019, 888, 21.

Department of Biophysical Chemistry (3)

Photoinduced charge separation in chromophore-protein systems

We have constructed protein (azurin) mutants with a covalently attached organometallic photooxidant capable of oxidizing the azurin Cu center 1.9 and 2.3 nm apart within ~60 ns upon irradiation, by electron hopping through tryptophan residues. We demonstrated that hopping through one and two tryptophans results in ca. 100 and 1000-fold electron-transfer acceleration. Experimental and theoretical results of electron transfer provide knowledge for constructing photoactive protein-based systems.

Collaborating entity: Beckman Institute, California Institute of Technology, Pasadena, USA



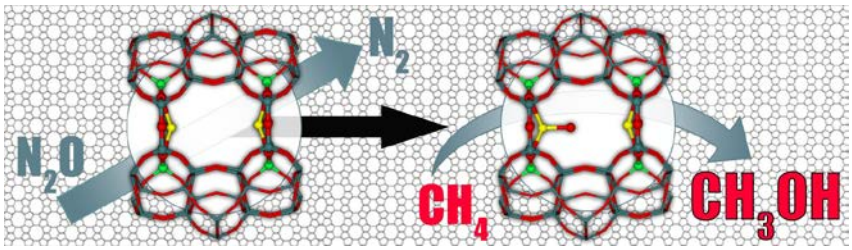
Electron transfer dynamics in protein (azurin) mutants with a covalently attached organometallic photooxidant. *Electron transfer sequence in protein (azurin) mutants with a covalently attached Rhenium organometallic photooxidant. Arrows in the upper part of the figure indicate individual electron transfer hops through individual tryptophans to the metal center. Time values correspond to single electron transfer steps. Blue arrow at the bottom of picture represents the back electron transfer and time of this process.*

Takematsu, K.; Williamson, H. R.; Nikolovski, P.; Kaiser, J. T.; Sheng, Y. L.; Pospíšil, P.; Towrie, M.; Heyda, J.; Hollas, D.; Záliš, S.; Gray, H. B.; Vlček, A.; Winkler, J. R., Two Tryptophans Are Better Than One in Accelerating Electron Flow through a Protein, Acs Central Science, 2019, 5, 192.

Department of Structure and Dynamics in Catalysis (4)

Binuclear cationic centers – highly active structures for selective oxidation of methane to methanol

A unique new type of redox catalysts has been developed using a new type of catalytic centers stabilized in zeolite matrices. These binuclear cation centers based on transition metal cations are capable to decompose molecular oxygen or N_2O even at room temperature to form highly active oxidic species. These oxo-species are subsequently capable to selectively oxidize methane to methanol at room temperature. The discovery of this system opens new possibilities in the utilization of natural gas.



Binuclear cationic centers in the zeolite. *Reduced binuclear cationic center stabilized in the zeolite ferrierite matrix and its oxidized form formed by oxidation by molecular oxygen.*

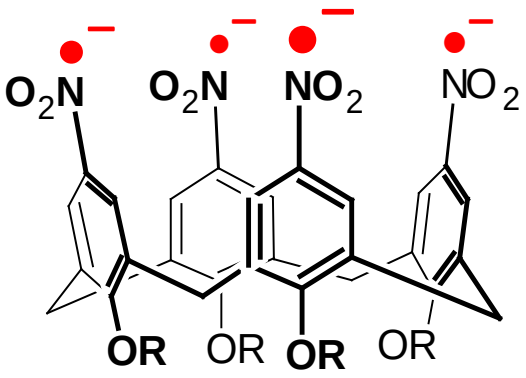
E. Tabor, M. Lemishka, Z. Sobalík, K. Mlekodaj, P. C. Andrikopoulos, J. Dědeček, S. Sklenák, Low-temperature selective oxidation of methane over distant binuclear cationic centers in zeolites, Communications Chemistry, 2019, 2, 71.

DOI: 10.1038/s42004-019-0173-9.

Department of Molecular Electrochemistry and Catalysis (5)

Electrochemically generated ligand – probably the first published case

Four-electron electrochemical reduction of the cone-tetranitrocalix[4]arene in dimethyl fumarate (DMF) results in the stable tetraradical tetraanion. The positive shift of the second reduction potential of the title compound with an increasing concentration of alkali metal ions is caused by complex formation. The tetraradical tetraanion of the parent tetranitrocalix[4]arene thus represents the first example of an electrochemically generated ligand – a promising receptor/sensor – for heavier alkali metal ions (K, Rb, Cs). Observed stoichiometries and corresponding stability constants for individual complexes were determined. The immobilization and reduction of nitrocalixarenes on the electrode surface offers new applications in electroseparation of alkali metal ions in electroanalytical chemistry.



Structure of the new electrochemically generated polydentate radical ligand. *The relatively high stability of the M4CX complexes can be justified by the effect which can be called a "stereochemical vector": the organized system of four fixed and charged nitroradicals oriented in space offering larger electrostatic coordination ability.*

A. Liška, P. Vojtíšek, J. Ludvík, The cone-tetranitrocalix[4]arene tetraradical tetraanion as an electrochemically generated ligand for heavier alkali metal cations, Chem. Commun., 2019, 55, 2817.

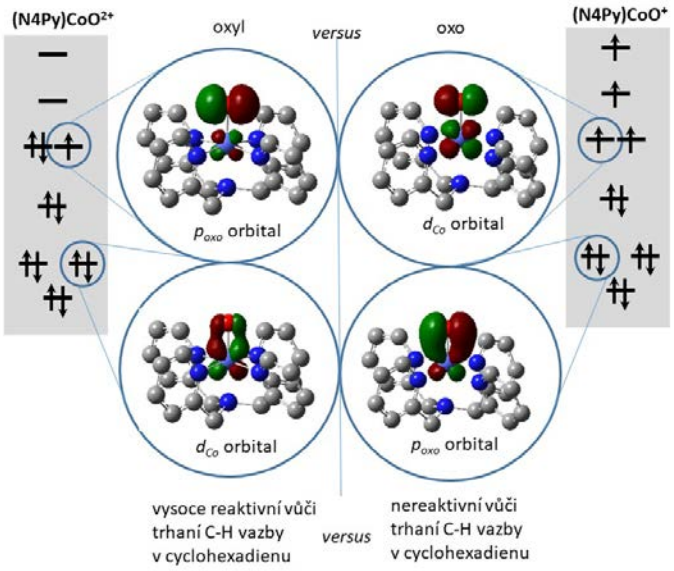
DOI: 10.1039/c8cc09662g

Department of Computational Chemistry (6)

Spectroscopic and catalytic properties of complexes with the cobalt(III)-oxyl and cobalt(III)-oxo units capable of the C-H bond activation.

Employing photodissociation spectroscopy and multireference calculations, electronic structures of the cobalt(III)-oxyl and cobalt(III)-oxo complexes were investigated along with their contributions to C-H bond reactivity. The importance of the work is twofold: first, the cobalt is capable of the formation of the bond with the oxo group, which was experimentally elusive for a long time; second, the variable bonding interaction between Co and oxo is directly linked to reactivity.

Collaborating entity: Radboud University, Netherlands, prof. Jana Roithová



Electronic structures of the cobalt(III)—oxyl and cobalt(III)—oxo complexes (left and right, respectively) and the comparison of their reactivity towards C-H bond activation. *The first complex (left) has a significant radical character with one unpaired electron localized on the oxygen moiety, while the oxygen in the second complex (right) has all electrons paired. Such a difference causes a different reactivity of the two complexes.*

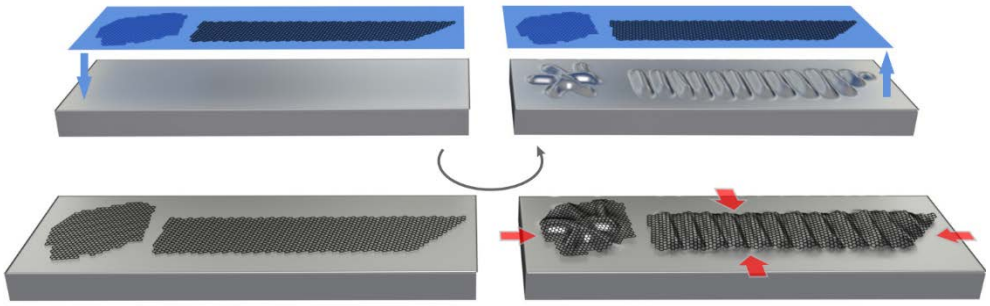
Andris E., Navrátil R., Jašík J., Srnec M., Rodríguez, M., Costas M., Roithová J., M-O Bonding Beyond the Oxo Wall: Spectroscopy and Reactivity of Cobalt (III)-Oxyl and Cobalt (III)-Oxo Complexes. Angew. Int. Chem., 2019, *58*, 9619.

Department of Electrochemical materials (7)

Strain engineering in graphene

Substantial advances have been achieved in the controlling the structure and surface of graphene through permanent deformation/shaping of its substrate – polymers (Sampathkumar et al. 2019a, Sampathkumar et al. 2019b) and lithographically prepared nanopillar fields (Verhagen et al. 2019).

Collaborating entities: FORTH/ICE-HT Patras, IPHT Jena, Institute of Physics of the Czech Academy of Sciences, Faculty of Mathematics and Physics of the Charles University, Faculty of Mechanical Engineering of the Czech Technical University.



Mutual sculpturing of graphene on a compliant polymer. *Controlled deformation fields – wrinkles were formed in graphene via heating or plasma treatment of compliant polymers. The wrinkles were, in turn, imprinted into the polymer upon its solidification.*

Sampathkumar K., Diez-Cabanes V., Kovaříček P., del Corro E., Bouša M., Hosek J., Kalbac M., Frank O., On the Suitability of Raman Spectroscopy to Monitor the Degree of Graphene Functionalization by Diazonium Salts, J. Phys. Chem., 2019, C 123, 22397.

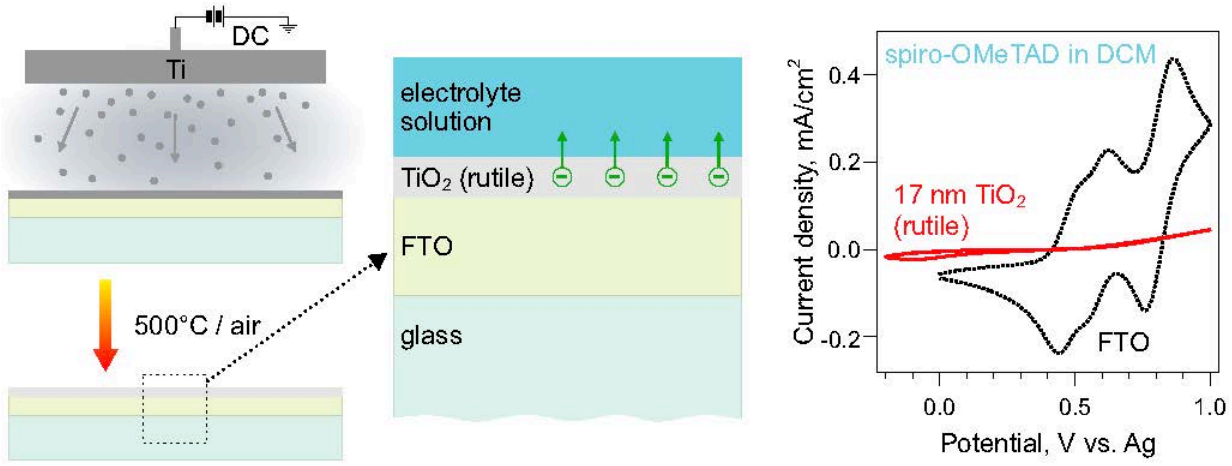
Sampathkumar K., Androulidakis C., Koukaras E. N., Rahova J., Drogowska K., Kalbac M., Vetushka A., Fejfar A., Galiotis C., Frank O., Sculpturing graphene wrinkle patterns into compliant substrates, Carbon, 2019, 146, 772.

Verhagen T., Pacakova B., Bousa M., Hübner U., Kalbac M., Vejpravova J., Frank O., Superlattice in collapsed graphene wrinkles, Sci. Rep., 2019, 9, 9972.

Electron- and hole-selective interfaces for perovskite photovoltaics

Compact thin films of oxide semiconductors (TiO2, SnO2) were developed for the electron-selective contacts in perovskite solar cell. These films transport electrons from the photoexcited perovskite to the current collecting terminal which is fabricated from conducting glass and prevent recombination of these electrons with the photoabsorber. New type of hole conductor based on CuSCN and reduced graphene oxide was developed for the same solar cell application. It provides a device with efficiency approaching 20 %.

Collaborating entities: EPF-Lausanne, University of Chemistry and Technology Prague, Institute of Physics of the CAS



Scheme of the fabrication and electrochemical testing of thin films from z TiO_2 (rutile). *In the first step, a thin layer of titanium is deposited by magnetron sputtering. It is subsequently transformed to TiO_2 (rutile) by calcination in air at 500°C. The right chart shows a cyclic voltammogram of spiro-OMeTAD in dichloromethane, documenting the perfect blocking function of this layer on the substrate from F-doped SnO_2 (FTO).*

L. Kavan, Conduction Band Engineering in Semiconducting Oxides (TiO_2, SnO_2): Applications in Perovskite Photovoltaics and Beyond, Catal.Today, 2019, 328, 50.

J. Krysa, H. Krysova, Z. Hubicka, S. Kment, J. Maixner, L. Kavan: "Transparent Rutile TiO_2 films Prepared by Thermal Oxidation of Sputtered Ti on FTO Glass", Photochem. Photobiol. Sci., 2019,18, 891.

L. Kavan, Z. Vlckova-Zivcova, P. Hubik, N. Arora, M. I. Dar, S. M. Zakeeruddin, M. Grätzel, Electrochemical Characterization of CuSCN Hole-Extracting Thin Films for Perovskite Photovoltaics", ACS Appl.Energy Mater., 2019,2, 4264.

H. Krysova, M. Zlamalova, H. Tarabkova, J. Jirkovsky, O. Frank, M. Kohout, L. Kavan, Rutile TiO_2 Thin Film Electrodes with Excellent Blocking Function and Optical Transparency, Electrochim. Acta, 2019, 321, 134685.

Cobalt pyridinoporphyrazine film as a platinum group metal-free mediator in electrochemical hydrogen oxidation and hydrogen evolution reactions

Cobalt pyridinoporphyrazine film-modified electrode exhibited electrocatalytic activity to hydrogen oxidation reaction and decreased overvoltage of hydrogen evolution reaction compared to bare surfaces. The hydrogen oxidation reaction mediated by cobalt pyridinoporphyrazine represents the first observation of such reaction on porphyrazine-based mediator in absence of platinum group metals. This finding may have a significant impact in hydrogen energetics.

M. Klusáčková, P. Janda, H. Tarábková, Hydrogen evolution reaction enhanced by water soluble metallopyridinoporphyrazine complex adsorbed on highly oriented pyrolytic graphite, Internat. J. Hydrogen Energy, 2019, 44, 11431.

M. Klusáčková, H. Tarábková, P. Janda, Cobalt pyridinoporphyrazine film as a platinum group metal-free mediator in hydrogen electrochemistry, Monatsh.Chem., 2019 150, 1643.

Department of Electrochemistry in Nanoscale (8)

Tuning the contact conductance of anchoring groups in single molecule junctions by molecular design

Molecular electronics requires anchoring of individual molecules on the conducting substrate that would lead to the formation of highly stable electronic structures. At the same time, these connectors should not dictate the conductance of these structures. Unique combination of the single molecule break junction measurements and theoretical analysis confirmed that the principle of tripodal anchoring brings the solution to this problem.

Collaborating entity: Karlsruhe Institute of Technology, Germany

The molecular wire with the tripodal anchoring group between two gold electrodes. *The illustration depicts the molecular wire with the tripodal anchoring group between two gold electrodes in the configuration of scanning tunneling microscopy. The tripodal anchoring group enables high stability of molecular junctions that is required for the construction of functional elements for molecular electronic applications.*

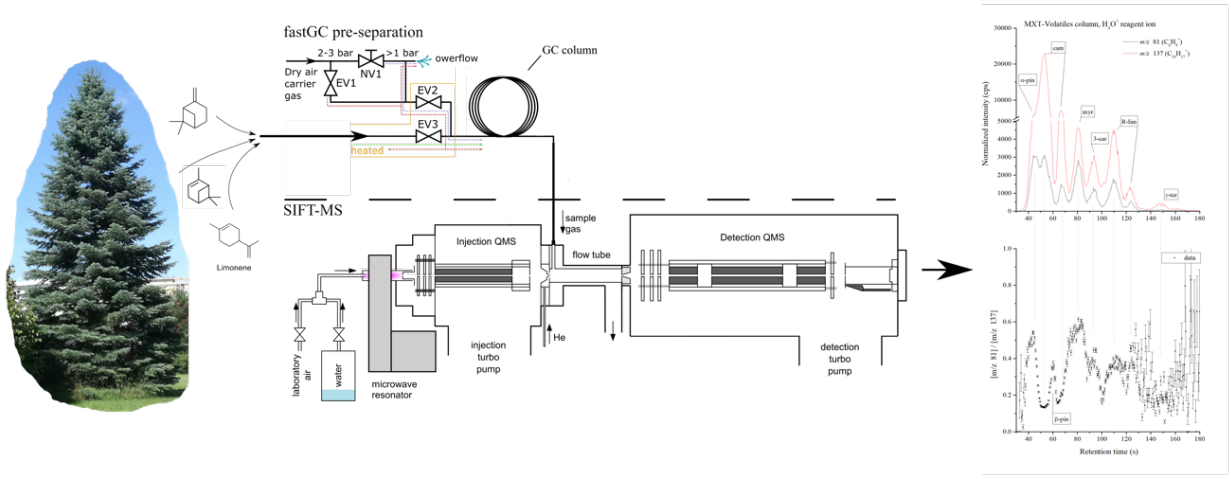
J. Šebera, M. Lindner, J. Gasior, G. Meszáros, O. Fuhr, M. Mayor, M Valášek, V. Kolivoška, M. Hromadová, Tuning contact conductance of anchoring groups in single molecule junctions by molecular design, Nanoscale, 2019, 11, 12959.

Department of Chemistry of Ions in Gaseous Phase (9)

Addition of fast gas chromatography to selected ion flow tube mass spectrometry for analysis of individual monoterpenes in mixtures

The selected ion flow tube mass spectromentry (SIFT-MS) is a technique used for a trace gas analysis in real time. The study deals with the limitation of SIFT-MS techniques – analysis of isomeric molecules – due to their identical atomic composition. Addition of fast gas chromatography, using a short metallic column and a direct ohmic heating, allowed to identify monoterpenes originated from coniferous tree samples.

Collaborating entity: Max-Planck-Institut für Chemie



Scheme of experiment for measurement of monoterpenes. *Combination of fast gas chromatography and selected ion flow tube mass spectromerty allowed to analyze and identify monoterpenes in pine trees samples.*

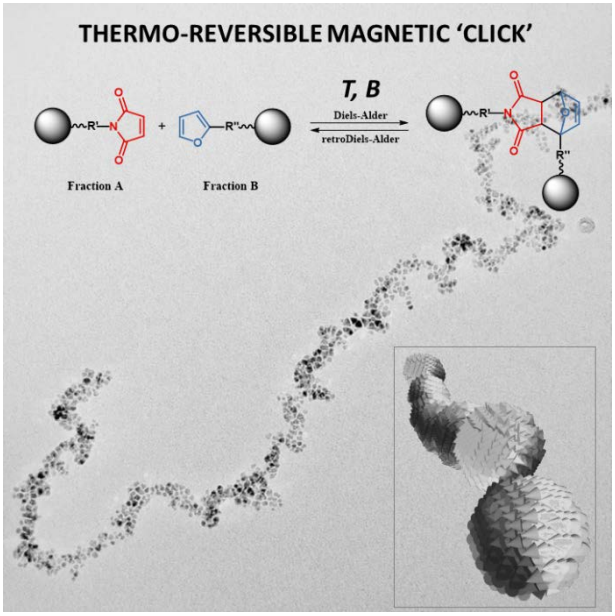
Lacko, M., Wang, N., Sovová, K., Pásztor, P., Španěl, P., Addition of fast gas chromatography to selected ion flow tube mass spectrometry for analysis of individual monoterpenes in mixtures. Atmospheric Measurement Techniques, 2019, 12, 4965.

Department of Low-dimensional Systems (10)

Thermoreversible magnetic nanochains

The reversible assembly of nanomagnets into organized systems is of considerable interest for many applications, including theragnostic strategies *in vivo*. Here, we develop a new approach based on the thermoreversible Diels–Alder (D–A) reaction in the presence of an external magnetic field that enables the assembly of magnetic nanoparticles into narrow chains with lengths of several micrometers. Moreover, the chains can be again disassembled at elevated temperatures through a retro-D–A reaction.

Collaborating entity: Faculty of Mathematics and Physics of the Charles University



Mikšátko, J., Aurélio, D., Kovaříček, P., Michlová, M., Veverka, M., Fridrichová, M,; Matulková, I., Žáček, M., Kalbáč M., Vejpravová, J. Thermoreversible magnetic nanochains, Nanoscale 2019, 11, 16773-16780.

Influence of Carbonaceous Residues on the Genotoxicity of Heat-Treated Silicalite-1 Film

Silicalite-1 film (***SF***) was investigated as a potential prosthetic material. The role of calcination of ***SF*** in the genotoxicity in osteoblast-like cells was addressed. Polycyclic aromatic hydrocarbons created on ***SF*** increased level of DNA damage. Thus, further optimization of the ***SF*** calcination procedure is required. Irradiation of PAHs led to the formation of singlet oxygen, which may act to sterilize ***SF*** in its application for the coating of the metallic prosthetic materials.

Collaborating entity: Institute of Physiology, Czech Academy of Sciences.

Ivan Jirka, Ivana Kopová, Pavel Kubát, Edyta Tabor, Lucie Bačáková, Milan Bouša and Petr Sajdl, Influence of Carbonaceous Residues on the Genotoxicity of Heat-Treated Silicalite-1 Film, MATERIALS, 2019, 12, 567.

DOI: 10.3390/ma12040567

Stable catalysts for the removal of oxygen in an acidic environment

A new type of oxidic catalysts for oxygen scavenging in an acidic environment has been developed. It is based on lanthanide-stabilized Ru and Ir pyrochlores. The newly prepared materials have an activity comparable to IrO_2 (industry standard), but they exceed its stability. This new type of catalysts will reduce the demand for IrO_2 in polymer electrolyte electrolyzers by stabilizing the more abundant and active Ru.

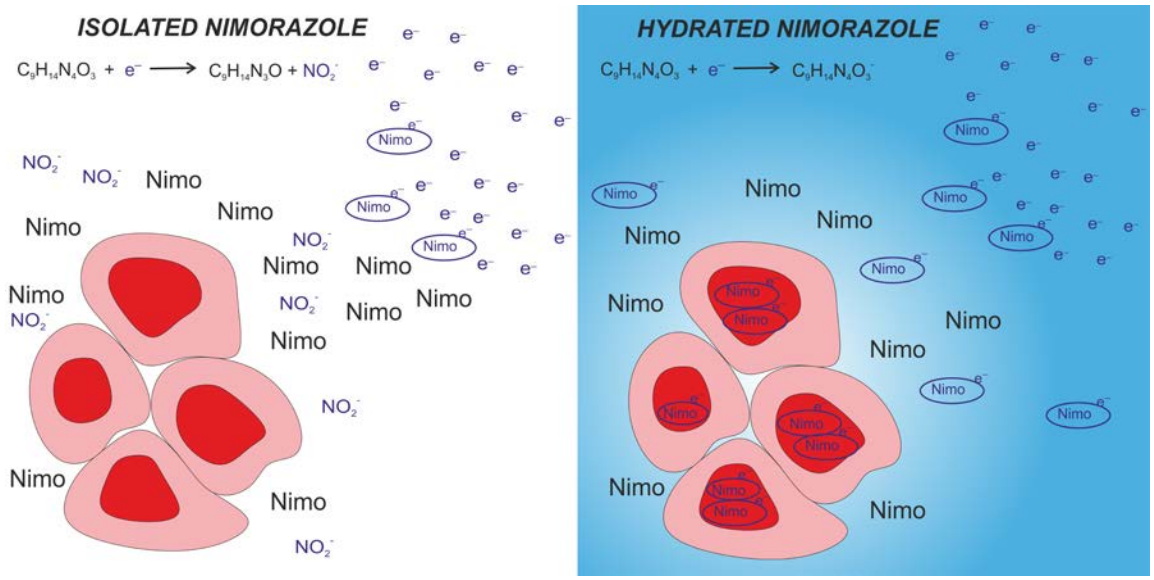
Collaborating entity: PSI Villigen

Abbott, D. F., Pittkowski, R., Nebel, R., Minhová Macounová, K, MArelli, E., Fabbri, E., Castelli, I. E., Schmidt, TJ., Krtil, P., Design and Synthesis of Ir/Ru Pyrochlore Catalysts for the Oxygen Evolution Reaction Based on Their Bulk Thermodynamic Properties. ACS Appl. Mater. Interfaces, 2019, 11, 37748.

Department of Dynamics of Molecules and Clusters (11)

Influence of Carbonaceous Residues on the Genotoxicity of Heat-Treated Silicalite-1 Fil

The method to study hydrated molecules in vacuum developed at JHI was used in an international study to elucidate the interaction of electrons with nimorazole in water. Nimorazole is a radiosesitizer used in the cancer therapy. The study published in Nat. Comm. demonstrates stabilization of the nimorazole anion, which enables its accumulation in cells. The study, selected as "Editors Highlight", changes the general view on electrons as “bond breakers” in the radio-sensitization mechanism.



Artistic view on the fundamental processes explaining mechanism of action of nimorazole radiosensitizer, based on the presented study. *In the environment rich on low energy electrons, isolated Nimorazole can dissociate and form NO2-. We demonstrated that hydrated nimorazole, however, does not dissociate and form stable parent anion. Such change may explain nimorazole transport and accommodation in cancer cells under hypoxic conditions.*

The study has been conducted in collaboration with University of Innsbruck and other foreign organizations. key experiments and data interpretations took place at the Department of Dynamics of Molecules and Clusters.

R. Meißner, J. Kočišek, L. Feketová, J. Fedor, M. Fárník, P. Limão-Vieira, E. Illenberger, and S. Denifl, Low-energy electrons transform the nimorazole molecule into a radiosensitizer, Nature Communications, 2019, 10, 2388

DOI: https://doi.org/10.1038/s41467-019-10340-8.

Department of Nanocatalysis (12)

Establishing the department and instrumentation of its new labs in 2019

In the first year of the department, complex plans of the remodeling of the laboratory spaces to accommodate planned experiments and instrumentation were designed and realized. In December of 2019, the preparatory efforts were completed by the transfer of four unique laboratories from the Argonne National Laboratories, including two high-vacuum apparatuses for the synthesis of cluster-based nanocatalysts and five catalysts testing apparatuses.

Collaborating entity: Argonne National Laboratory and US Department of Energy

Cluster laboratory. *View of the basic units of the cluster fabrication apparatuses shortly after the move-in.*

At the same time, publications following the experimental work of S. Vajda were completed.

Halder, M.-A. Ha, H. Zhai, B. Yang, M. J. Pellin, S. Seifert, A. N. Alexandrova, S. Vajda, Oxidative Dehydrogenation of Cyclohexane by Cu vs Pd Clusters: Selectivity Control by Specific Cluster Dynamics, ChemCatChem., 2019, in press, (on-line Nov 4, 2019), Front Cover

DOI: 10.1002/cctc.201901795

Halder, A. Ngo, X. Luo, H.-H. Wang, J. G. Wen, P. Abbasi, M. Asadi, C. Zhang, D. Miller, D. Zhang, J. Lu, P. C. Redfern, K. C. Lau, R. Amine, R. S. Assary, Y. J. Lee, A. Salehi-Khojin, S. Vajda, K. Amine, L. A. Curtiss, In situ Formed Ir3Li Nanoparticles as Active Cathode Material in Li-Oxygen Batteries, J. Phys. Chem. A, 2019,123, 10047-10056

DOI: 10.1021/acs.jpca.9b06875

Y. Liu, N. Marcella, J. Timoshenko, A. Halder, B. Yang, L. Kolipaka, M. J. Pellin, S. Seifert, S. Vajda, P. Liu, A. I. Frenkel, Mapping XANES spectra on structural descriptors of copper oxide clusters using supervised machine learning, J. Chem. Phys., 2019, 151, 164201 Editor's Pick, Front Cover, DOI: 10.1063/1.5126597

Scientometric achievements:

The results of science and research achieved by the staff of HIPC in 2019 were published in 182 articles in international impact journals, 2 monographs and 1 chapter in a book, and are listed in the ASEP database:

https://asep-analytika.lib.cas.cz/Publication/asep/ufch-w/gqz

These works have been cited more than 410 times as of the date of this report. Chronologically selected publications are regularly published on the institute's website in the section 'News - Important publications':

https://www.jh-inst.cas.cz/node/2228

Applied Organometallic Chemistry, 2019, e5318
Harmless glucose-modified ruthenium complexes suppressing cell migration of highly invasive cancer cell lines
Martin Lamač, Michal Horáček, Lucie Červenková Šťastná, Jindřich Karban, Lucia Sommerová, Hana Skoupilová, Roman Hrstka, Jiří Pinkas
DOI: 10.1002/aoc.5318.

Angewandte Chemie International Edition, 2019, 58, 17169–17174.
Straightforward Synthesis and Properties of Highly Fluorescent [5]- and [7]-Helical Dispiroindeno[2,1-c]fluorenes
Reinhard P.Kaiser, David Nečas, Timothee Cadart, Gyepes, Robert, , Ivana Císařová, Jiří Mosinger, Lubomír Pospíšil, Martin Kotora
DOI: 10.1002/anie.201908348

Applied Surface Science, 2019, 491, 16-23.
Non-destructive depth profile reconstruction of single-layer graphene using angle-resolved X-ray photoelectron spectroscopy
J. Zemek, J. Houdková, P. Jiříček, T. Ižák, Martin Kalbáč

Chemical Reviews, 2019, 119 (19), 10856-10915.
Quantum Chemistry in the Age of Quantum Computing
Yudong Cao, Jonathan Romero, Jonathan P. Olson, Matthias Degroote, Peter D. Johnson, Maria Kieferová, Ian D. Kivlichan, Tim Menke, Borja Peropadre, Nicolas P. D. Sawaya, Sukin Sim, Veis Libor, Alan Aspuru-Guzik.

Nanoscale, 2019, 11 (36), 16773-16780.
Thermoreversible magnetic nanochains
Jiří Mikšátko, Aurelio David, Petr Kovaříček, Magdaléna Michlová, Miroslav Veverka, Michaela Fridrichova, Irena Matulková, Martin Žáček, Martin Kalbáč, Jana Vejpravová

Electrochimica Acta, 2019, 318, 108-119.
Oxidation potentials of guanine, guanosine and guanosine-5 '-monophosphate: Theory and experiment
Alan Liška, Iveta Třísková, Jiří Ludík, Libuše Trnková

Chemistry - A European Journal, 2019, 25 (52), 12068-12073.
Mechanochemical Pretreatment for Efficient Solvent-Free Synthesis of SSZ-13 Zeolite

Veronika Pashková, Kinga Mlekodaj, Petr Klein, Libor Brabec, Žouzelka Radek, Jiří Rathouský, Věnceslava Tokarova, Jiří Dědeček

The Journal of Chemical Physics, 2019, 151, 164201.
(Picture on Journal Front Cover)
Mapping XANES spectra on structural descriptors of copper oxide clusters using supervised machine learning
Yang Liu, Nicholas Marcella, Janis Timoshenko, Avik Halder, Bing Yang, Lakshmi Kolipaka, Michael. J. Pellin, Soenke Seifert, Štefan Vajda, Ping Liu, and Anatoly I. Frenkel

Chemical Communications, 2019, 55 (71), 10563-10566.
Prebiotic synthesis at impact craters: the role of Fe-clays and iron meteorites
Adam Pastorek, Jana Hrnčířová, Luboš Jankovič, Lukáš Nejdl, Svatopluk Civiš, Ondřej Ivanek, Violetta Shestivska, Knížek Antonín, Petr Kubelík, Jiří Šponer, Lukáš Petera, Anna Křivková, Cassone, Giuseppe, Markéta Vaculovičova, Judit E.Sponer, Martin Ferus

Free Radical Biology & Medicine, 2019, 143:240-251.
Redox properties of individual quercetin moieties
E. Heřmánková, M. Zatloukalová, M. Biler, R. Sokolová, M. Bancířová, A. G. Tzakos, V. Křen, M. Kuzma, P. Trouillas , J. Vacek

Nanoscale, 2019, 11, 12959-12964.
Tuning the contact conductance of anchoring groups in single molecule junctions by molecular design
Jakub Šebera, Marcin Lindner, Jindřich Gasior, Gábor Mészáros, Olaf Fuhr, Marcel Mayor, Michal Valášek, Viliam Kolivoška and Magdaléna Hromadová

Nature Communications, 2019, 10, 2388.
Low-energy electrons transform the nimorazole molecule into a radiosensitiserR. Meissner, J. Kočišek, L. Feketeová, J. Fedor, M. Fárník, P. Limao-Vieira, E. Illenberger, S. Denifl

Angewandte Chemie International Edition, 2019, 58, 2 – 8.
M−O Bonding Beyond the Oxo Wall: Spectroscopy and Reactivity of Cobalt (III)-Oxyl and Cobalt(III)-Oxo Complexes
E. Andris, R. Navrátil, J. Jašík, M. Srnec, M. Rodríguez, M. Costas, J. Roithová

ACS Applied Materials & Interfaces, 2019, 11 (18), 16506-16516.
Selectivity Control of the Photo-Catalytic Water Oxidation on SrTiO3 Nanocubes via Surface Dimensionality
K. M. Macounová, R. Nebel, M. Klusáčková, M. Klementova, P. Krtil

Analytical Chemistry, 2019, 91, 8, 5380-5388.
Electrostatic Switching and Selection of H3O+, NO+, and O-2(+center dot) Reagent

Ions for Selected Ion Flow-Drift Tube Mass Spectrometric Analyses of Air and Breath
P. Španěl, A. Spesyvyi, D. Smith

Carbon, 2019, 146, 772-778.
Sculpturing graphene wrinkle patterns into compliant substrates, K. Sampathkumar,

C. Androulidakis, E. N. Koukaras, J. Rahova, K. Drogowska, M. Kalbáč, A. Vetushka, A. Fejfar, C. Galiotis, O. Frank

The Journal of Physical Chemistry Letters, 2019, 10, 2024−2030.
Experimental Evidence of the Existence of Interleaflet Coupled Nanodomains: An MC-FRET Study
Ivo S. Vinklárek, Lukáš Vel'as, Petra Riegerová, Kristián Skála, Ilya Mikhalyov, Natalia Gretskaya, Martin Hof, and Radek Šachl

Chemical Communications, 2019, 55 (23), 3351-3354.
Probabilistic mapping of single molecule junction configurations as a tool to achieve the desired geometry of asymmetric tripodal molecules
Viliam Kolivoška, Jakub Sebera, Táňa Sebechlebská, Marcin Lindner, Jindřich Gasior, Gábor Mészáros, Marcel Mayor, Michal Valášek and Magdaléna Hromadová

Chemical Communications, 2019, 55 (19), 2817-2820.
The cone-tetranitrocalix[4]arene tetraradical tetraanion as an electrochemically generated ligand for heavier alkali metal cations
Alan Liška, Pavel Vojtíšek, Jiří Ludvík

ChemSusCHem, 2019, 12 (3), 556-576.
Tuning the Aluminum Distribution in Zeolites to Increase their Performance in Acid-Catalyzed Reactions
Jiří Dědeček, Edyta Tabor, Štěpán Sklenák

Journal of Chermical Theory and Computation, 2019, 15 (2), 803-812
Structure and Dynamics of the Hydration Shell: Spatially Decomposed Time Correlation Approach
Eva Pluhařová, Pavel Jungwirth, Matubayasi Nobuyuki, Maršálek Ondřej

Angewandte Chemie - International Edition, 2019, 58 (5), 1324-1328
Spatially Resolved Covalent Functionalization Patterns on Graphene
Leoš Valenta, Petr Kovaříček, Václav Valeš, Zdeněk Bastl, Karolina A. Drogowská, Timotheus A.Verhagen, Radek Cibulka, Martin Kalbáč

ACS Central Science 2019, 5 (1), 192-200.
Two Tryptophans Are Better Than One in Accelerating Electron Flow through a Protein
Kana Takematsu, Heather R Williamson, Pavle Nikolovski, Jens T. Kaiser, Yuling Sheng, Petr Pospíšil, Michael Towrie, Jan Heyda, Daniel Hollas, Stanislav Záliš, Harry B. Gray, Antonín Vlček, and Jay R. Winkler

Applied Catalysis B: Environmental, 2019, 240, 358-366.
Feasibility of application of iron zeolites for high-temperature decomposition of N2O under real conditions of the technology for nitric acid production
Edyta Tabor, Galina Sadovská, Milan Bernauer, Petr Sazama, Jana Nováková, Vlastimil Fila, Tomas Kmjec, Jaro

III. 2 Important projects

In 2019, HIPC participated in 8 research projects with the support of foreign funders and 95 research projects financially supported by several different domestic funders, in which the researchers from the HIPC acted as principal investigators / co-investigators or project partners.

RESEARCH PROJECTS FINANCIALLY SUPPORTED BY SEVERAL DIFFERENT DOMESTIC FUNDERS

FUNDER	NUMBER OF PROJECTS
Czech Science Foundation	56
Ministry of Education, Youth and Sports	21
Technology Agency of the Czech Republic	7
Czech Academy of Sciences	6
Ministry of Industry and Trade	3
Ministry of the Interior	1
Other	1
Foreign	8

Selected research projects

Nanomaterials and Nanotechnologies for Environment Protection and Sustainable Future (acronym of the research infrastructure - NanoEnviCz), : Principal investigator Martin Kalbáč, partner institutions: Technical University of Liberec/Institute for Nanomaterials, Advanced Technologies and Innovation; E. Purkyně University in Ústí nad Labem/Faculty of Science; Palacký University in Olomouc/ Faculty of Science; Institute of Inorganic Chemistry, CAS; Institute of Experimental Medicine, CAS. The project was supported by programme Large Research Infrastructures (2010-2019).

The portfolio of operating facilities and expertise provided by NanoEnviCz covers various areas of research into nanomaterials, surfaces and nanocomposites, as materials for environmental protection and other related applications.

Concert of lipids, ions, and proteins in cell membrane dynamics and function (Technology Agency of the Czech Republic, STARFOS), principal investigator: Martin Hof, partner institution: Institute of Organic Chemistry and Biochemistry, CAS. The aim of the project is to present a new perspective on the closely intertwined interplay between lipids, ions and proteins, which significantly affects membrane processes such as cell signaling and membrane transport. (2019 2023)

Selected strategic projects

ERA chair, (acronym **J. Heyrovský chair**), project leader: J. Hrušák, international project of Horizon 2020 programme, funder: European Commission.

The J. Heyrovský chair is appointed to Dr Stefan Vajda since January 2019. The department of nanocatalysis was also established in January 2019. During the year, most of the positions of the scientific team of the department were filled by experts with experience from foreign research organizations and two of experts already working at the HIPC joined. At the same time, the equipment was installed in two new laboratories. Two male and one female student started master and doctoral studies.

Capacity development of HIPC, project leader: M. Kalbáč, Funder: MEYS, programme RKV I.

More than ten years ago, the European Commission issued recommendations in the European Charter for Researchers and in the Code of Conduct for the Recruitment of Researchers (C&C, 2005/251/ES) and specified a set of principles for improving the research system. The implementation of C&C principles in research institutions is supported by the **Human Resources Strategy for Researchers (HRS4R)**.

At the beginning of 2019, the HIPC officially joined the research organizations that received the **HR Excellence in Research award**. It shows progress in harmonizing our human resources policy with international standards and it identifies the HIPC as an excellent workplace in quality management and human resource development in science and research. In addition, the HIPC is the first institute of CAS to get this award. Now, we are gradually achieving the objectives we have set in the Action Plan. The whole process is managed by the Steering and Monitoring Committee, which members are representatives of scientists, administrative and technical staff. After two years, we will review the relevance of the Action Plan, and after another three years, we will be visited by independent experts, because to win the HR Award means not only a recognition of our current status, but also a permanent commitment to creating favorable conditions for the employees of the HIPC.

In 2019, we succeeded in fulfilling several important tasks that we set ourselves in the HRS4R action plan:

- We launched a new, modern website of HIPC.

- We publish newly created documents simultaneously in Czech and English.

- We translated several directives and internal regulations into English, we are revising the basic documents of HIPC so that they are up-to-date and accessible for employees that do not understand Czech language.

- We created manuals that contribute to transparency in the evaluation of scientific work, specifically the Criteria for the evaluation of scientific work, the Evaluation Manual, the Manual for the Evaluation Commission and the Employee Handbook.

- The evaluation of researchers took place in 2019 in accordance with the recommendation of the international advisory board, which was appointed by the director of HIPC and which members are scientists with extensive experience in the field of science leadership.

- We have published a unified template for advertising a vacancy for a scientific job. Experience from the course of selection procedures for open positions of the new department of nanocatalysis, which took place in accordance with the principles of the European Research

Area ERA, the so-called *Open, Transparent & Merit Based Policy*, was used in a new methodology for the selection of researchers.

- There were a number of trainings developing the knowledge and skills of employees in several areas of interest. The examples are: the training of members of the bankruptcy commission, training of team leaders for open competitions, management training for managers and teaching English to members of the economic department.

https://www.jh-inst.cas.cz/basic-page/human-resources-strategy-researchers-hrs4r

ESFRI The Chair of the European Strategy Forum on Research Infrastructures (ESFRI) is our employ RNDr. Jan Hrušák, CSc. From 1st January 2019. He was elected at 65th plenary meeting of ESFRI for a period of two years with the possibility of extension for one year. The Chairman's Office and its Secretariat are located at HIPC.

Jan Hrušák as a chairman of ESFRI coordinates the strategic discussion on the main priorities for European research infrastructures after 2020 and he prepares the process of updating the ESFRI Roadmap, which will be completed at the end of 2021. The activity of ESFRI chairman secretariat is supported by EU projects StR-ESFRI and StR-ESFRI II (Horizon 2020) on the basis of a consortium agreement in the amount of EUR 283,375.00, by project of the Ministry of Education, Youth and Sports CZERA 3 (INTER-EXCELLENCE programme, INTER-INFORM sub-programme) whose activities are fulfilled by the National Information Center for European Research (NICER) of the Technology Center of CAS.

Jan Hrušák has also been appointed an independent expert on the Steering Committee for the creation of the European Open Science Cloud (EOSC), a gigantic service infrastructure combining distributed data storages from all scientific disciplines, computing capacities of HPC and other service infrastructures. The EOSC is one of the biggest challenges of current European science policy. The EOSC Steering Committee meets almost every month. Simultaneously, Jan Hrušák is one of the members of the European Research Area and Innovation Committee (ERAC), which creates European policy in science and research. As an author, he contributed to the OECD publication "Reference Framework for Assessing the Scientific and Socio-Economic Impact of Research Infrastructures," published in March 2019.

The activity of the chairman of ESFRI means not only a prestigious representation for the Czech Republic, but it also helps to shape and direct Czech policy in research a development area in Europe. The support team of the chairman of ESFRI at HIPC participates in the drafting of documents for negotiations on all aspects of ESFRI and EOSC. It participates in developing Czech positions and projecting European Union policies into the Czech Republic agenda in area of research (e.g. Structural Funds). These activities are carried out in coordination with Technological Centre of CAS and the Ministry of Education, Youth and Sports.

III. 3 Significant awards

The following scientists and students were awarded in 2019 for the results of their research activities:

Mgr. Juraj Fedor, Ph.D. - The Award of the Learned Society of the Czech Republic in the category "junior researcher" for significant scientific contribution to the experimental study of the interactions of electrons with molecules was awarded by the Learned Society of the Czech Republic.

doc. RNDr. Lubomír Pospíšil, CSc. - The Metrohm Award for his lifelong contribution to electroanalytical chemistry, specifically for his contribution to the use of polarography in elucidating important physicochemical processes was awarded by Methrohm AG.

prof. RNDr. Ladislav Kavan, CSc., DSc., prof. RNDr. Jiří Ludvík, CSc., prof. RNDr. Zdeněk Samec, DrSc. - Commemorative medals for important contributions to the field of electrochemistry were awarded by the Faculty of Science of Charles University on the occasion of the 60th anniversary of prof. Jaroslav Heyrovský's the Nobel Prize. The medals were awarded by the dean of the faculty prof. RNDr. Jiří Zima, CSc.

doc. RNDr. Ing. Martin Kalbáč, Ph.D. - The Academic Award for outstanding scientific personalities who are the bearers of research at the top international level was awarded by the President of the CAS, prof. Eva Zažímalová.

Ing. Daniel Bím, Ph.D. - Doctorandus Award for natural sciences in the Czech Head competition. Awarded by the Czech Head initiative.

Mgr. Adéla Melcrová, Ph.D. - which is intended for talented students in bachelor, master or PhD programmes who have demonstrated exceptional skills and creative thinking in their field, and for young talented researchers of the CAS up to 33 years of age. Awarded by the Hlávka Foundation.

Mgr. Ing. Eva Krupičková Pluhařová, Ph.D., RNDr. Viliam Kolivoška, Ph.D., MBA and Ing. Petr Kovaříček, Ph.D. - which is intended for talented students in bachelor, master or PhD programmes who have demonstrated exceptional skills and creative thinking in their field, and for young talented researchers of the CAS up to 33 years of age. Awarded by the Zažímalová.

For the archive of all awards follow the link:

https://web.jh-inst.cas.cz/cs/prizes

III. 4 Promotion and popularization

The cooperation of HIPC with the different media in various forms to popularize the results of the activities of scientists takes place throughout the year. In the first half of 2019, HIPC presented its results to the public through press releases generated in cooperation with the PR agency Konektor. As of June 30, the cooperation with the PR agency Konektor was terminated and as of September 1, a new employee was hired as a PR manager. As a result of these structural changes, we managed to renew close cooperation with the Division of Media Communication of the CAS in the field of media coverage of research results and popularization of science to the target group, which is primarily the general public.

During 2019, the research activities of the HIPC scientists were regularly presented to the public through popularization articles in the daily press, magazines, internet servers and in the form of interviews on radio and television. Dozens of articles, interviews and reports were published in the media in this way. A selection of the most important media outlets is publicly available on the institute's website;

http://web.jh-inst.cas.cz/media

In the course of 2019, the HIPC also issued a total of 12 press releases, covering research results and significant events directly related to the HIPC. All press releases in full and with subsequent responses in the media are regularly published on the website of HIPC;

https://web.jh-inst.cas.cz/cs/press-releases

Special attention was paid to the 60th anniversary of prof. Jaroslav Heyrovský's Nobel Prize for his discovery of a new analytical method of polarography. Prof. Heyrovský was a Czech scientist and founder of the Polarographic Institute, predecessor of the J. Heyrovský Institute of Physical Chemistry. On this occasion, the HIPC organized a ceremonial meeting, with the participation of the President of the CAS, the rectors of Czech universities and other important guests. This meeting was followed by the grand opening of the laboratories of the Department of Nanocatalysis.

Popularization of results of research and development through programs for those interested in natural sciences:

In 2019, the HIPC organized 120 popularization and educational events/programs for university students, high school students and elementary school pupils, preschoolers and the general public. **These events were visited by a total of 8,550 visitors.**

A detailed schedule of 2019 programs entitled *60 let Nobelovky 2019* (60 Years of Nobel Prize 2019) is archived in the web application of the popularization project Tři nástroje (Three Tools):
http://www.3nastroje.cz/detail.php?p=50

An overview of the most important popularization and education programs and events in 2019: at the festival *Science and Technology Week 2019*, the researchers of HIPC have prepared for the public a meeting with science and research in the form of various programs spread over 5 different days. A rich presentation of science was created that was attended by a total of 360 visitors.

For high school students and teachers, the program *Den (s) vědcem* (A day with a scientist) continued, including workshops, practical measurements or popularization lectures and excursions. Pupils from primary and middle schools and preschoolers from all over the Czech Republic attended the workshops *Chemie není nuda* (Chemistry is not boring, middle school) or chemical shows presenting chemistry and the profession of scientist *Posviť si citronem na duhu* (Shine a lemon on a rainbow, primary school and preschoolers). Those interested in chemistry attended two chemistry clubs (25 children in total, three hours once a month). The program of Saturday workshops (once a month) called *Cesta za nobelovkou* (The Road to the Nobel Prize) was also dedicated to general public. 35 children (5–15 years) had the opportunity to get acquainted with chemistry and physics through experimentation in our EDU classroom and laboratory. 24 high school students from 17 schools from all over the Czech Republic visited the traditional August event *NANOškola 2019* (NANOschool, August 19-23, 2019), which was supported for the fourth time by the Ministry of Education, Youth and Sports project in the Support program for gifted high school and elementary school students (project 0033/7/NAD/2019).

15 high school students completed year-round internships in the project *Otevřená věda AV ČR 2019* (Open Science of the ASCR CAS) at HIPC. Other 23 high school students participated in extracurricular internships (with the support of the project Ministry of Education, Youth and Sports 0038/7/NAD/2019 in the program Support for gifted high school and middle school students). Other students completed professional internships: 7 students from several Prague schools and from Střední průmyslová škola chemická akademika Heyrovského (Academician Heyrovský Secondary Industrial School of Chemistry in Ostrava). A one-week course in chemical experiments called Neon took place in the town Bor as part of this project. The course was attended by 10 high school students.

HIPC continued to participate in the education of secondary school students within 2 projects of the program *Šablony SŠ* (High School Templates) supported by Structural Funds of the Ministry of Education, Youth and Sports (Masaryk Secondary School of Chemistry, Prague 1 and Bishop Grammar School, Žďár nad Sázavou).

In 2019, the HIPC organized a total of 10 exhibitions: own traveling exhibition *Příběh kapky* (The Story of a Drop) five times. The exhibition reminds the scientist Jaroslav Heyrovský and it took place in Strakonice (28th exhibition), in Prague (29th and 31st exhibitions) and for a week in the HIPC. The part of the exhibition was installed in Karolinum (the seat of Charles University) for one day on the occasion of the ceremonial commemoration of the 60th anniversary of the award of the Nobel Prize to J. Heyrovský (10th December 2019). 30th exhibition was organized in Frýdek Místek. The virtual version of the exhibition, which has been running since 2009 and has been visited by around 31,000 visitors throughout its duration, is updated on its website at http://www.heyrovsky.cz). The independent exhibitions on different themes took place in the HIPC chamber gallery 4P: the traditional annual exhibition of works by scientists from the HIPC entitled *Nejen prací živ je vědec* (A scientist has life outside of work). The exhibition *Svět podle Hieronyma Bosche* (The World According to Hieronymus Bosch, by *Svatopluk Civiš*), which took place twice: once in Gallery 4P and once in Gymnázium Botičská (high school in Prague 2). The exhibition *Jiří Suchý: Grafiky* (Graphics, see fig.) and the exhibition of photographs by Josef Zoser: *Tiché návraty* (Silent Returns) took place in the Gallery 4P.

Exhibitions *in the lobby of the HIPC, called Gallery 4P, are an opportunity for meetings between science and art.*

III. 5 Scientific and pedagogical collaboration of HIPC with universities

In 2019, the HIPC participated in the training of **55 PhD students** (in full-time and part-time form of study; of this number, 12 defended their dissertation during 2019). 18 university students were trained by researchers from HIPC as part of their bachelor's and master's theses.

Every year, these students present the results of their internships (bachelor's and master's diploma theses and dissertations) at a student conference called **Seminář studentů ÚFCH JH** (Student Seminar of HIPC). The conference took place in the conference center of the CAS in the Liblice Chateau (April 29 - 30 2019). 27 university students (5 of them foreign) and 1 high school student gave their presentations, mostly in English. The conference was also attended by almost 30 scientists from HIPC. Student contributions are summarized in the proceedings:

https://www.jh-inst.cas.cz/index.php/scientific-meetings/student-seminar-of-jhi-2019

Thirty researchers participated in the **teaching** of bachelor's, master's and PhD students **at ten universities**, and during the *summer/winter* semester a total of *589/1179* hours in *19/49* semester cycles of lectures, seminars and practice exercises.

In 2019, 15 scientists were members of subject area boards of the doctoral study programmes (scientific advisory boards of PhD study). 15 scientists were members of examining committees for state bachelor, master and PhD exams, and for dissertation defense in the field of physical chemistry at several universities and colleges (Faculty of Science and Faculty of Mathematics and Physics, Charles University in Prague; Czech Technical University in Prague; University of Chemistry and Technology, Prague; University of Pardubice; Masaryk University in Brno; Palacký University Olomouc and University of South Bohemia in České Budějovice).

In 2019, HIPC again successfully collaborated in 27 grant projects with different universities. The employees of HIPC were principal investigators or project participants.

Another educational and at the same time popularization activity is educating **high school youth** and working with talented high school students who are interested in studying natural sciences (lectures, excursions, workshops and internships). This activity is carried out

beyond everyday research activities since 2005. 54 one-hour lectures on various topics in the field of physical chemistry were given to high school students in 2019. Students who completed high school internships at the HIPC defended their work in various competitions, such as SOČ (High-School Expert Activity) or Amavet (Association for Youth, Science and Technology). The students submitted their work also as seminar papers and final exam papers (almost twenty works in total). 3 students advanced to the national round of SOČ competition. One student took 2nd place in the field of Physics and another student took 3rd place in the field of Healthcare.

In 2019, HIPC also continued programs focused on the **education of primary and middle school pupils** (teaching by experimentation, workshops) and preschoolers (chemical show). HIPC cooperates with more than a hundred schools (high schools, primary and middle schools and kindergartens) from the regions of the Czech Republic, including Prague. HIPC regularly cooperates, for example, with the Department of Projects and Grants of the CAS: project *Otevřená věda AV ČR 2019* (Open Science project of the CAS 2019) and with the National Institute of Further Education of the Ministry of Education, Youth and Sports: programs of educational visits in HIPC *Den (s) vědcem*, A day (with) a scientist. HIPC also collaborates with the Nadační fond Jaroslava Heyrovského (Jaroslav Heyrovský Endowment Fund) on competition *SOČ* (High school expert activity) and with Goethe Institute in Prague (competition Bystré hlavy, Bright Heads). HIPC participates in joint projects with high schools.

Regularly updated web pages are dedicated to popularization of results of research and development: http://www.3nastroje.cz and http://www.heyrovsky.cz.

Educational programs: *The range of chemical programs (from the shows for kindergartens, through workshops and groups for primary and middle school students to all-day programs with lectures, workshops and internships in laboratories for high school students throughout the school year) is complemented by holiday programs: one-week NanoŠkola (Nanoschool), chemistry course Neon in the town Bor and workshop programs for suburban or summer camps. High school students from all over Czech Republic have internships in HIPC. Their instructors are more than 20 scientists and PhD students from HIPC.*

III. 6 Collaboration of the HIPC with other institutions and with the business sector

The results of cooperation with the business and other organizations obtained in a project

In 2019, the HIPC collaborated with the business sector on 7 projects.

Analysis and quantification of discharge products of the gas Novec 4710

Program: The replacement of gas SF6 in distribution boards

Result: Identification and quantification of discharge products of the gas Novec 4710

Application: Knowledge of plasma chemistry during partial discharge in high-voltage distribution boards filled with this gas.

Funder: Technology Agency of the Czech Republic

Partner organization: Eaton Elektrotechnika s.r.o.

Synthesis and optimization of cathode materials for 48V Li battery for the automotive industry

Program: Research and design of 48V lithium batteries for the automotive industry / TRIO programme

Result: 1) The optimized NMC material with hollow sphere morphology was used as a cathode in a battery module with a theoretical capacity of 121.7 Ah and an energy of 450.5 Wh. The tested battery provided 78.3% of the theoretical capacity and 73% of the theoretical energy after 10 formatting cycles and showed stable operation after more than 200 charging/discharging cycles at C/10 speed. 2) Electrochemical testing of NMC materials with higher NiO concentrations confirmed greater capacity/energy losses during formatting due to higher Ni^{+4} reactivity during charging.

Funder: Ministry of Industry and Trade of the Czech Republic

Partner organization: HE3DA, s.r.o.

Publication: M. Zukalova, J. Prochazka, A. Zukal and L. Kavan, Electrochemical Performance of LiNixMnyCozO2 (NMC) Materials with Hollow Spheres Morphology, ECS Trans, 95(1), 55-63 (2019). DOI: 10.1149/09501.0055ecst

Innovative photocatalytic concretes and concrete screeds

Program: Innovative photocatalytic screeds and concrete additives

Result: Innovative photocatalytic concretes and concrete screeds with solar self-cleaning and antimicrobial effect

Application: The company Betosan, s.r.o., project partner in joint project FV20234, plans the production and future application of the developed materials in construction industry.

Funder: Ministry of Industry and Trade of the Czech Republic

Partner organization: The company Betosan, s.r.o.

Publication: 2 utility model applications

Innovative nanocomposite coatings with photocatalytic self-cleaning and disinfection function

Program: Photoactive nanocomposite systems for environmental improvement

Result: Colloidal system based on nanoparticles of titanium dioxide and silica for photocatalytic self-cleaning and disinfection surface treatment of historic buildings and other monuments

Application: The company BAL Teluria, s.r.o., project partner in the joint project TH04030090, plans to use the developed materials for the preventive surface treatment of historic buildings and other monuments.

Funder: Technology Agency of the Czech Republic

Partner organization: The company BAL Teluria, s.r.o.

Results of collaboration with other organizations and businesses obtained on the basis of contracts

In 2019, the HIPC continued to fulfill the obligations of 4 contracts for work (domestic and foreign business and other entities). As part of the performance of these contracts, results were achieved, mostly submitted as technical reports.

Influence of chain length of nonpolar lipids on the stability of the lipid layer of the mucosal film - computer modeling

Client: Santen SAS, Francie

Abstract: We explained the mechanism of destabilization of the mucosal film in the presence of non-polar short-chain lipids using computer modeling.

Application: Support in the design and development of ophthalmic drugs

Production of zeolite SSZ-13 with mechanochemical activation

Client: UNICRE a.s.

Abstract: A procedure for the synthesis of zeolite SSZ-13 without the use of solvent (water) was developed by mechanochemical activation of the synthesis mixture.

Application: The use of this process significantly increases the yield of the synthesis of the zeolitic catalyst and at the same time reduces its impact on the environment.

Publication: Mechanochemical Pretreatment for Efficient Solvent-Free Synthesis of SSZ-13 Zeolite, V. Pashkova, K. Mlekodaj, P. Klein, L. Brabec, R. Žouželka, J. Rathouský, V. Tokarová, J. Dědeček, Chemistry – A European Journal 25 (2019) 12068-12073.

Characterization of plasma modified surfaces of polymeric materials by XPS method

Client: Czech Technical University in Prague, The Faculty of Mechanical Engineering

Abstract: The surface composition and population of oxygen-containing functional groups of a series of 21 samples prepared by plasma surface treatment under various experimental conditions were determined by XPS spectroscopy.

Application: The results are used to optimize the conditions of plasma modifications of surfaces of polymeric materials by microwave plasma in order to develop new composites for pressureless technologies, 3D printing, Rotational molding, etc.

Evaluation of nanomorphology of the surface of the corrosion layer of Zr alloy samples by AFM method

Client: ÚJP PRAHA a.s.

Abstract: Evaluation of nanomorphology of the surface of the corrosion layer of Zr alloy samples by AFM method when assessing the corrosive effects of the environment corresponding to the VVER reactor on nanomorphological changes in the surface of Zr alloy tubes for nuclear fuel deposition.

Application: For assessing the corrosive effects of the environment corresponding to the VVER reactor on nanomorphological changes in the surface of Zr alloy tubes for nuclear fuel deposition.

Joint research and development projects supported by public funds

In 2019, 2 patents and 1 utility model were granted.

Patent

A method of producing a porous diamond layer and a thick porous diamond layer reinforced by nanofibers

The invention describes a method of manufacturing a porous diamond layer and a porous diamond body reinforced with nanofibers. This method of preparation includes the step of inoculating diamond nanoparticles into nanofibers of any material capable of withstanding plasma-assisted deposition conditions.

Date of grant of the patent:: 12th June 2019

Originators: V. Mortet, Vincent, A. Taylor, L. Kavan, O. Frank, Z. Vlčková Živcová, H. Krýsová, V. Petrák

Application: Innovative nanocomposite coatings with photocatalytic self-cleaning and disinfection function

Patent

Process for producing zeolite SSZ-13 with mechanochemical activation

A process for the synthesis of zeolite SSZ 13 without the use of solvent (water) was developed by mechanochemical activation of the synthesis mixture.

Date of grant of the patent: 4th December 2019

Originators: V. Pashková, K. Mlekodaj, J. Dědeček, V. Tokarová

Application: The use of this procedure significantly increases the yield of the synthesis of the zeolitic catalyst and at the same time reduces its impact on the environment.

Utility model

Cyclopentadienyl-arene complexes of ruthenium for the preparation of drugs suppressing the migration and invasiveness of tumor cells

The presented solution deals with ruthenium complexes with arene and cyclopentadienyl ligands and their use in the preparation of drugs useful for the treatment of cancer. The main expected effect is the suppression of cancer cell migration and invasiveness in selected types of invasive tumors (ovarian cancer, breast cancer and others).
Date of grant: 19th February 2019

Originators: R. Hrstka, L. Sommerová, J. Pinkas, J. Karban

Application: Innovative nanocomposite coatings with photocatalytic self-cleaning and disinfection function.

Information on the employees of the HIPC who held positions in the governing bodies of major international scientific organizations

RNDr. Jan Hrušák, CSc. Name of the organization: European Strategy Forum for Research Infrastructures (ESFRI), position: Chairman, term of office: 2019 - 2021

Mgr. Magdaléna Hromadová, PhD., PhD., name of the organization: International Society of Electrochemistry, position: officer of Division 6 (Molecular Electrochemistry). Term of office: 2017 - 2019

doc. Ing. Petr Krtil, CSc., name of the organization: International Society of Electrochemistry, position: executive secretary. Term of office: 2019 - 2023

III. 7 International scientific collaboration

Within the framework of international cooperation, the HIPC solved a total of 8 projects financed by the European Commission within the Horizon 2020 program. Furthermore, the HIPC participated in 12 international projects, within the framework of international scientific cooperation outside the EU framework programs and outside the projects of the Structural Funds.

Projects funded by the European Commission under the HORIZON 2020 program

Ion–Molecule Processes for Analytical Chemistry Technologies, (acronym IMPACT), coordinator: University of Birmingham, investigator: prof. RNDr. Patrik Španěl, Dr. rer. nat. The project was launched in 2016 and continues until 2020.

Trans-Spin NanoArchitectures: from birth to functionalities in magnetic field (acronym TSuNAMI), coordinator: Charles University in Prague, investigator: doc. RNDr. Ing. Kalbáč Martin, Ph.D. The project was launched in 2017 and continues until 2021.

Electrochemical Conversion of Renewable Electricity into Fuels and Chemicals (Acronym: ELCOREL), coordinator: J. Heyrovský Institute of Physical Chemistry (Czech Republic), investigator: doc. Ing. Petr Krtil, CSc. The project was launched in 2017 and continues until 2021.

ERA chair at J. Heyrovsky Institute of Physical Chemistry AS CR-The institutional approach towards ERA, (acronym Heyrovsky Chair), coordinator: J. Heyrovský Institute of Physical Chemistry (Czech Republic). The project leader is RNDr. Jan Hrušák, CSc. The project includes an international advisory board. The project was launched in 2018 and continues until 2023.

Transformative Chemistry for Sustainable Energy Future (Acronym: Energy-X), coordinator: The Technical University of Denmark, investigator: doc. Ing. Petr Krtil, Ph.D. The project was launched in 2019 and continues until 2020.

Proton Transport and Proton-Coupled Transport (Acronym: PROTON), coordinator: Peter Pohl, investigator: prof. Martin Hof, Dr. rer.nat, DSc. The project was launched in 2019 and continues until 2023.

Solar Energy for Circular Economy (Acronym: SUNRISE), coordinator: University of Leiden, investigator: prof. RNDr. Antonín Vlček, CSc. The project was launched in 2019 and continues until 2020.

Support to Reinforce the European Strategy Forum on Research Infrastructures (Acronym: StR-Esfri2), coordinator: United Kingdom Research and Innovation, project participant: RNDr. Jan Hrušák, CSc. The project was launched in 2017 and continues until 2022.

International projects that were carried out in the framework of international scientific cooperation outside the EU framework programs

OVERVIEW OF INTERNATIONAL PROJECTS THAT ARE CARRIED OUT IN THE FRAMEWORK OF INTERNATIONAL SCIENTIFIC COLABORATION

Funder	N. of Projects
INTER-EXCELLENCE (MEYS) sub-programme INTER-ACTION	2
INTER-EXCELLENCE (MEYS) sub-programme INTER-COST	3
Program Mobility (MEYS)	4
International Cooperation Program – Visegrad Group (MEYS)	1
International mobility of researchers (MEYS- Operational Program Research, Development and Education)	2

III. 8 Conferences and foreign guests

In 2019, the HIPC organized or co-organized 6 conferences with international participation, which were attended by 452 guests, including 145 foreigners. Additionally, HIPC organized or co-organized 8 national conferences with a total participation of 426 guests (47 foreigners).

Conferences with international participation

Nanocatalysis Day
11th April 2019, Venue: HIPC, number of participants: 80, foreigners: 20

39th Modern Electrochemical Methods

20th-24th May 2019, Venue: Jetřichovice, number of participants: 85, foreigners: 31

The Second International Conference on Soft Chemical Ionization Mass Spectrometry and its Applications to Trace Gas Analysis

10th-13th June 2019, Venue: HIPC, number of participants: 52, foreigners: 41

52nd Heyrovský Discussion
16th-20th June 2019, Venue: Liblice Chateau, number of participants: 48, foreigners: 16

Dynamic covalent chemistry: Frontiers & Perspectives
27th June 2019, Venue: HIPC, number of participants: 102, foreigners: 23

51th Symposium on Catalysis
4th-5th November 2019, Venue: HIPC, number of participants: 85, foreigners: 14

Significant national scientific events organized or co-organized by HIPC

Výzkum meziplanetární hmoty a extrasolárních systémů
(Research of interplanetary matter and extrasolar systems)

8th -10th November 2019, Venue: Horský hotel Charbulák, number of participants: 25

Prague Membrane Discussions 2019 – Spring Event
21st March 2019, Venue: HIPC, number of participants: 52

The student seminar of JHI 2019
29th-30th April 2019, Venue: Liblice chateau, number of participants: 58, foreigners: 5

Potlach č. VII (Potlatch N. 7)
15th October 2019, Venue: HIPC, number of participants: 69, foreigners: 6

Na hranici Země a vesmíru (At the border of Earth and Space)
23rd – 24th October 2019, Venue: Hvězdárna a radioklub lázeňského města Karlovy Vary o.p.s. (Observatory and Radioclub of Spa City of Carlsbad)
number of participants: 13

60th Anniversary of Jaroslav Heyrovský Nobel Prize in Chemistry
11th November 2019, Venue: HIPC, number of participants: 90, foreigners: 20

Heyrovský Memorial Lecture
10th December 2019, Venue: Faculty of Science, Charles University, number of participants: 47, foreigners: 3

Odpoledne s elektrochemií (Afternoon with Electrochemistry)
9. 12. 2019, Venue: HIPC, number of participants: 72, foreigners: 13

Foreign guests of the HIPC

In 2019, **13 foreign guests visited** HIPC. The guests gave lectures during their stays at the HIPC.

Prof. Renato Zenobi, ETH Zurich, Switzerland gave a 29th **R. Brdicka Memorial Lecture:** "Nanoscale Chemical Analysis and Imaging using Tip-Enhanced Raman Spectroscopy". Another important lecture was given by **prof. Jean-Marie Lehn, Institut de Science et d'Ingénierie (Supramoléculaire Université de Strasbourg, France)** "Perspectives in Chemistry: Towards Adaptive Chemistry".

prof. Renato Zenobi

Eidgenössische Technische Hochschule
Zürich
Switzerland

prof. Jean-Marie Lehn

Institut de Science et d'Ingénierie
Supramoléculaire
Université de Strasbourg, France

Other distinguished guests were:

prof. Emilio Pérez Álvarez, IMDEA Nanoscience, Madrid, Spain, with the lecture „Diversions and junctions in the road of science: from carbon nanotube rotaxanes to covalent organic frameworks",

prof. Euan Kay, School of Chemistry, University of St. Andrews, United Kingdom,with the lecture „Manipulating the Monolayer: Dynamic Covalent Nanoparticle Building Blocks" and

prof. Max von Delius, Institute of Organic Chemistry and Advanced Materials, University of Ulm, Germany with the lecture „New Tools and Uses of Dynamic Covalent Chemistry".

IV. Assessment of additional and other activity

In addition to its main activity, in 2019 the HIPC leased non-residential space in the building of cafeteria and in the main building to the following companies:

RENTAL OF NON-RESIDENTAL SPACE

TENANT	IDENTIFICATION NUMBER
HE3DA s.r.o.	28949935
Advanced Materials - JTJ s. r. o.	26763842
Institute of Thermomechanics of the CAS	61388998
FN-NANO s.r.o.	05079233
GODS, s.r.o.	45787956
Dana Kapková Dekolab-sklo	69482292
Ivan Černý	42531772
Lukáš Svoboda	70752648
Zdeňka Beranová	41798473
IVR FS s.r.o.	24277169
LAGET, spol. s r.o.	15030091
M-CATERING	25099671
Three Bond Czech, s. r. o.	27194639
Institute of Physics of the CAS	68378271

HIPC provided accommodation for its employees and foreign guests if needed. HIPC did not carry out any other activities.

V. Information on measures to eliminate deficiencies in economic management and a report on how the measures to eliminate deficiencies imposed in the previous year have been implemented

In 2019, the Czech Science Foundation inspected the using of financial funds in all grants supported by it. The audit was carried for 2018 and partly also for 2017. The audit found an unauthorized use of the allocated funds, in conflict with the terms of the contract. The Czech Science Foundation reduced the subsidy by CZK 167,330.27. Given that these costs were incurred as justified but ineligible, the sum was credited to account 542/100, where non-deductible expenses are recorded, as these costs are related to previous accounting periods, i.e. 2017 and 2018. Based on the results of the audit, a more rigorous monitoring and control of eligible costs was implemented according to individual grant agreements.

In the financial year 2019, older receivables in the amount of CZK 40,072.73 were written off. The receivables are practically irrecoverable. The major part of the amount is the write-off of receivables for foreign employees. These receivables were for accommodation and for lunches, when the billing of these short-term foreign employees was received by the accounting entity only after their departure from HIPC or from the Czech Republic. These receivables are from previous years, when we unsuccessfully tried to recover them. The group of written-off receivables also includes the write-off of a receivable, when payment by card was deducted twice and the complaint was not accepted.

VI. Financial information about facts that are relevant to the assessment of the economic position of the institution and may affect its development

In 2019, no events occurred that would affect the economic position of the HIPC to any significant extent. The financial results made it possible to meet the planned formation of a reserve for the repair of the real estate in Michle, Prague.

VII. Expected development of HIPC activities

In 2020-2022, the HIPC will develop scientific and research activities in the field of physical chemistry and relevant other fields on the basis of a strategy approved by the institute board. The main component of the activity will be the formulation of research and development projects and their implementation on the basis of targeted funding in the form of grant projects.

The ERA chairs project **Heyrovský Chair** is especially important. This project helps elevate scientific institutions among the best in the world. The HIPC is only the second scientific center in the Czech Republic that achieved this prestigious funding. In total, the HIPC obtained almost 2.5 million euros (over 60 million CZK), which was used, among other things, to acquire a world-renowned scientist on the basis of an international tender. The position was appointed to prof. Štefan Vajda from Argonne National Laboratory and Institute for Molecular Engineering of the University of Chicago. In 2020, the team of the Nanocatalysis Department will start full-scale experimental research.

The strategy also includes expanding the participation of the HIPC in EU projects and supporting young researchers in developing their scientific careers. The HIPC received the prestigious HR Award, fully entitled "HR Excellence in Research Award", awarded by the European Commission for excellence in the care of human resources in the scientific environment. Obtaining the HR Award is not only a sign of quality, but also a lasting commitment to continued development and the creation of favorable conditions for employees. Therefore, an action plan has been developed describing in a binding manner the concrete steps to bring the procedures in line with the "European Charter for Researchers" and the "Code of Conduct for the Recruitment of New Staff". After two years, a mid-term evaluation will be carried out, and then the HIPC will be evaluated every three years.

In 2020, the administrative support of scientific work will be improved in the form of process management, especially in the areas of grant support (creation of a new grant group as the basis of the future grant department), recruitment (OTM-R), intellectual property protection, open access to information, transfer technologies and their licensing.

VIII. Activities in the field of environmental protection

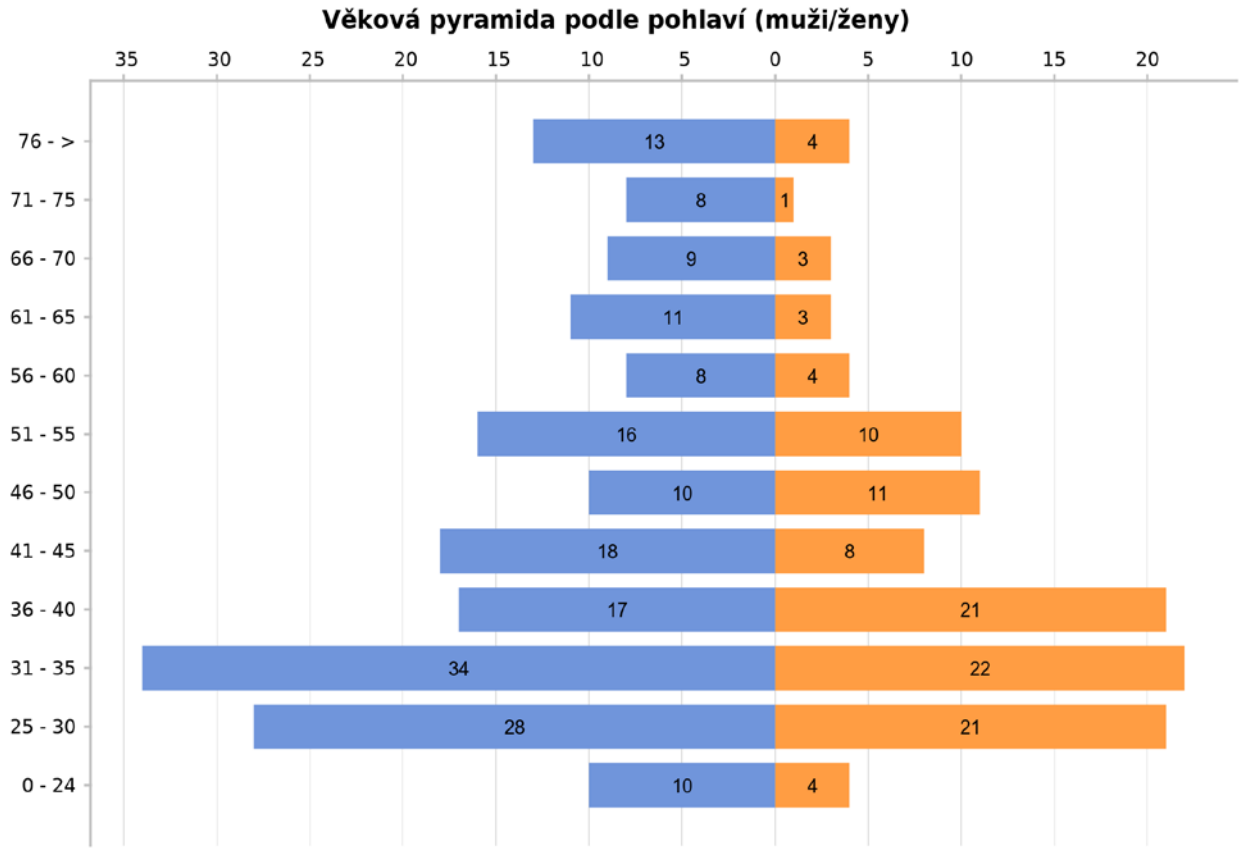
HIPC participates in research projects related to environmental protection, both in basic research of environmentally important physical chemistry and in applied research in cooperation with industry.

HIPC carries out regular disposal of waste generated in connection with research activities, especially chemicals and depreciated office equipment using the services of specialized companies, in cooperation with the city district office. The HIPC also sorts the waste produced, namely glass, paper, plastics, batteries and accumulators.

IX. Activities in the field of labor relations

An overview of the number of employees and the distribution of personnel costs are given in the Notes to the Financial Statements. The number of employees as on 31st December 2019 was 294, the average recalculated number for 2019 was 240. The classification of the HIPC's employees into the categories of professionals and researchers on the basis of the updated internal salary regulations and career rules of the CAS is based on the evaluation of scientific work by heads of departments and evaluation commissions based on specific criteria.

NUMBER OF EMPLOYES 31st December 2019	
TOTAL NUMBER OF EMPLOYES	294
AVERAGE RECALCULATED NUMBER OF EMPLOYEES	240
NUMBER OF EMPLOYES (SCIENTIFIC POSITIONS)	234
PhD STUDENTS	47
N. OF FOREIGN SCIENTISTS (SCIENTIFIC POSITIONS)	88 (38 %)
N. OF WOMEN (SCIENTIFIC POSITIONS)	82



X. Provision of information under Act No. 106/1999 Coll., On Free Access to information

No request for information was submitted under Act No. 106/1999 Coll., On Free Access to information.

Stamp

signature of the director of the institute

OTHER MANDATORY INFORMATION

This document was created with support of the project Rozvoj kapacit ÚFCH JH, v.v.i. pro výzkum a vývoj (reg. No. CZ.02.2.69/0.0/0.0/ 16_028/0006251) financed by the Ministry of Education, Youth and Sports and the European Structural and Investment Funds in the Operational Program Research, development and education.

EUROPEAN UNION
European Structural and Investment Funds
Operational Programme Research,
Development and Education