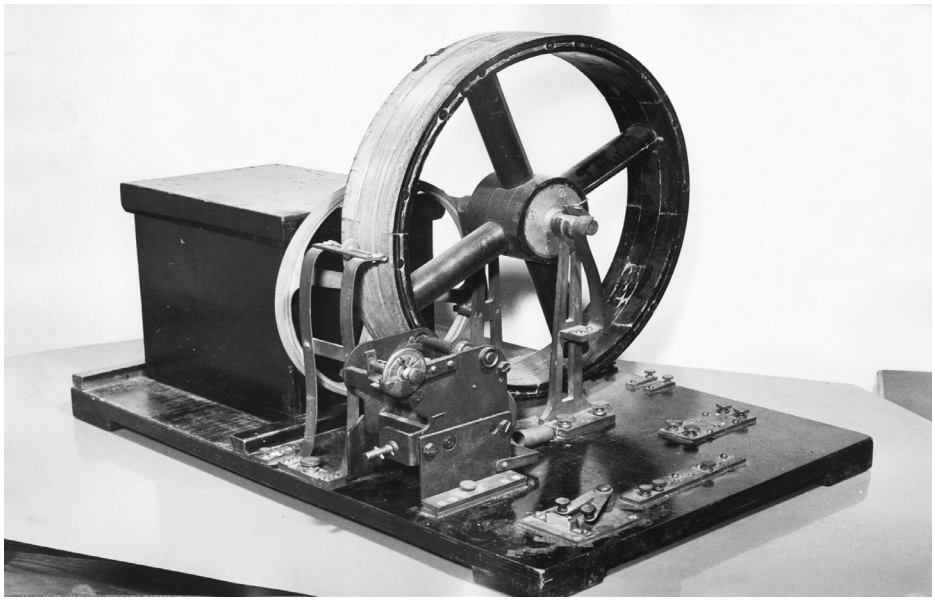
J. Heyrovský Institute of Physical Chemistry



J. Heyrovský Institute of Physical Chemistry

ANNUAL REPORT

ON ACTIVITY AND ECONOMIC MANAGEMENT 2021

J. Heyrovský Institute of Physical Chemistry (JHIPC, Institute)
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 26 May 2022
Approved by the Institute Board on 20 June 2022
In Prague on 22 June 2022

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 Institute

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

appointed effective from 1 May 2017

The Institute Board

Elected on:	23 January 2017; members:
Chairman:	prof. RNDr. Patrik Španěl, Dr. rer. nat.
Vice-chairman:	prof. RNDr. Ladislav Kavan, CSc., DSc.

Internal members (JHIPC)

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: Mgr. Otakar Frank, Ph.D.
J. Heyrovský Institute of Physical Chemistry of the CAS

Members: Ing. Jana Bludská, CSc.,
Institute of Inorganic Chemistry of the CAS

prof. Ing. Jiří Homola, CSc., DSc.
Institute of Photonics and Electronics of the CAS

prof. Mgr. Iva Matolínová, Dr.
Faculty of Mathematics and Physics, Charles University in Prague

B) Changes in the bodies of the Institute

In 2021, there were no changes in the bodies of the J. Heyrovský Institute of Physical Chemistry (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 11 times in 2021 of which one was the meeting of the broader director's board. The conclusions of the meetings are published on the internal website of JHIPC.

b) Submission of the draft budget for 2021 to the Supervisory Board for comments and the Institute Board for approval.

c) Submission of the Annual Report on Activities and Economic Management for 2020 to the Supervisory Board for an opinion and to the Institute Board for approval after the auditor's verification of the closing financial statement.

d) Submission of proposals for the Otto Wichterle Award, the Praemium Academiae Award, the František Běhounek Medal, the Josef Hlavka Award and the Česká Hlava Award,

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 2021.

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

h) Appointment of members of commissions (e.g., selection committees).

i) Setting up new processes to increase the effectiveness of the JHIPC management.

j) Facilitating operational measures in connection with the COVID-19 pandemic, when, despite epidemiological measures, the operation of the JHIPC was maintained, including laboratory research, and the risk of infection was reduced by working from home in cases that made it possible.

International Advisory Board acts as an advisory body to the director; its members are:

prof. Dr. Ulrike Diebold, Vienna University of Technology, Austria

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. Joachim Heberle, Free University of Berlin, Germany

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

prof. Dr. Leticia Gonzales, Universitat Wien, Austria

The Institute Board

In 2021, meetings of the Institute Board took place a total of 30 times, of which 27 meetings took place in the form of voting by mail (per rollam).

13. meeting of the Institute Board (2 February 2021)

- The Institute Board approved the minutes and resolutions of the 12 meeting of the Institute Board (of 7 September 2020).
- The Institute Board approved the minutes and resolutions of the voting by mail of 29 September 2020, 2 October 2020, 9 November 2020, 8 December 2020, 14 December 2020, 11 January 2021.
- The Institute Board supported the nomination of Ing. Matěj Velický, Ph.D. for the Lumina quaeruntur Award.

- The Institute Board proposed the award of the František Běhounek Medal to the Dean of the Faculty of Science of Charles University in Prague, prof. RNDr. Jiří Zima, CSc.

14. meeting of the Institute Board (25 May 2021)

- The Institute Board approved the minutes and resolutions of the 13 meeting of the Institute Board (of 2 February 2021).

- The Institute Board approved the minutes and resolutions of the voting by mail of 15 February 2021, 18 February 2021, 3 March 2021, 18 March 2021, 27 March 2021, 1 April 2021, 15 April 2021, 21 April 2021 and 7 May 2021.

- The Institute Board approved the announcement of the Selection Procedure for the position of the Director of the Institute from 1 November 2021.

- The Institute Board decided on the next election to the Institute Board: all the candidates will be in one group, i.e., without "election baskets".

- The Institute Board has agreed to publish its Resolutions not only in Czech, but also in English.

15. meeting of the Institute Board (8 November 2021)

- The Institute Board approved the minutes and resolutions of the 14 meeting of the Institute Board (of 25 May 2021).

- The Institute Board approved the minutes and resolutions of the voting by mail of 9 June 2021, 24 June 2021, 9 July 2021, 22 July 2021, 23 August 2021, 7 September 2021, 15 September 2021, 21 September 2021, 27 September 2021, 6 October 2021, 11 October 2021 and 3 November 2021.

- The Institute Board recommended the publication of the advertisement for the post of the Director of the Institute in the discussed version by 10 November 2021 at the latest, on the website of the Institute, on the website of the Academy of Sciences of the Czech Republic and in Hospodářské noviny.

- The Institute Board approved the text of the Election Rules of the Institute, including Annex 1 and Annex 2.

- The election will take place on January 13, 2022, from 10 a.m.

- The Institute Board has approved a change in the Internal Wage Regulation of the Institute so that the minimum wage for categories O1 and O2 will be increased to CZK 16,200 with effect from 1 January 2022.

The Institute Board approved the following resolutions by mail:

- The Institute Board supported the submission of a total of 72 grant project proposals.

- The Institute Board approved the documents of the Rules for Drawing Social Fund of the J. Heyrovský Institute of Physical Chemistry of the CAS, p.r.i. for 2021 and the Social Fund Utilization Budget for 2021 as submitted.

- The Institute Board approved the Rules of Procedure of the J. Heyrovský Institute of Physical Chemistry of the CAS, p.r.i. as submitted.

- The Board of the Institute **did not recommend** supporting the proposal of the start-up grant of the Experientia Foundation to support the establishment of a new scientific group due to the current topic of the Department of Structure and Dynamics in Catalysis. At the same time, taking this into account, the Board recommended that the head of this department discuss with the director of the Institute the possibility of recruiting a new scientist in the field of organic reactions on zeolites.

- The Institute Board agreed to conclude the document "Agreement on corporation" between the J. Heyrovský Institute of Physical Chemistry of the CAS, p.r.i. and MBN Research Center GmbH as submitted.

- The Institute Board agreed to the following nominations for the Otto Wichterle Award: Pamir Nag, Ph.D., Haider Golam, Ph.D. and Carlos Mauricio Maldonado Domínguez, Ph.D.

- The Institute Board recommended to submit an application for support from the Programme of Support for Prospective Human Resources - Wage Support for Postdocs at the Institutes of the CAS to the candidates: Mgr. Vojtěch Hrdlička, Ph.D. and MSc. Béla Urbán, Ph.D.

- The Institute Board approved the presented the submitted budget of the Institute for 2021.

- The institute board notes the submitted Annual Report on Activities and Management for 2020, including the attached report of the independent auditor, and agreed with its wording.

- The Institute Board agreed to conclude the submitted Cooperation Agreement between JHIPC and Roplass s.r.o.

- The Institute Board consented to the conclusion of the submitted Cooperation Agreement between the JHIPC and R&D centre for plasma and nanotechnology surface modifications CEPLANT.

- The Institute Board agreed to conclude the Consortium Agreement as submitted.

- The Institute Board approved the submitted Organizational Rules of the JHIPC.

- The Institute Board recommended nominating prof. RNDr. Antonín Vlček, CSC for the Jaroslav Heyrovský Honorary Medal for Merit in Chemical Sciences.

- The Institute Board agreed to the conclusion of the submitted Memorandum of Understanding between JHIPC and The Industrial Technology Research Institute and the Memorandum of Cooperation between JHIPC and the Ministry of Labour and Social Affairs of the Czech Republic.

- The Institute Board agreed to the involvement of ÚFCH JH in the solution of the proposed research program "Breakthrough technologies of the future of sensor

technology, digitization, artificial intelligence, and quantum technologies Strategy AV21", for five years, starting from 2022.

- The Institute Board agreed to JHIPC's involvement in the solution of the proposed research program Strategy AV21 with the theme of Sustainable Energy.

- The Institute Board agreed to conclude the submitted Cooperation Agreement on the research project Slavia between JHIPC on the one hand and S.A.B. Aerospace s.r.o on the other.

- The Institute Board appointed a Selection Committee for the assessment of submitted applications and registered candidates for the selection procedure for the appointment of the Director of the J. Heyrovský Institute of Physical Chemistry of the CAS, p.r.i. Its members are prof. Patrik Španěl (chair), prof. Ladislav Kavan, RNDr. Zdeněk Havlas, DrSc., RNDr. Antonín Fejfar, CSc., prof. Pavel Matějka, prof. Tomáš Obšil, doc. Ing. Ivan Richter, Dr.

- The Institute Board approved the Initial Gender Equality Plan 2021 2024 as presented.

Supervisory Board

In 2020, a meeting of the Supervisory Board of the J. Heyrovský Institute of Physical Chemistry of the CAS, p.r.i. took place on 14 June 2021. Eight meetings by mail took place due to 5 February 2021, 11 May 2021, 17 May 2021, 11 October 2021, 2 November 2021, 6 December 2021, 20 December 2021 and 22 December 2021.

All members of the Supervisory Board and the Institute 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 2021.

Meeting of the Supervisory Board on 14 June 2021

- P. Bobák introduced two new members of the Supervisory Board of the JHIPC: the Academic Council of the CAS appointed Mgr. Otakar Frank, Ph.D., as Vice-President at its 42nd meeting on 12 January 2021, and Ing. Jana Bludská, CSc. as a new member, with effect from 20 January 2021 until 19 January 2026.

- Director's report – presentation: Director of the Institute M. Hof presented the leading scientific and research results of the Institute in 2015-2020 in the form of a projection. He informed the board about the structure of the institute and staff policy, young prospective researchers, and the growing number of foreign employees. The director also talked about the trends in research in the Institute, publications, grants, and plans for the future and justified the intention of adding a new building and using it to construct new laboratories.

- The Supervisory Board appreciated the research and publication activities of the Institute very positively. The Supervisory Board took note of the report of the director of the JHIPC.

- The Supervisory Board discussed and took note of the Annual Report of JHIPC for the year 2020, the Auditor's Report for 2020 and the Institute's Register of Contracts for 2020.

- The supervisory board discussed and took note of the Appendix to the Financial Statements, the Balance Sheet and the Profit and Loss Statement. It also takes note of the presented information on the management and investments of the Institute.

- The Supervisory Board acknowledges and agrees with the Draft Budget of the Institute for 2021. The meeting discussed the draft budget and the outlook for 2022/23, and the Supervisory Board recommended adding a medium-term outlook for 2022/23.

- The Supervisory Board appoints Ing. L. Ježek as the auditor for the financial statements for the year 2021 according to the Audit Agreement.

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

The Supervisory Board approved the following resolution by mail:

1) The Supervisory Board agrees with Appendix No. 3 pursuant to Article XIII. article 2 to the contract of 1 March 2018 registration no. 2018/003 On the Lease of Non-residential Premises (Catering) between the JHIPC, p.r.i. and M Catering, s.r.o. - reduction of the lease until 30 April 2021 due to state of emergency.

The approval took place by mail No. 59 as of February 5, 2021.

2) The Supervisory Board agrees with Appendix No. 4 pursuant to Article XIII. article 2 to the contract of 1 March 2018 registration no. 2018/003 On the Lease of Non-residential Premises (Catering) between the JHIPC, p.r.i. and M Catering, s.r.o. - reduction of the lease until 30 June 2021 or to the end of the state of emergency.

The approval took place by mail No. 60 as of May 5, 2021.

3) The Supervisory Board agrees with the Application for prior written consent to allocate investment funds to the NMR spectrometer with accessories (M. Horáček, M. Lamač). Estimated price including VAT is 19 500 000 CZK.

The approval took place by mail No. 61 as of May 17, 2021.

4) The Supervisory Board agrees with the Contract on the establishment of easement with PRE distribuce, a. s.

The approval took place by mail No. 62 as of October 11, 2021.

5) The Supervisory Board agrees with the Application for prior written consent for the approval of the investment plan – acquisition of SPECS NAP XPS equipment as part of the upcoming ERC-2022-SYC Synergy Grants (Š. Vajda).

The approval took place by mail No. 63 as of November 2, 2021.

6) The Supervisory Board agrees with the Agreement on Assignment of the Lease of Business Premises between JHIPC p.r.i. and IVR FS s.r.o. and VORY Energy, a.s.

The approval took place by mail No. 64 as of December 6, 2021.

7) The Supervisory Board agrees with the documents sent from the economic department No. 1 – 9.

The approval took place by mail No. 65 as of December 20, 2021.

8) The Supervisory Board agrees with Amendment No. 1 to the Contract No. 2014/063 on the Lease of Business Premises between JHIPC p.r.i. and GODS, s. r. o.

The approval took place by mail No. 65 as of December 22, 2021.

II. Information on changes in the foundig deed

No changes were made to the founding deed in 2021.

III. Assessment of the main activity

In accordance with the valid founding deed, the JHIPC 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 22 June 2010, the main activity of the JHIPC 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 JHIPC activity and for control of experiments and processing of results of the JHIPC. Through its activities, the JHIPC contributes to increasing the level of knowledge and education and to the use of the results of scientific research in practice. JHIPC 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, JHIPC 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. JHIPC 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. JHIPC carries out projects independently and in cooperation with universities and other scientific and expert institutions.

In 2021, the JHIPC 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 centre.

The JHIPC actively supports collaboration at the international level: currently, there are 78 foreign scientists in the JHIPC, and the total number of scientists is 198.

III. 1. The most important results

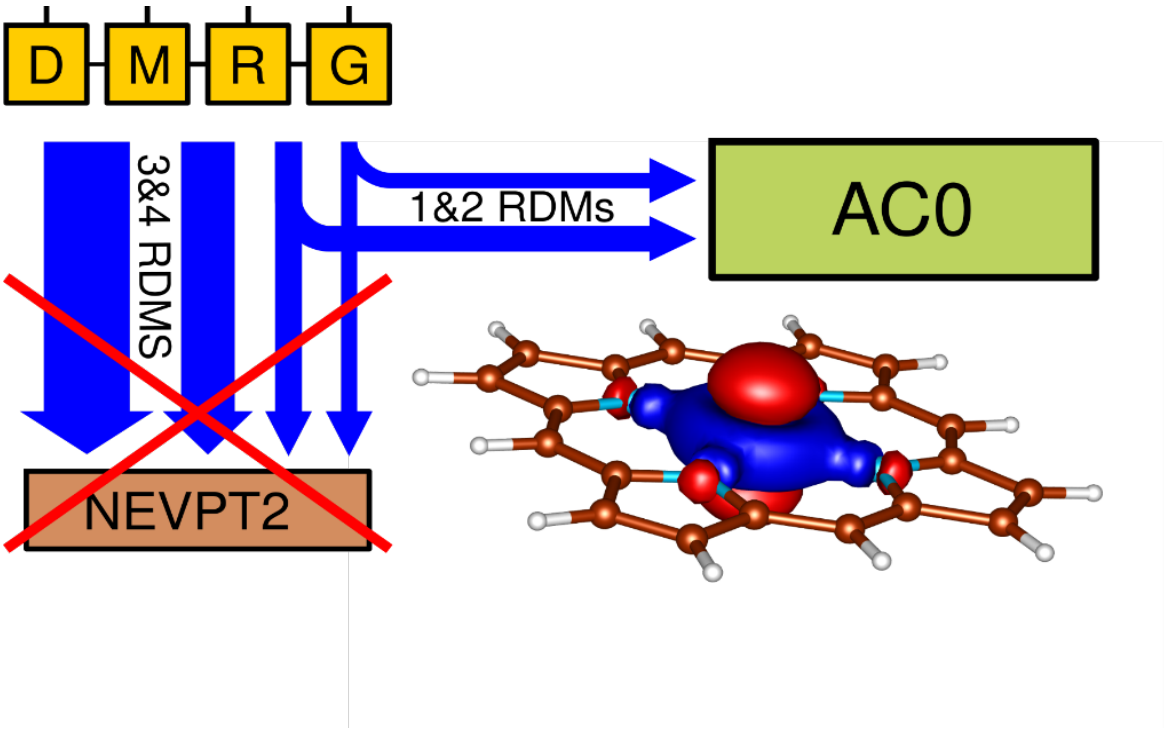
The research plan and the grants achieved important results that are described in this section according to the departments.

Department of Theoretical Chemistry (1)

Density matrix renormalization group with dynamical correlation via adiabatic connection

We have developed a new computational approach to the electronic structure problem of strongly correlated molecules, which combines DMRG with the adiabatic connection. The former is responsible for an accurate description of strong correlation, whereas the later accounts for the missing dynamical electron correlation. This unique connection offers a favorable scaling and high accuracy, which was demonstrated on the examples of n-acenes (n = 2 - 7), Fe(II)-porphyrin, and the Fe3S4 cluster.

Collaborating entity: Institute of Physics, Lodz University of Technology, Poland



Scheme of DMRG-AC0 method*. Scheme of the DMRG-AC0 method emphasizing the need for only up to two-body active space reduced density matrices and thus favorable computational scaling.*

Density matrix renormalization group with dynamical correlation via adiabatic connection. P. Beran, M. Matousek, M. Hapka, K. Pernal, L. Veis. J. *Chem. Theor. Comput.*, 17, 12, 7575-7585 (2021), doi.org/10.1021/acs.jctc.1c00896

Department of Spectroscopy (2)

Application of a dielectric breakdown induced by high power lasers for a laboratory simulation of meteor plasma

It can be literally stated that terawatt lasers enable the impossible: under controlled laboratory conditions, scientists can mimic phenomena incapable of being explored using any other standard experimental approach. Such a case represents also spectra of meteor plasma, their dynamics and dominant spectral features are mostly a subject of mathematical modelling and computations. In our study, we show application of such extreme laser sources for simulation of falling stars.

Collaborating entity: PALS Research Center, Institute of Physics, CAS

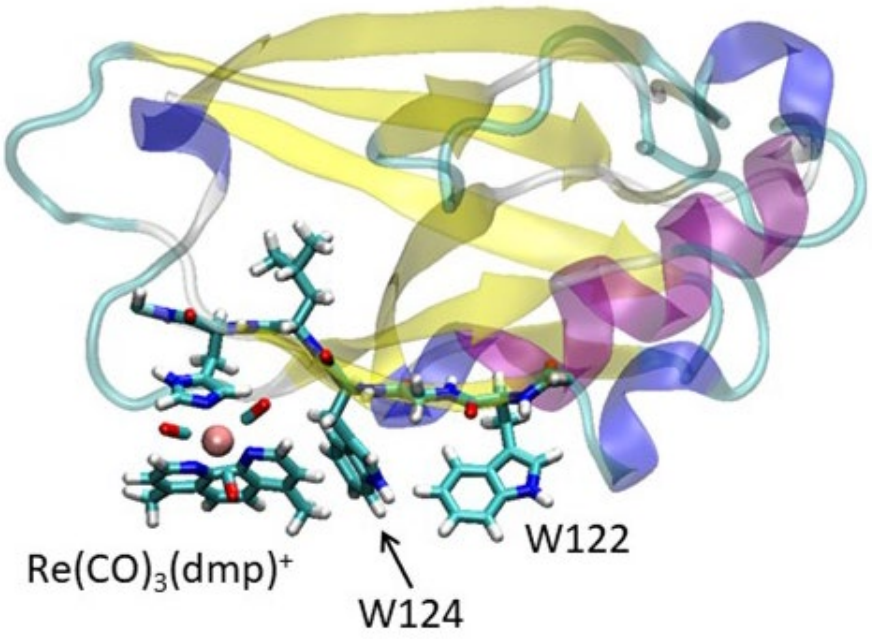
Myriads of falling stars can be simulated by high power laser. *Time lapse of falling stars. Interpretation of their spectra provides information about elemental composition of meteoroids, while their trajectory and origin can be calculated based on photographic records. High power laser experiments are crucial for accurate interpretation of spectral data and help us to understand physics of atmospheric plasma.*

Application of a Dielectric Breakdown Induced by High Power Lasers for a Laboratory Simulation of Meteor Plasma. A. Křivková, L. Petera, V. Laitl, P. Kubelík, E. Chatzitheodoridis, L. Lena, J. Koukal, A. Knížek, R. Dudžák, D. Páclík, S. Civiš, M. Krůs, M. Ferus. Experimental Astronomy, 51, 425–451 (2021), doi.org/10.1007/s10686-020-09688-3

Department of Biophysical Chemistry (3)

Dynamics of photoinduced charge separation through tryptophan protein residues
Electron hopping through tryptophan activates and protects enzymes. Chromophore energetics and positions relative to indoles are evolution-optimized in natural photosystems. Our analysis of modified blue copper proteins using molecular and quantum dynamics revealed the roles of electronic coupling, adiabaticity, electrostatic-field fluctuations, and solvation dynamics in driving charge transport over long distances and pointed to the importance of solvation of redox-active sites in the design of bioinspired light-harvesting systems and functional photocatalysts.

Collaborating entity: California Institute of Technology (USA), Queen Mary University of London (UK)

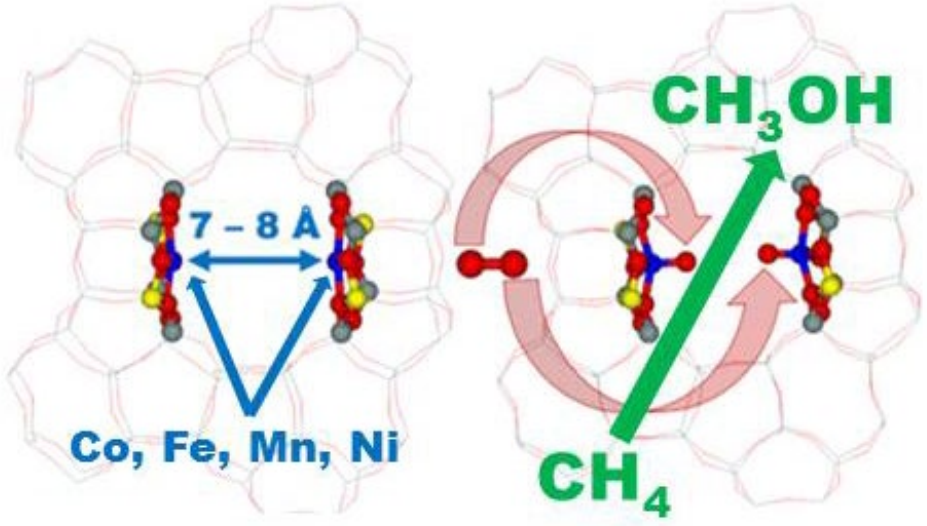


***Investigated blue copper protein**. The active electron transfer part of the system consisting of the rhenium-based organometallic chromophore and two tryptophans was investigated by quantum dynamics while the rest of the system was treated classically by molecular mechanics*

Photoinduced hole hopping through tryptophans in proteins. S. Záliš, J. Heyda, F. Šebesta, J.R. Winkler, H. B. Gray, A. Vlček. *Proc. Natl. Acad. Sci. U.S.A.*, 2021, *118*, e2024627118, doi.org/10.1073/pnas.2024627118

Department of Structure and Dynamics in Catalysis (4)

Catalysts for activation of dioxygen and selective oxidation of methane to methanol
We have recently developed binuclear catalytic centers of two iron ions in a ferrierite zeolite that split dioxygen and subsequently oxidize methane to methanol. The newly obtained results show that the binuclear centers of other metals also activate oxygen and oxidize methane. Moreover, the geometric parameters of these centers necessary for oxygen dissociation and methane oxidation were found. These discoveries provide the basis for developing an industrially relevant methane catalyst.



Oxidation of methane to methanol over zeolite catalyst. *Arrangement of binuclear cationic site of two coopeating transition metal ions stabilized in the zeolite matrix (left), split dioxygen forming two highly reactive α-oxygens capable to oxidize methane to methanol (right).*

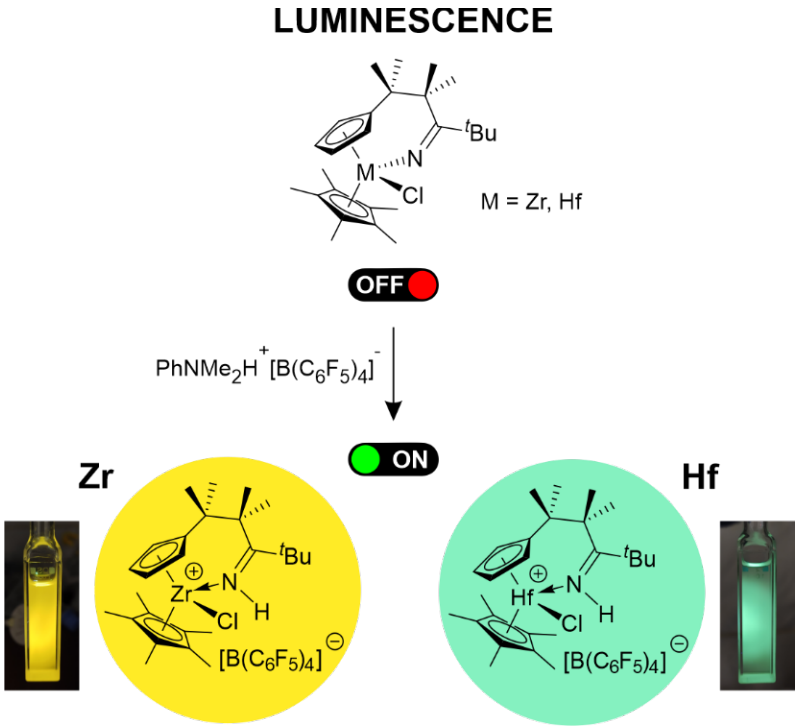
Splitting dioxygen over distant binuclear Fe sites in zeolites. Effect of the local arrangement and framework topology. E. Tabor, M. Lemishka, J. E. Olszowka, K. Mlekodaj, J. Dedecek, P. C. Andrikopoulos, S. Sklenak, *ACS Catal.* 11 (2021) 2340-2355, doi.org/10.1021/acscatal.0c04459
Splitting dioxygen over distant binuclear transition metal cationic sites in zeolites. Effect of the transition metal cation, J. Dedecek, E. Tabor, P. C. Andrikopoulos, S. Sklenak. *Int. J. Quant. Chem.*, 121 (2021) Article Number: e26611, doi.org/10.1002/qua.26611

Department of Molecular Electrochemistry and Catalysis (5)

Luminescent cationic group 4 metal complexes

New cationic group 4 metallocene complexes stabilized by pendant imine and pyridine groups were prepared as crystalline borate salts. Compared to the corresponding neutral species, the cationic Zr and Hf derivatives exhibited significantly enhanced green to yellow photoluminescence predominantly from triplet ligand-to-metal excited states with lifetimes up to 62 μs and quantum yields up to 58% in the solid state. DFT calculations were performed to explain their experimentally observed structural, spectral, and electrochemical properties.

Collaborating entity: Institute of Inorganic Chemistry, CAS



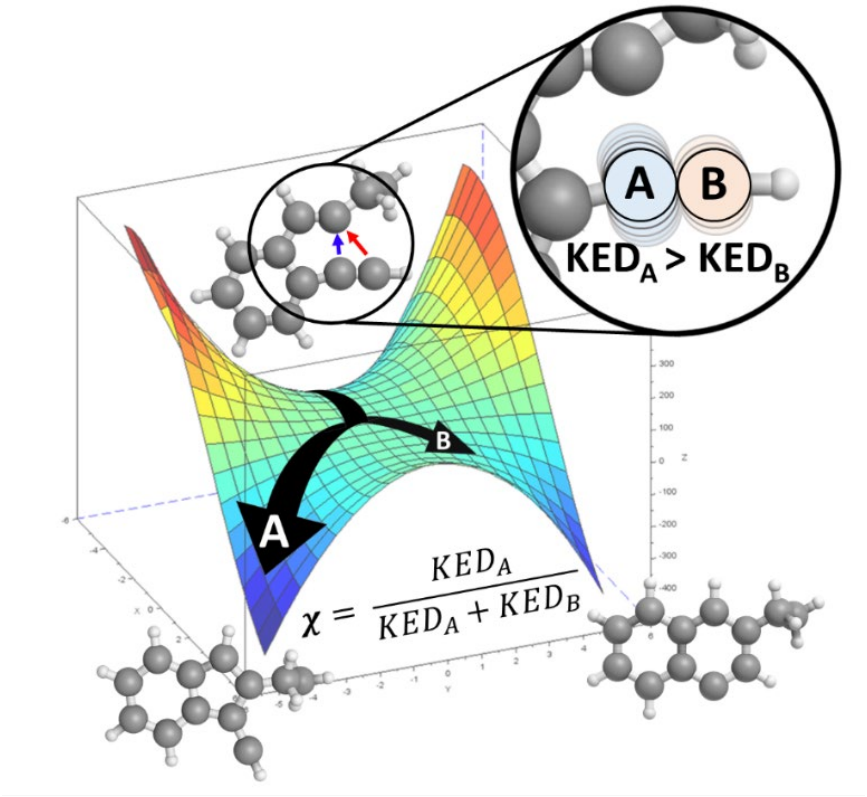
Switching on luminescence in group 4 metallocene complexes. *Protonation of the ketimide ligand moiety in Zr and Hf complexes activates an intense photoluminescence, while the emitted light color depends on the central metal atom.*

Luminescent Cationic Group 4 Metallocene Complexes Stabilized by Pendant N-Donor Groups. D. Dunlop, M. Večeřa, R. Gyepes, P. Kubát, K. Lang, M. Horáček, J. Pinkas, L. Šimková, A. Liška, M. Lamač. *Inorg. Chem.* 2021, 60, 7315-7328, doi.org/10.1021/acs.inorgchem.1c00461

Department of Computational Chemistry (6)

Bifurcating reactions: distribution of products from energy distribution in a shared reactive mode

We developed a method to reliably predict the product ratio in branched reactions leading to two products across one single barrier. The method uses inexpensive calculation and analysis of the energy distribution within reactive mode at the top of the barrier. At the same time, the predictability is comparable to or higher than when using more demanding methods. The result brings a new perspective on chemical reactivity and helps to aim at higher reaction selectivity in these reactions.



Potential energy surface for a bifurcation reaction. *Product outcome of bifurcation reactions given by the distribution of kinetic energy at the top of barrier*

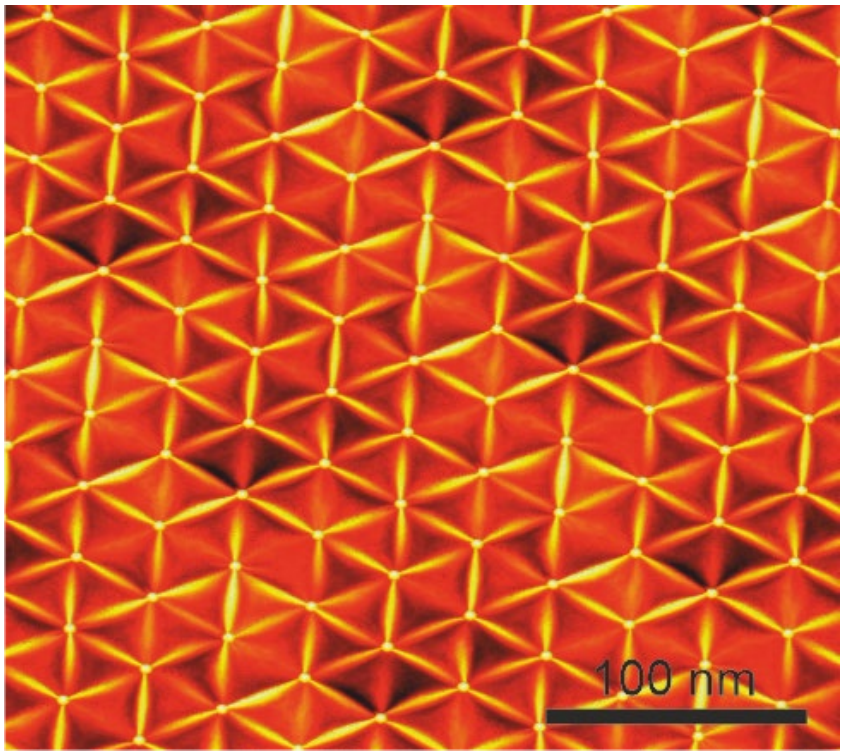
Bifurcating reactions: distribution of products from energy distribution in a shared reactive mode. P. Bharadwaz, M. Maldonado-Domínguez, M. Srnec. *Chem. Sci.*, 2021,12, 12682-12694, doi.org/10.1039/D1SC02826J

Department of Electrochemical materials (7)

Local deformation of two-dimensional materials

Two-dimensional materials like graphene belong to the strongest materials known. At the same time, their optoelectronic properties, applicable, for example, in sensorics, are very sensitive to external forces. We have, therefore, focused on the study and description of such deformation-related phenomena at the nanoscale. We have revealed even more pronounced alterations when compared with those accomplished by ordinary methods.

Collaborating entities: Institute of thermomechanics, CAS, University of Vienna, University of Thessaloniki, FORTH-ICE/HT Patras



Solar energy from monolayer MoS_2? *Optoelectronic properties of monolayer semiconducting MoS_2 seem to predestine this material for solar energy harvesting. However, for a successful large-scale application, it is essential to solving the riddle of its large-area growth, especially concerning the unwanted growth of the insulating oxidic interlayer.*

Strong localization effects in the photoluminescence of transition metal dichalcogenide heterobilayers. A. Rodriguez, M. Kalbac, O. Frank. *2D Materials* 8(2), 025028 (2021), doi.org/10.1088/2053-1583/abe363

Wrinkle development in graphene sheets with patterned nano-protrusions: A molecular dynamics study. J. Varillas, O. Frank. *Carbon* 173, 301-10 (2021), doi.org/10.1016/j.carbon.2020.11.003

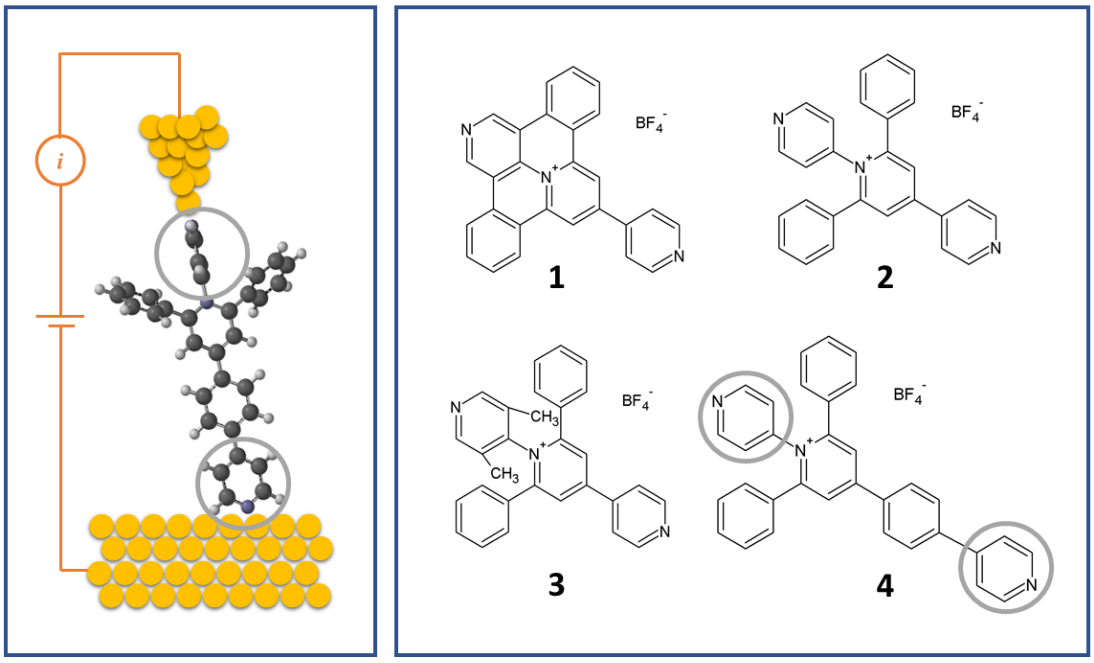
Franckeite as an Exfoliable Naturally Occurring Topological Insulator. W. S. Paz, M. G. Menezes, N. N. Batista, G. Sanchez-Santolino, M. Velicky, M. Varela, R. B. Capaz, J. J. Palacios. *Nano Letters* 21(18), 7781-8 (2021), doi.org/10.1021/acs.nanolett.1c02742

Department of Electrochemistry in Nanoscale (8)

Environmental control of single-molecule junction evolution and conductance

Environmental control of single molecule junction evolution and conductance has been demonstrated. Studied systems represent the smallest unit designed for the signal transfer in the electric circuits based on the individual molecules. Our results showed the potential of the environmental control for such a design. The environmental control concept was verified on the example of organic pyridinium-based cations.

Collaborating entity: P. P. Lainé, Université de Paris, Francie



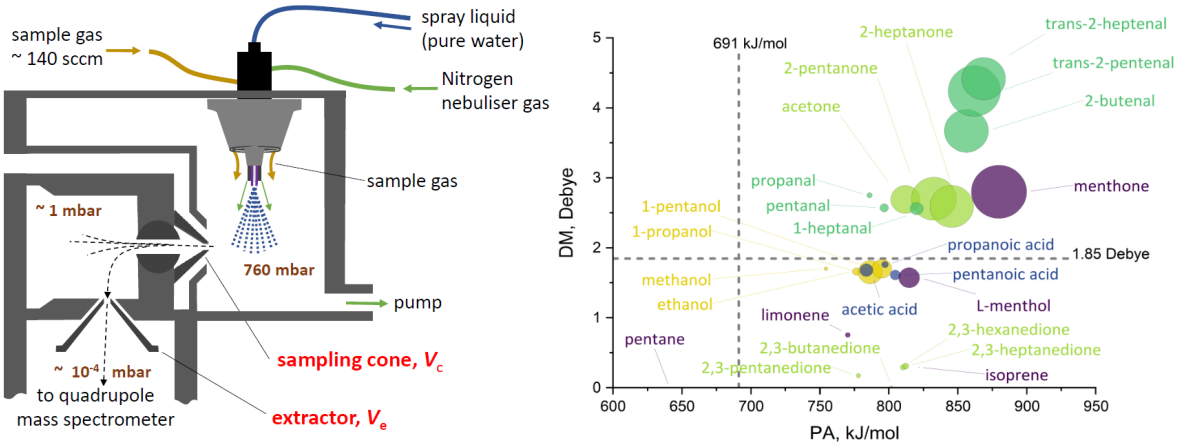
Metal-molecule-metal junction for molecular electronics. *Metal-molecule-metal junction in the electric circuit arrangement (left) and molecular systems studied (right). Anchoring groups are indicated by gray circles.*

Environmental Control of Single-Molecule Junction Evolution and Conductance: A Case Study of Expanded Pyridinium Wiring. Š. Nováková Lachmanová, V. Kolivoška, J. Šebera, J. Gasior, G. Meszáros, G. Dupeyre, P. P. Lainé, M. Hromadová. *Angewandte Chemie International Edition* 60 (2021) 4732–4739, doi.org/10.1002/anie.202013882

Department of Chemistry of Ions in Gaseous Phase (9)

Sensitivity of secondary electrospray ionization mass spectrometry to a range of volatile organic compounds: Ligand switching ion chemistry and the influence of Zspray™ guiding electric fields

Sensitivities of SESI-MS were determined for several classes of VOCs by introducing samples of suitably varying concentrations as quantified online using SIFT-MS. The complex ion chemistry occurring in the SESI ion source, primarily involving gas-phase ligand switching, results in widely variable sensitivities for different classes of VOCs. The sensitivity is observed to depend on the dipole moment and proton affinity of the analyte VOC molecule.



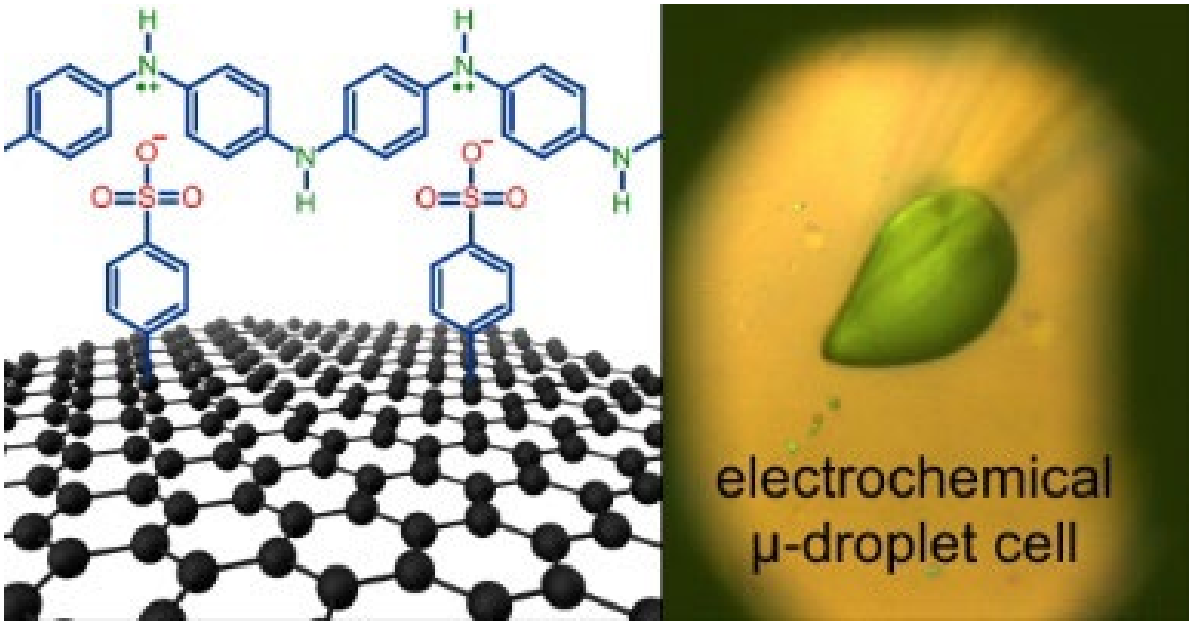
Zspray™ ion source adapted for SESI-MS, and the associated ion sampling and E-field arrangements and sensitivity data obtained for a range of volatile organic compounds (VOCs). *The VOC in air samples, continuously analyzed by SIFT-MS, are introduced to the ion source chamber via a coaxial cone with the electrospray. A bubble plot shows the combined effect of dipole moment, DM, and proton affinity, PA. The positions of the bubbles labelled by the compound names indicate PA and DM values, whilst their area corresponds to the value of the measured SESI-MS sensitivity.*

Sensitivity of secondary electrospray ionization mass spectrometry to a range of volatile organic compounds: Ligand switching ion chemistry and the influence of Zspray (TM) guiding electric fields. K. Dryahina, M. Polasek, D. Smith, P. Spanel. *Rapid Commun Mass Spectrom*. 2021; 35(22), doi.org/10.1002/rcm.9187

Department of Low-dimensional Systems (10)

Two-dimensional CVD–graphene/polyaniline supercapacitors

Supercapacitors complement lithium batteries in applications needing high power density. We developed well-defined two–dimensional graphene/polyaniline heterostructures, employed them as supercapacitors, and showed the reversibility of polyaniline redox transitions and graphene electrochemical doping. The heterostructure capacitance is one order of magnitude higher than the capacitance of pristine graphene.



Conducting polymer, polyaniline. *Prepared on the surface of sulfonated graphene by oxidation of anilinium monolayer. The formed heterostructure was investigated by microscopic spectroelectrochemical methods.*

Two-Dimensional CVD–Graphene/Polyaniline Supercapacitors: Synthesis Strategy and Electrochemical Operation. M. Bláha, M. Bouša, V. Valeš, O. Frank, M. Kalbáč, *ACS Applied Materials & Interface,* 2021, 13, 34686-34695, doi: 10.1021/acsami.1c05054

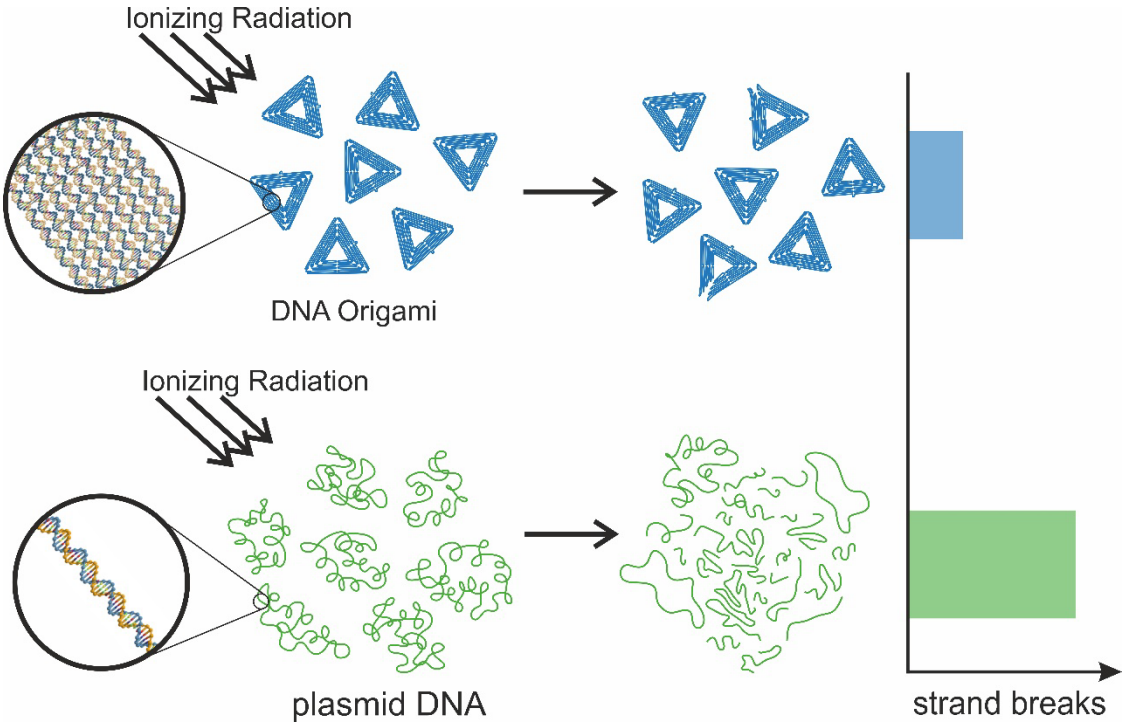
Department of Dynamics of Molecules and Clusters (11)

Folding enhances resistance of DNA to ionizing radiation

This work results from our efforts to implement DNA origami methods in CZ. DNA origami nanostructures are usually used as templates for experiments with short DNA segments. We show that DNA folded into nanostructure itself can serve as a sample, suggesting a new experimental approach to studying DNA. Observed radio-protective effect of the DNA scaffold with parallel DNA strands can be used in the development of novel radio-resistant materials and drug carriers for combined chemo-radiation therapy.

Collaborating entity: Hybrid nanostructures group (I. Bald) at the University of Potsdam, Germany

Department of Radiation Dosimetry(M. Davídková) at the Nuclear Physics Institute of the CAS, CZ



DNA folded into nanostructure is protected against ionizing radiation more than „free" plasmid DNA. *Artistic view on irradiation experiments with DNA folded into origami nanostructures and corresponding plasmid DNA, showing much lower damage to the folded DNA.*

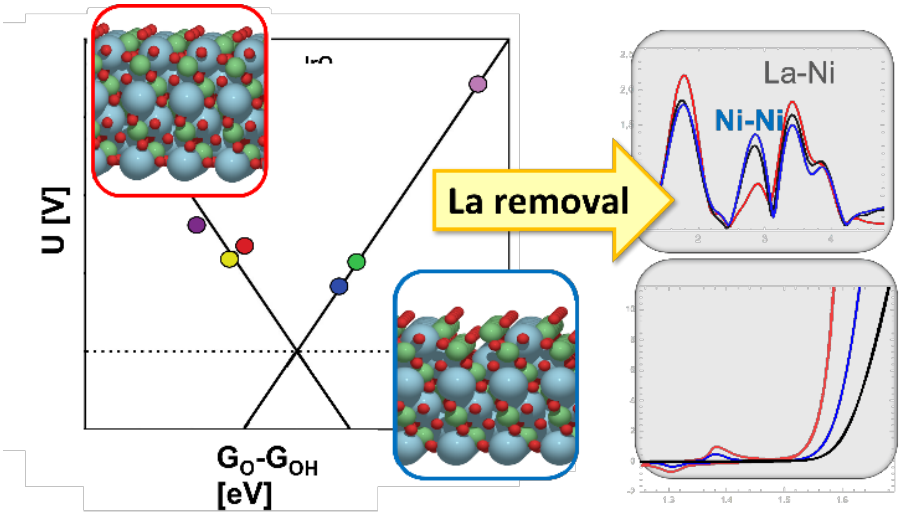
Folding DNA into origami nanostructures enhances resistance to ionizing radiation. L. Sala, A. Zerolová, A. Rodriguez, D. Reimitz, M. Davídková, K. Ebel, I. Bald, J. Kočišek. *Nanoscale* 13, 11197, 2021, doi.org/10.1039/D1NR02013G

Department of Nanocatalysis (12)

Synthetic activation of perovskite based catalysts for efficient oxygen evolution

We have developed a novel synthetic approach for Ni based perovskites with intentionally built defect structure. Planar defects introduced during synthesis are centre of selective lanthanide removal of subsequent surface reconstruction. The exfoliated reconstructed materials show significantly enhanced OER activity resulting from precise control of the Ni oxidation state in the reconstructed surfaces. This leads to a superior utilization of the catalyst and in principle, enables the preparation of novel anodes for alkaline water electrolyzers.

Collaborating entity: University Copenhagen, Leicester University, Northeastern University, Institute of physics, CAS



Activation of LaNiO perovskites for efficient oxygen evolution. *The figure illustrates the role of partial exfoliation of the lanthanide from perovskite structure (with subsequent surface reconstruction) plays in control of surface reactivity. The reconstructed lanthanide deficient surface (the formation of which was proved by X-ray absorption spectroscopy) facilitates the oxygen evolution reaction making it prospective anode material for alkaline water electrolyzers.*

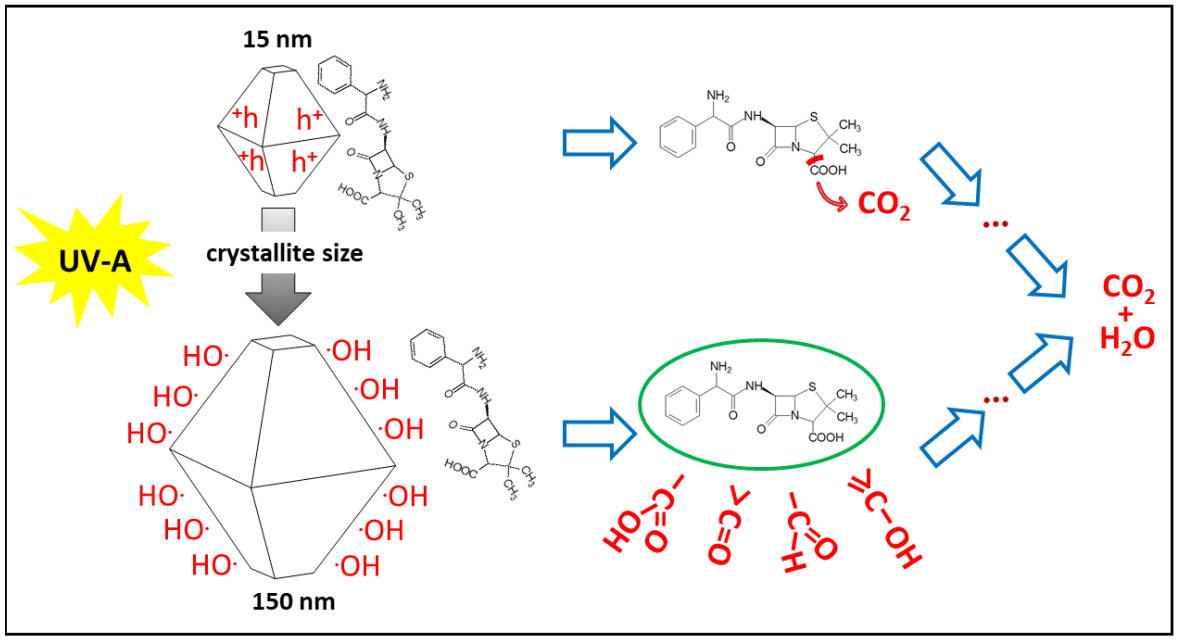
Engendering Unprecedented Activation of Oxygen Evolution via Rational Pinning of Ni Oxidation State in Prototypical Perovskite: Close Juxtaposition of Synthetic Approach and Theoretical Conception. R. Pittkowski, S. Divanis, M. Klementová, R. Nebel, S. Nikman, H. Hoster, S. Mukerjee, J. Rossmeisl, P. Krtil, *ACS Catalysis*, 11 (2021), 985-997, doi.org/10.1021/acscatal.0c04733

Center for Innovations in the Field of Nanomaterials and Nanotechnologies (13)

Efficient removal of emerging aqueous pollutants

High concentrations of pharmaceuticals have been detected in greywater effluents treated using up-to-date technologies. Practically relevant concentrations of naproxen, metformin, sulfamethoxazole, and antibiotics were efficiently removed using heterogeneous photocatalysis. The high degree of mineralization achieved suppressed the formation of potentially toxic products. The degradation pathway mechanism determined by DFT modeling was in very good agreement with the outcomes of the experiments.

Collaborating entity: UCT Prague, Institute of physics, CAS



Scheme of the photocatalytic degradation of ampicillin antibiotic. The scheme shows the different mechanism of photocatalytic degradation of the ampicillin molecule depending on the crystal size of the anatase form of titanium dioxide.

Photocatalytic Removal of Pharmaceuticals from Greywater. B. Ojobe, R. Zouzelka, B. Satkova, M. Vagnerova, A. Nemeskalova, M. Kuchar, J. Bartacek, J. Rathousky, *Catalysts* 2021, 11, 1125, doi.org/10.3390/catal11091125

Removal of Ampicillin by Heterogeneous Photocatalysis: Combined Experimental and DFT Study. L. Belhacova, H. Bibova, T. Marikova, M. Kuchar, R. Zouzelka, J. Rathousky. *Nanomaterials* 2021, 11, 1992, doi.org/10.3390/nano11081992

Hierarchical TiO2 Layers Prepared by Plasma Jets. R. Zouzelka, J. Olejnicek, P. Ksirova, Z. Hubicka, J. Duchon, I. Martiniakova, B. Muzikova, M. Mergl, M. Kalbac, L. Brabec, M. Kocirik, M. Remzova, E. Vaneckova, J. Rathousky. *Nanomaterials* 2021, 11, 3254, doi.org/10.3390/nano11123254

Scientometric achievements:

The results of science and research achieved by the staff of JHIPC in 2021 were published in 174 articles in international impact journals, 1 monograph and 6 chapters in a book, and are listed in the ASEP database:
https://asep.lib.cas.cz/arl-cav/cs/vyhledavani/
These works have been cited more than 364 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://web.jh-inst.cas.cz/publications-news/important-publications-released-2020-2024

ACS Catalysis, 2021, 11, 4, 2340–2355
Splitting Dioxygen over Distant Binuclear Fe Sites in Zeolites. Effect of the Local Arrangement and Framework Topology
Edyta Tabor, Mariia Lemishka, Joanna E. Olszowka, Kinga Mlekodaj, Jiri Dedecek, Prokopis C. Andrikopoulos, and Stepan Sklenak
doi/10.1021/acscatal.0c04459

Chemistry of Materials, 2021, 33, 5, 1781–1788
Synthesis of the Zeolites from SBU: An SSZ-13 Study
Kinga Mlekodaj, Milan Bernauer, Joanna E. Olszowka, Petr Klein, Veronika Pashkova and Jiri Dedecek
doi.org/10.1021/acs.chemmater.0c04710

Advanced Sustainable Systems, 2021, Volume 5, Issue11, 2000298
Synergistic Effect of Cu,F-Codoping of Titanium Dioxide for Multifunctional Catalytic and Photocatalytic Studies
Miguel Díaz-Sánchez, Roxana Nicoleta Murgu, Diana Díaz-García, José M. Méndez-Arriaga, Sanjiv Prashar, Béla Urbán, Jiří Pinkas, Martin Lamač, Michal Horáček, Santiago Gómez-Ruiz
doi.org/10.1002/adsu.202000298

Proceedings of the National Academy of Sciences, 2021, 118 (11) e2024627118
*P*hotoinduced hole hopping through tryptophans in proteins
Stanislav Záliš, Jan Heyda, Filip Šebesta, Jay R. Winkler, Harry B. Gray, Antonín Vlček
doi.org/10.1073/pnas.2024627118

ChemElectroChem, 2021, Volume8, Issue11, Pages 2137-2149
Electrochemical Reduction of Carbon Dioxide on 3D Printed Electrodes
Eva Vaněčková, Milan Bouša, Violetta Shestivska, Jiří Kubišta, Pavel Moreno-García, Peter Broekmann, Motiar Rahaman, Martin Zlámal, Jan Heyda, Milan Bernauer, Táňa Sebechlebská, Viliam Kolivoška
doi.org/10.1002/celc.202100261

Inorganic Chemistry, 2021, 60, 10, 7315–7328

Luminescent Cationic Group 4 Metallocene Complexes Stabilized by Pendant N-Donor Groups
David Dunlop, Miloš Večeřa, Róbert Gyepes, Pavel Kubát, Kamil Lang, Michal Horáček, Jiří Pinkas, Ludmila Šimková, Alan Liška, and Martin Lamač
doi.org/10.1021/acs.inorgchem.1c00461

Advanced Functional Materials, 2021, Volume31, Issue29, 2102196
Superradiant Emission from Coherent Excitons in van Der Waals Heterostructures
Golam Haider, Krishna Sampathkumar, Tim Verhagen, Lukáš Nádvorník, Farjana J. Sonia, Václav Valeš, Jan Sýkora, Peter Kapusta, Petr Němec, Martin Hof, Otakar Frank, Yang-Fang Chen, Jana Vejpravová, Martin Kalbáč
doi.org/10.1002/adfm.202102196

Renewable Energy, 2021, Volume 168, 1015-1026
Improvement of thermal energy accumulation by incorporation of carbon nanomaterial into magnesium chloride hexahydrate and magnesium nitrate hexahydrate
Pavla Honcová, Galina Sádovská, Jana Pastvová, Petr Koštál, Jürgen Seidel, Petr Sazam, Radim Pilař
doi.org/10.1016/j.renene.2020.12.115

Sensors and Actuators B: Chemical, 2021, Volume 344, 130252
Flow amperometric uric acid biosensors based on different enzymatic mini-reactors: A comparative study of uricase immobilization
Sofiia Tvorynska, Jiří Barek, Bohdan Josypčuk
doi.org/10.1016/j.snb.2021.130252
Nanomaterials, 2021**,** 11(12), 3254
Hierarchical TiO2 Layers Prepared by Plasma Jets
Radek Zouzelka, Jiri Olejnicek, Petra Ksirova, Zdenek Hubicka, Jan Duchon, Ivana Martiniakova, Barbora Muzikova, Martin Mergl, Martin Kalbac, Libor Brabec, Milan Kocirik, Monika Remzova, Eva Vaneckova and Jiri Rathousky
doi.org/10.3390/nano11123254
Journal of Materials Chemistry A, 2021,9, 17512-17520
Does the Seebeck coefficient of a single-molecule junction depend on the junction configuration?
František Vavrek, Olena Butsyk, Viliam Kolivoška, Štěpánka Nováková Lachmanová, Táňa Sebechlebská, Jakub Šebera, Jindřich Gasior, Gábor Mészárosb and Magdaléna Hromadová
doi.org/10.1039/D1TA05324H

ACS Applied Materials & Interfaces, 2021, 13, 29, 34686–34695
Two-Dimensional CVD-Graphene/Polyaniline Supercapacitors: Synthesis Strategy and Electrochemical Operation
Michal Bláha, Milan Bouša, Václav Valeš, Otakar Frank, and Martin Kalbáč
doi.org/10.1021/acsami.1c05054

American Chemical Society, 2021, 143, 47, 19909–19918
Sequestration of Proteins in Stress Granules Relies on the In-Cell but Not the In Vitro Folding Stability

Sara S. Ribeiro, Mailin Becker, Emeline Laborie, Roland Pollak, Stepan Timr, Fabio Sterpone, Simon Ebbinghaus
doi/10.1021/jacs.1c09589

Chemistry A European Journal, 2021, Volume27, Issue71, 17889-17899
On the Supra-LUMO Interaction: Case Study of a Sudden Change of Electronic Structure as a Functional Emergence
Alexis Gosset, Štěpánka Nováková Lachmanová, Sawsen Cherraben, Gildas Bertho, Jérémy Forté, Christian Perruchot, Henri-Pierre Jacquot de Rouville, Lubomír Pospíšil, Magdaléna Hromadová, Éric Brémond, Philippe P. Lainé
doi.org/10.1002/chem.202103136

Chemical Science, 2021,12, 12682-12694
Bifurcating reactions: distribution of products from energy distribution in a shared reactive mode
Priyam Bharadwaz, Mauricio Maldonado-Domínguez and Martin Srnec
doi.org/10.1039/D1SC02826J

American Chemical Society, 2021, 143, 36, 14694–14702
On-Surface Strain-Driven Synthesis of Nonalternant Non-Benzenoid Aromatic Compounds Containing Four- to Eight-Membered Rings
Benjamin Mallada, Bruno de la Torre, Jesús I. Mendieta-Moreno, Dana Nachtigallová, Adam Matěj, Mikulas Matoušek, Pingo Mutombo, Jiri Brabec, Libor Veis, Timothée Cadart, Martin Kotora and Pavel Jelínek
doi.org/10.1021/jacs.1c06168

Biomaterials Science, 2021,9, 7379-7391
Probing polymer brushes with electrochemical impedance spectroscopy: a mini review
Judita Anthi, Viliam Kolivoška, Barbora Holubová, Hana Vaisocherová-Lísalová
doi.org/10.1039/D1BM01330K

The Journal of Physical Chemistry C, 2021, 125, 40, 21803–21809
Electrolyte versus Dielectric Gating of Two-Dimensional Materials
Matěj Velický
doi.org/10.1021/acs.jpcc.1c04795
Sensors and Actuators B: Chemical, 2021, Volume 347, 130583
Screen-printed amalgam electrodes

Bohdan Josypčuk, Jan Langmaier, Sofiia Tvorynska
doi.org/10.1016/j.snb.2021.130583

Journal of Chemical Theory and Computation, 2021, 17, 12, 7575–7585
Density Matrix Renormalization Group with Dynamical Correlation via Adiabatic Connection
Pavel Beran, Mikuláš Matoušek, Michał Hapka, Katarzyna Pernal and Libor Veis
doi.org/10.1021/acs.jctc.1c00896

III. 2 Important projects

In 2021, JHIPC participated in 9 research projects with the support of foreign funders and 106 research projects financially supported by several different domestic funders, in which the researchers from the JHIPC acted as principal investigators / co-investigators or project partners.

RESEARCH PROJECTS SUPPORTED BY DOMESTIC FUNDERS

FUNDER	NUMBER PROJECTS
Czech Science Foundation	51
Ministry of Education, Youth and Sports	27
Czech Academy of Sciences	19
Technology Agency of the Czech Republic	7
Ministry of Industry and Trade	1
Ministry of the Interior	1

Selected fundamental research projects

Concert of lipids, ions, and proteins in cell membrane dynamics and function (GACR, EXPRO), 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)

Modernization and improvement of a large research infrastructure Nanomaterials and Nanotechnologies for Environment Protection and Sustainable Future (Ministry of Education, Youth and Sports, Pro-NanoEnviCz II), principal investigator: Martin Kalbáč, partner institutions: Technical University of Liberec and E. Purkyně University in Ústí

nad Labem. The project is directly linked to the existing research infrastructure NanoEnviCz and complements it in the area of critically lacking instruments and expertise. (2020-2022)

ÅrchitectRonics of Two-dimensional crystals via synergy of chiral electro-chemical and opto-electronic concepts on Å-scale.

(GACR, EXPRO), principal investigator: Martin Kalbáč, partner institutions: Technical University of Liberec and E. Purkyně University in Ústí nad Labem. The aim of the project is to achieve electrochemical and chiral manipulation of excitons / superradiance on platforms based on ultrapure 2D gratings and chiral entities, i.e. with the coexistence of geometric and Berry phases of induced chirality. (2020-2024)

Investigation and transformation of matter by electrons in liquid microcatteries

(GAČR, EXPRO), investigator: Juraj Fedor, other participants of the project VŠCHT. The aim of the project is to develop new concepts for the use of electrons in liquid spectroscopy and to use the newly developed technique to study interphases.

Selected applied research projects

Use of a catalyst for the production of methanol from methane, wherein the catalyst comprises a zeolite having vapors in the skeleton based on the total number of all aluminum atoms in the zeolite, and a transition metal cation.

Team: Jiří Dědeček, Zdeněk Sobalík, Edyta Tabor, Štěpán Sklenak, Kinga Mlekodaj. A catalyst with binuclear transition metal centers that is capable of selectively oxidizing methane to methanol and other liquid products at low temperatures and without the use of an effluent to release the products.

Utilization: Negotiations on intellectual property protection and commercialization take place.

Selected strategic projects

AV21 Strategy is a project of the Academy of Sciences of the Czech Republic, which was established in 2015, whose motto is "Top research in the public interest". This project is implemented mainly through coordinated research programs of mutually cooperating institutes of the CAS and other organizations. Research takes place in long-term interdisciplinary programs that focus on solving current problems and challenges and emphasize the practical application of results in economically and socially important areas. At the same time, the AV21 strategy retains the determinative role of basic research, which conditions the development of all scientific disciplines.

In 2021, J. Heyrovský Institute of Physical Chemistry was involved in programs:
Nanostructured materials for energy conversion
Nanostructured materials for catalysis and environmental protection

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

Under the direction of Štefan Vajda in the position of "J. Heyrovský chair,' another four apparatus for testing the catalytic activity of the cluster were put into operation this year. The apparatus were imported from the United States of America. Chemical studies of nanocatalysts have expanded. Members of the department published three articles, submitted four publications, received several grants, organized an international conference, Cluster Meeting 2021, and continued to educate secondary school students.

Capacity development of JHIPC, project leader: M. Kalbáč, project leader: M. Kalbáč, Funder: Ministry of Education, Youth and Sports, programme RKV I.

Capacity development of JHIPC II, project leader: M. Kalbáč, Funder: Ministry of Education, Youth and Sports programme RKV I., programme RKV II.

Our Institute is one of the first institutions in the Czech Republic and one of the first institutes of the Czech Academy of Sciences to obtain the **"HR Excellence in Research"** (HR Award) certification. After two years of implementation of the steps of the HR Award Action Plan, a revised Interim Assessment Action Plan has been sent to the European Commission, describing the changes that have taken place since the HR Award. In February 2021, the Institute received the so-called Consensus report containing recommendations for the next three years. Then, the Action Plan will be revised again, evaluated on site by a commissioners visit, and the certification will be granted or withdrawn. The Institute received positive feedback in this Interim evaluation, and all criteria were met without corrective measures.

The certification obtained is a motivating factor for aligning human resources policy with international standards. It demonstrates the efforts of the Heyrovský Institute to create a friendly atmosphere and to involve employees in the process of directing the institution and the internationalization of the institution. The HR Award signifies quality and a permanent commitment to continuing development and creating favorable conditions for workers, as it must be defended in three-year cycles.
In December 2021, the **Gender Equality Plan** (GEP, 2021 2024), which is part of the HR Award Action Plan, was approved by the management of the Institute. This Plan is based on the outputs of an internal gender audit in accordance with the Gender Audit Standard (Government of the Czech Republic, 2016). The plan was developed according to the requirements of the European Commission for funding from Horizon Europe and meets the procedural conditions of the programme and the recommended thematic orientations. The work of the Plan focuses on the following:

- Promotion of work-life balance and organizational culture
- Representation of under-represented groups (most often women) in leadership and decision-making
- Fair recruitment and career development conditions
- Integration of the gender dimension into research and teaching content

- Prevention and treatment of discriminatory behavior, including sexual harassment in the workplace

The Gender Equality Officer organizes the implementation of GEP. The implementation of the plan in the area of prevention of discriminatory behaviour is supported by internal training and peer training of employees working within the STOPPER project (the Ministry of Labour and Social Affairs of the Czech Republic). In particular, the plan aims at building internal capacities for work in a fair and open working environment. Another goal is to eliminate unconscious prejudices and stereotypes and improve working conditions for various workers, especially women, so they can fully develop their personal and professional potential in their work at the Institute.

In 2021, in addition to building the GEP, we dealt with several critical activities:

- The researcher recruitment process corresponding to the principles of OTM R has been revised considering the previous year's experience. The process has been simplified, and the recruitment documents have been modified.
- The staff of the Technology Transfer Office continued to develop cooperation with scientists. The second part of the database of intellectual property results, part of industrial property, has been launched. Thanks to this, it is possible to detect scientific results with application potential before they are published.
- Employees had the opportunity to attend courses in soft managerial skills, knowledge in intellectual property and technology transfer, foundations of scientific work in English, popularization of science, and mentoring. Employees of support departments participated in English courses to support international cooperation in science and research.
- The first round of young researchers (doctoral students) evaluations with an emphasis on career development took place.
- A questionnaire survey took place to identify the needs of non-Czech-speaking employees, which will help to better integrate these foreign employees into the Institute's strategic planning.
- In the Heyrovský Open Access Funding (RKVII) program, 12 articles were published through the so-called golden path of Open Access in the total financial amount of 1.1 million CZK incl. VAT.
- A mentoring program for young scientists was prepared, the first run of which is scheduled for spring 2022.

The process implementation is supervised by the Steering Committee and the Monitoring Committee and coordinated by the Implementation Coordinator.

More information can be found at this link:
www.jh-inst.cas.cz/cs/zakladni-stranka/strategie-lidskych-zdroju-pro-vyzkumne-pracovniky-hrs4r-2

JHIPC provides facilities for the office of Jan Hrušák, **President of the European Strategic Forum for Research Infrastructures (ESFRI)**. JHIPC is also the recipient of the StR ESFRI 2 project (H2020 Grant agreement ID: 823711).

In 2021, ESFRI joined the debate at the European Union level on the new European Research Area(era) and anchored the role of research infrastructures as one of the key era actions in the era governance model. The Strategic Forum continued to implement the objectives of the ESFRI White Paper 2020: Making Science Happen – A New Ambition for Research Infrastructures in the European Research Area. One of the key objectives is to promote a connected ecosystem of research infrastructures and to connect our forum with the wider professional public. Therefore, the Institute organized several so-called "ESFRI open sessions", where we discussed the involvement of infrastructures and their contribution to the development of individual scientific disciplines and developed the concept of ESFRI stakeholder forum as a platform for communication. The Forum further strengthened the dialogue with the EOSC (European Open Science Cloud) platform, including two joint workshops addressing the role of research infrastructures in implementing EOSC and their linkages with other Open Science actors. The main event in 2021 was an international conference held under the auspices of the Slovenian Presidency of the Council of the EU. President Jan Hrušák presented an update of the Roadmap for Research Infrastructures at the conference. The Roadmap, together with the analysis of the landscape of research infrastructures (EFRI RI landscape analysis), i.e., another important ESFRI strategic document, form the basis of the EU's R&D policy and in building the ERA. In 2021, Forum President Jan Hrušák spoke as an invited speaker at several dozen conferences and workshops.

The activities of the President of ESFRI not only represent a prestigious representation for the Czech Republic and help shape and steer Czech research, development, and innovation policy in Europe. The support team of the chairman of ESFRI at JHIPC participates in drafting documents for negotiations on all aspects of ESFRI and EOSC. It engages in developing Czech positions and projecting European Union policies into the Czech Republic's agenda in research (e.g., Structural Funds). These activities are coordinated with the Technological Centre of the CAS and the Ministry of Education, Youth and Sports.

III. 3. Significant awards

The following scientists and students were awarded in 2021 for the results of their research activities:

prof. RNDr. Ladislav Kavan, CSc., DSc. - The Metrohm Award for lifetime contribution to the development of electro-analytical chemistry. Awarded by Metrohm.

prof. RNDr. Patrik Španěl, Dr. rer. nat.- Praemium Academiae for outstanding scientific contribution. Awarded by the CAS.

doc. RNDr. Lubomír Pospíšil, CSc. - Medal of Prof. Ferdinand Schulz for many years of exemplary work in the Scientific Council of the Faculty of Environmental Protection Technology of the University of Chemistry and Technology Prague; awarded by the University of Chemistry and Technology Prague.

Haider Golam, Ph.D - Otto Wichterle's award for excellence in nanosciences and technologies (graphene); awarded by the CAS.

Mgr. Magdaléna Hromadová, Ph.D. - Diploma for the lecture "Heyrovský Lecture 2021" at Charles University; awarded by the Czech Chemical Society.

Mgr. Lukáš Petera - Academia Award for the thesis entitled The Consequences of the Great Bombing Era for the Chemical and Prebiotic Evolution of Early Mars and Earth. Part of the award is the publication of his work in a book; awarded by the Academia Publishing House.

Mgr. Sofiia Tvorynska - Best poster prize 2021 at the international conference 72 Annual Meeting of the International Society of Electrochemistry, 29 August - 3 September 2021, Hybrid Meeting Jeju Island, Korea/Online.

Mgr. Sofiia Tvorynska - 2 place in the Marta Sališová Prize 2021 competition for the presentation of the results at 73 Congress of chemists in Slovakia; awarded by the Slovak Chemical Society.

For the archive of all awards follow the link:
web.jh-inst.cas.cz/cs/prizes

III. 4. Promotion and popularization

The cooperation of JHIPC with the different media in various forms to promote the results of the activities of scientists takes place throughout the year. JHIPC cooperates with the the Division of Media Communication of the CAS in the field of media coverage of research results and promotion of science to the target group, which is primarily the general public.

During 2021, the research activities of the JHIPC 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. A total of 658 articles, interviews or reports

were published in this way in the media (197 without content duplicates). A selection of the most important media outlets is publicly available on the JHIPC's website:

web.jh-inst.cas.cz/media

In the course of 2021, the JHIPC also issued a total of 10 press releases, covering research results and significant events directly related to the JHIPC. Martin Ferus's cooperation on the Czech Space Mission Slavia, which received the support of the European Space Agency, as well as online broadcast of chemical experiments for the children of Květa Stejskalová at the time of lockdowns (both July 2021), were the most popular in the media.

All press releases in full and with subsequent responses in the media are regularly published on the website of JHIPC:

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

Outputs on TV and radio:
Czech Television 1 – Open Week at the Academy of Sciences – Příběh kapky

(The Story of the Drop) (2 November 2021)

ČRo Radiožurnál - Celkem 9 vědců převezme už za 2 hodiny od Akademie věd prestižní ocenění (A total of 9 scientists will receive a prestigious award from the Academy of Sciences in just 2 hours) (5 November 2021)

We inform the general and professional public about the activities and research results of our scientists on the social networks Twitter and LinkedIn.

News about current events with the Institute is regularly brought by the information TV panel in the Institute's lobby and the monthly Newsletter. We send the Newsletter to all employees as an e-mail. We provide all employees with up-to-date information about important events, awards, important publications or vacancies within the Institute.

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

In 2021, the EDU educational laboratory and classroom could only operate in a limited mode (for smaller groups of students) with its programs for lower and secondary school pupils. Nevertheless, a total of 142 programs for 4200 participants were organized online or on site.

The scientific results are promoted regularly by:

- web application of the long-term educational project of the JHIPC Tři nástroje (Three tools):

www.3nastroje.cz

exhibition website The Story of a Drop about Jaroslav Heyrovský:

www.heyrovsky.cz

- the JHIPC website:

www.jh-inst.cas.cz

A detailed schedule of the 2021 programs entitled Věda v roušce? (Science with a respirator?) is archived on the website of the project Tři nástroje.

An overview of the most important popularization and education programs and events in 2021:

Even this year, at a time when the restrictions associated with Covid 19 allowed, some researchers at JHIPC participated in the education of students and teachers with their lectures, laboratory practices and other activities in various programs educating students and teachers.

During the year, there were chemistry clubs and Saturday courses, high school internships, chemical theatres and workshops for pupils of middle and high schools, August summer school NANO2021 and summer biochemical course Kyslík v Boru (Oxygen in Boron, the town of Bor). We also managed to organize the two planned exhibitions for the public Dotkni se (exo)planet (Touch (exo)planets) and Příběh kapky (The Story of a Drop) in the premises of the Institute. Two members of the popularization team PEXED JHIPC (Popularization EXperimental EDucation) took part in the online lectures (organized by the CAS) for pupils of lower, middle and high schools and gave 57 lectures at thirty schools.

We also actively continued the educational programme for teachers: with our teaching programme, we participated in a course organized by the Open Science project of the CAS for teachers (August, Čtyřkoly, teaching chemistry through experimentation). Our accredited program for teachers of high and middle schools called Modern Physical Chemistry and Nanosciences was visited in November by teachers from the Skalice Lower and Middle School near Česká Lípa. Also this year, we have been involved in teaching chemistry and physics in projects called Šablony SŠ (High School Templates) in various schools (in the teaching module "expert from practice"), e.g. in Polná u Jihlavy Lower and Middle School, Kraslice Lower and Middle School, Bishop Grammar School, Žďár nad Sázavou).

Thirteen high school students completed year-round internships in the project Otevřená věda AV ČR 2021 (Open Science of the CAS) at JHIPC under supervision of 7 instructors. A total of 31 students and 15 lecturers were involved in other internships of the Institute, supported by our project No. 0022/7/NAD/2021. As part of this project, a one-week August course in chemical experiments called Kyslík v Boru (Oxygen in Bor) took place, which was attended by 12 high and middle school students.

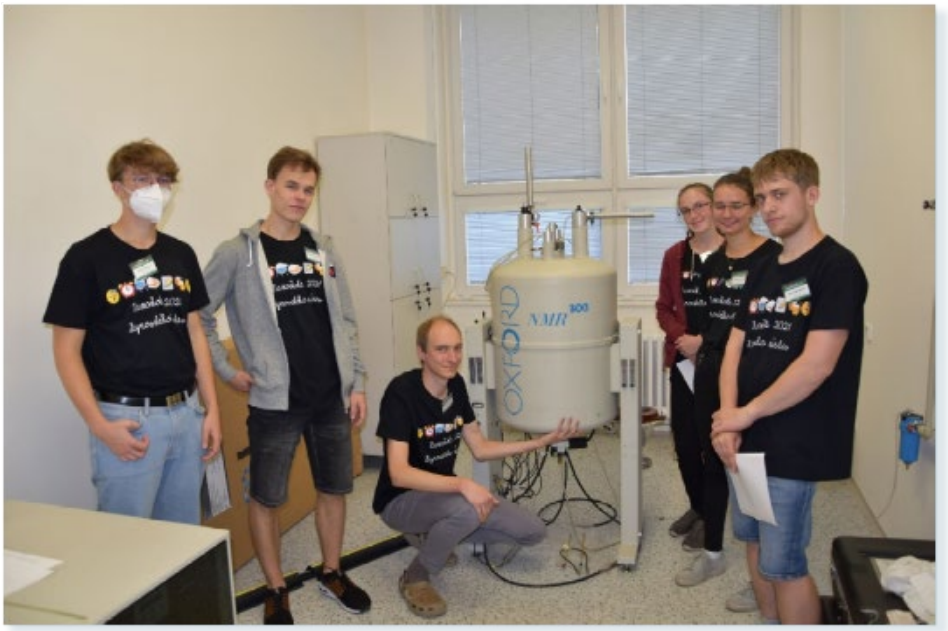
In 2021, the Institute could organize at least two exhibitions again. For a month, the lobby hosted an exhibition with astrochemical themes created by a team of scientists from the Department of Spectroscopy called Dotkni se (exo)planet (Touch (exo)Planets). The successful exhibition already has its other fans, so, it will be travelling in 2022-23. For two weeks in November, also as part of the AV ČR Week festival, the public had the opportunity to visit the 32 exposition of the traveling exhibition about Jaroslav Heyrovský entitled The Story of a Drop.

For the annual Týden vědy a techniky TVT 2021 (Science and Technology Week festival), the researchers of the JHIPC prepared a colorful program. The events were organized in a full-time manner, with three public lectures also being streamed and archived on the JHIPC Youtube channel. Programmes of workshops and chemical theatres took place in the EDU classroom with the participation of all registered children and parents. The total number of visitors to our Science Week programmes (including both exhibitions) was 700.

The website www.3nastroje.cz, which presents all the educational and popularization activities of JHIPC scientists online achieved recording 4,500 visits and 14,400 views in 2021.

The exhibition Touch (exo)planets interested both adults and children, as well as students and pupils from various schools.

Several different classes from the Modřany Gymnasium (Modřany High School) visited the Story of the Drop exhibition and the result of the visit was, for example, the processing of team projects with the theme the life of and research by Jaroslav Heyrovský.



Some students who attended the NANO2021 summer school and got acquainted with various techniques in the form of internships (here at the NMR laboratory), also expressed interest in continuing cooperation in the form of a year-long internship in the laboratory.

Teaching by experimentation is a great success for students of lower, middle and high schools. Therefore, our offer of topics is constantly growing, so today a teacher can choose from dozens of thematically different workshops.

The Ministry of Education accredited our Modern Physical Chemistry and Nanosciences programme for the education of teachers. In addition to lectures, we carry out practical measurements in laboratories during workshops. The teachers then follow up on this programme by visiting with their students.

III. 5. Scientific and pedagogical collaboration of JHIPC with universities

In 2021, the JHIPC participated in the training of 57 PhD students (in full-time and part-time forms of study; of this number, 7 defended their dissertation during 2021). 20 university students were trained by researchers from JHIPC as part of their bachelor's and master's theses.

Unfortunately, in 2021, due to the limitations associated with Covid 19 disease, as in the previous year, it was impossible to hold an annual Student Seminar where students would present the results of their dissertations.

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 446/254 hours in 19/23 semester cycles of lectures, seminars and practice exercises.

In 2021, 15 scientists were members of subject area boards of the doctoral study programmes (scientific advisory boards of PhD study). Fifteen 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 2021, the JHIPC again successfully collaborated in 22 grant projects with different universities. The employees of JHIPC 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 has been carried out beyond everyday research activities since 2005. Eighty-two one-hour lectures on various topics in the field of physical chemistry were given to high school students in 2021, most of them on-line.

Students who completed high school internships at the JHIPC defended their work in various competitions, such as SOČ (High-School Expert Activity) or the conference of the project Otevřená věda (Open Science) of the CAS. The students submitted their work also as seminar papers and final exam papers (15 works in total). Two students advanced to the national round of SOČ competition.

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

In 2021, the JHIPC Technology Transfer Office (TTO) was further developed. JHIPC TTO was established in July 2020 as one of the outputs of the Capacity Development of JHIPC for research and development II, supported by the Operational Program Research, Development, Education. The main task of the TTO is to protect the Institute's intellectual property and its commercialization.

A specialist in the protection of intellectual property (0.2 part-time) was hired. The TTO externally employs a lawyer specializing in technology transfer. At the same time, a position of a technological scout was created in each department, aiming to identify results with a high potential for commercialization.

In 2021, CTT focused on further building the internal technology transfer system. The "Methodology for the Implementation of Commercial Procurement and Contractual Research with the Application Sector" was created, the internal directive SM 09 "Management of Intellectual Property and Protection and Application of Industrial Property Rights" was updated, and the Institute's Internal Intellectual Property Database was created. In addition to this database, the Institute was involved in creating the Results Database of the CAS.

During the year, many seminars and workshops were held for the staff of JHIPC with a focus on the protection of intellectual property and technology transfer.

Concerning the protection of industrial property of the JHIPC, the TTO registers a total of 18 active national patents and 7 utility models. In addition, the European patent application EP 18150610.6 and PCT application PCT/CZ2020/050018 are pending. This application has entered the national phase in China, the USA, Europe, and India. A Memorandum of Cooperation was concluded with the Taiwanese ITRI Institute to test this technology. A research funding agreement was concluded with the Lobodon, which is interested in this technology.

In 2021, two license agreements were concluded with Betosan, s.r.o., Eaton Elektronika, s.r.o.

In addition to licensing, establishing spin-off companies appears to be a necessary form of commercialization. The administration of the “Proposal for a material plan for the establishment of a spin-off of ÚFCH JH” continued in 2021. The proposal was submitted to the Supervisory Board of the Institute and the Property Commission of the CAS for approval. The company is expected to start operations in 2022.

Also, in 2021, the TTO was a member of the TRANSFER.CZ association. This association brings together many important technology transfer organizations throughout the Czech Republic. At the competition, Transfera technology Day 2021, organized annually by the

association, the technology of the JHIPC, Fabrics for cleaning surfaces of historical materials, took second place.

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

In 2021, the JHIPC collaborated with the business sector on three projects.

Photoactive nanocomposite systems for environmental improvement

Program: Photoactive nanocomposite systems for environmental improvement (FONASYS)

Result: 1) Application of photoactive nanocomposite materials for solar self-cleaning and prevention of algae growth on insulated objects (proven technology)

2) Application of innovative photoactive nanocomposite systems with photocatalytic self-cleaning and disinfection function to monumentally protected objects (proven technology)

3) Map of insulated panel houses attacked by algae in the Czech Republic

4) Mapping and cataloguing of historical objects on the territory of the capital city of Thresholds suitable for photoactive nanocomposite coating.

Application: The company Color and Laky Teluria, s. r. o., the project partner of the joint project TH04030090, plans to use the developed materials for the preventive surface treatment of historical buildings and other monumental buildings. The company PRAGOTHERM, servis fasád, s.r.o. plans to apply developed nanocomposite coatings with self-cleaning effect against algae growth for preventive treatment of the surface of insulated facades.

Funder: Technology Agency of the Czech Republic

Partner organisation: E Barvy a laky Teluria, s. r. o., PRAGOTHERM, servis fasád, s.r.o.

Hydrophobic Magnetic Sorbent Production Method (Patent 308890), Formulated

Hydrophobic Magnetic Sorbent Utility Model

Heavy Metal Sorbent Utility Model

Program: Progressive Materials for Protection against Serious Environmental Damage/ Epsilon

Result: Magnetic sorbents based on porous silicates, in the development of which we have participated, are materials for dealing with environmental accidents. The magnetic properties of the sorbent simplify its application by allowing easy collection of the used sorbent, a key part of the application of these materials in environmental accident remediation.

Application: Vakos a. s. will incorporate the developed sorbent into its production portfolio.

Funder: Technology Agency of the Czech Republic

Partner organizations: EOrlen UniCre a.s., Vakos a.s.,

Methodology for determining the effectiveness of photocatalytic technology in removing air pollutants

Program: Utilization of optimized photocatalytic nanocomposites for removal of airborne pollutants

Result: An experimental station was built and a methodology was developed to determine the efficiency of photocatalytic technology in removing the main groups of air pollutants (NOx, volatile organic compounds, ozone). Based on the correlations obtained between relevant process parameters (illumination intensity, concentration, humidity, flow character, etc.) and photocatalytic efficiency, it is possible to predict the applicability of this technology under realistic weather conditions.

Application: The results obtained are of fundamental importance for the application of photocatalytic technology for realistic outdoor and indoor air purification.

Funder: Ministry of Industry and Trade of the Czech Republic

Partner organization: Advanced Materials JTJ, s. r. o., Kamenné Žehrovice

Results of collaboration with other organizations and businesses obtained based on contracts

In 2021, the JHIPC continued to fulfill the obligations of one contract for work and concluded four new contracts. As part of the performance of these contracts, results were achieved, mostly submitted as technical reports.

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

Client: UJP PRAHA a.s.

Abstract: Evaluation of nanomorphology of the surface of the corrosion layer of Zr alloy samples by AFM.

Application: During 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 storage.

Investigation of paramagnetic centers in sensitized TiO2 during VIS irradiation using EPR spectroscopy

Client: Institute of Inorganic Chemistry of the CAS, p.r.i.

Abstract: The supplied samples were measured in an EPR spectrometer without and with irradiation at room and nitrogen temperature. An interpretation was proposed in collaboration with photochemists. In addition, one unplanned result was the improvement of the low-temperature system in the Dewar vessel, where helium gas was used to significantly reduce the occurrence of latent nitrogen boiling, thus preventing unwanted nitrogen bubbling in a sensitive part of the instrument. Its suppression made it possible to measure signals ten times weaker than previously possible with this technique, and this technique will undoubtedly be useful in the future.

Application: The results of the measurements of the EPR spectra of modified TiO2 during irradiation were an integral part of a wider investigation using other methods at other institutes. The result is the imidiately written publication "Effect of amines on the peroxo-titanates and photoactivity of annealed TiO2" submitted 5.1.2022 to the Arabian Journal of Chemistry (IF=5.165) (Q1)

Characterization of the surface composition of oxygen plasma modified LDPE samples by the XPS method

Client: Faculty of Mechanical Engineering, CTU in Prague

Abstract: Determination of the populations of individual oxygen-containing functional groups on the surface of LDPE generated by oxygen plasma under different conditions. These groups significantly affect the reactivity of the surface, which is important for technological applications of the polymer.

Application: Potential applications in the manufacture of LDPE/polyamide sandwich structures

Investigation of the applicability of hydroisomerization catalysts based on zeolites in commercial applications of chemical industry

Client: Ranido, s.r.o.

Abstract: The result includes: 1) Design of catalysts for hydroisomerisation

2) Selection and characterization of suitable zeolites

3) Consultation on the preparation of catalysts for hydroisomerisation

4) Characterisation of the zeolites used and the catalysts prepared

5) Laboratory scale testing of catalysts.

Application: Chemical industry.

Phonolite catalysts for heptane isomerization in commercial applications of chemical industry

Client: ORLEN UniCRE a.s.

Abstract: The result includes: a characterization of the structure and catalytic activity of the catalysts.

Application: Chemical industry.

Spin-off firm „AV Spin“

In order to achieve the most effective transfer of developed technologies, the staff of the Technology Transfer Office of the JHIPC actively participated in cooperation with CeTTAV of the CAS in the establishment of the spin-off company AV Spin, whose portfolio of activities will be based exclusively on the know-how created by the staff of our TTO.

The main fields of activity of the company to be established will be:

- use of photocatalytic and photochemical technologies for removal of environmental pollutants
- New methods for the comprehensive conservation of tangible cultural heritage based on advances in materials science and nanotechnology.

In addition to experimental testing, the spin-off company will provide professional services, consulting and advisory services in the above fields, and sell licenses and sublicenses. It will engage in research and development activities in collaboration with research organizations and commercial entities. Small-scale production of means for the comprehensive protection of historical materials is also possible.

The launch of the spin-off company is planned for mid-2022 after approval of all necessary documents by the Supervisory Board of the Institute and the Property Committee of the CAS.

Patents and utility models

In 2020, 1 patent and 1 utility model were granted. Two licensing agreements have been concluded.

Patent

Method of preparation of silane group modified polyolefins, catalytic system and its application (PV 2021-41)

The invention relates to a method for the preparation of a silyl group-terminated polyolefin (in particular, polyethylene, hereinafter referred to as SiPE). An essential part of the invention is the description of a catalytic system enabling the preparation of this material,

the key components of which are an organometallic complex of Ti, Hf, V or Nb, a cocatalyst (B(C6F5)3 or methylaluminoxane (MAO)) and a hydrosilane.

Originator: Mgr. Jiří Pinkas, Ph.D.

Application: Preparation of block copolymers of polyolefin with inorganic (polysiloxanes) and polar organic polymers (e.g. polymethacrylate).

Utility model

Photoacoustic gas analyzer with automatic calibration (PUV 2021-39397)

The subject of the technical solution is an autonomous gas analyzer that provides data on the concentration of a limited number of selected gases. According to the present technical solution, the analyzer comprises a laser module with a laser and temperature stabilization provided by a Peltier cell, a detection module connected to it, a phase-locked amplifier communicatively coupled to the detection module, and a control unit communicatively connected to the laser module, to the detection module and the phase-locked amplifier. Its essence is that the detection module is photoacoustic. The analyzer is based on photoacoustic spectroscopy (quartz enhanced photoacoustic spectroscopy method commonly known as QEPAS). The emphasis is on the self-calibration of the analyzer.

Originator: Ing. Jan Suchánek, Ph.D.

Application: Depending on the laser used, the detection set-up can be used for leak detection of hazardous gases, air quality monitoring, gas measurement in the field of occupational safety, and medicine for diagnostics by breath analysis.

Licensing agreement

I Innovative photocatalytic screed materials and concrete additives (2021/071)

Originator: RNDr. Jaromír Jirkovský, CSc

Application: Building industry

Licensing agreement

SF6 gas substitutes in switchboards (2021/070)

Originator: Mgr. Juraj Fedor, Ph.D.,

Application: Industrial wiring and power distribution equipment.

Information on the employees of the JHIPC 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. Name of the organization: International Society of Electrochemistry. Position: Vice-chair of Division 6 (Molecular Electrochemistry). Term of office: 2019-2020

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

prof. Ing. Tomáš Navrátil, PhD. Name of the organization: International Society of Electrochemistry. Position: Regional representative. Term of office: 2021–2025

RNDr. Radek Šachl, Ph.D. Name of the organization: Deutsche Geselschaft für Biophysik. Position: Speaker of the Membrane Biophysics section. Term of office: 2021-2024

III. 7. International scientific collaboration

Within the framework of international cooperation, the JHIPC solved a total of 7 projects financed by the European Commission within the Horizon 2020 program. Furthermore, the JHIPC participated in 9 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

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.

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 2022.

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.

Irradiation driven nanofabrication: computational modelling versus experiment (acronym RADON), coordinator: MBN Research Center, Germany, investigator: Mgr. Juraj Fedor, Ph.D. The project was launched in 2020 and continues until 2022.

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.

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.

Optical near-field electron microscopy (acronym: ONEM), coordinator: University of Vienna, investigator: Marianna Amaro, Ph.D. The project was launched in 2021 and continues until 2025.

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 COLLABORATION

Funder	N. of Projects
INTER-EXCELLENCE (MEYS) sub-programme INTER-ACTION	5
INTER-EXCELLENCE (MEYS) sub-programme INTER-COST	2
Program Mobility (MEYS)	6
International Cooperation Program – Visegrad Group (MEYS)	2
International mobility of research (MEYS- Operational Program Research, Development and Education)	8

III. 8. Conferences and foreign guests

Due to the global Covid 19 pandemic, the declaration of a state of emergency and the national safety regulations, it was not possible to carry out professional social activities.

Significant national scientific events organized or co-organized by JHIPC

Cluster Meeting 2021

18-23 July 2021, venue**:** JHIPC, number of participants: 96, of which from abroad 53

52. Symposium o katalýze (52nd Symposium on Catalysis)
8 - 9 November 2021, venue: JHIPC, number of participants: 180, of which from abroad 53

XL. Moderní Elektrochemické Metody (Modern Electrochemical Methods)

8 - 12 November 2021, venue: Jetřichovice

IV. Assessment of additional and other activity: economics department

In addition to its main activity, in 2020 the JHIPC leased non-residential space in the building of cafeteria and in the main building e.g. to technology companies, a catering company and the Institute of Physics of the CAS. JHIPC provided accommodation for its employees and foreign guests if needed in the hostel in the building ZJ or in the hostel in Michle. The apartment, which is owned by JHIPC, is provided accommodation for important invited guests.

We reduced the rent to 1/2 of the originally agreed price of the M-CATERING till 30 June 2021, due to emergency measures to protect the population from further spread of COVID 19 caused by the new coronavirus SARS CoV 2 (Act No. 94/2021 Coll., On emergency measures in the event of an epidemic of COVID 19 and amending some related laws), which have a significant impact outside other to the economic activity of the tenant (restriction of the activity of catering establishments). The company resumed operations in full after 30 June 2021. However, this reduction will not be covered by the subsidy from the CAS.

V. Information about the audit of the CAS

In 2021, the audit of the CAS took place, which was focused on management and administration. Minor administrative deficiencies were identified, which are to be remedied by the JHIPC by 31 October 2022.

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

In 2021, no events occurred that would affect the economic position of the JHIPC 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. However, the financial management and other activities of JHIPC are entirely dependent on subsidies from the founder, i.e., the CAS and grant agencies, or subsidies from ministries. Other revenues would not cover the activities of JHIPC.

VII. Expected development of JHIPC activities

In 2022-2022, the JHIPC will develop scientific and research activities in the field of physical chemistry and relevant other fields based on 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. At the same time, a "Sustainable Development Strategy of the CFCH JH is being developed with an overall vision in the long term". This document describes the following areas, based on the participation of all the Institute's senior scientists:

- Purpose and mission of the Institute
- Strategic focus of scientific work
- Societal relevance of research and technology transfer

- Institutional funding and goal-directed subsidies
- Human resources development – HR Award
- Gender Equality Plan
- Investment objectives
- Strategy for foreign cooperation
- Communication strategy
- Sustainability in terms of resources and waste, including energy and CO_2

In 2022, 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), intellectual property protection, open access to information, transfer of technologies and their licensing.

The objectives of the **strategy for international cooperation in research and development** are formulated primarily as:

Creation of a consolidated interinstitutional network enabling international cooperation, including scientific education, and the sharing of best practices in the field of scientific management, based on an analysis of existing cooperation at the level of the JHIPC and its departments.

Adopting a participatory approach to develop the concept of the European Research and Innovation Area. Coordination with international partners in formulating, presenting and promoting opinions, both on policy development and on specific program actions.

Close cooperation with international partners while sharing a unique scientific **infrastructure**, equipment and related services. Part of this goal is to fully expand the capacity of the JHIPC as a partner for international cooperation.

In the field of promoting diversity and equal opportunities, an audit will be carried out, and a Gender Equality Plan will be created on its basis.

Get talented students and researchers at an early stage and together with international partners to provide high-quality training in sophisticated scientific techniques in the wider field of physical chemistry. The medium-term goal is to intensify scientific cooperation with foreign universities aimed at awarding a "jointly awarded doctorate".

VIII. Activities in the field of environmental protection

JHIPC 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.

JHIPC carries out regular disposal of waste generated in connection with research activities, especially chemicals and depreciated office equipment using the services of specialised companies,

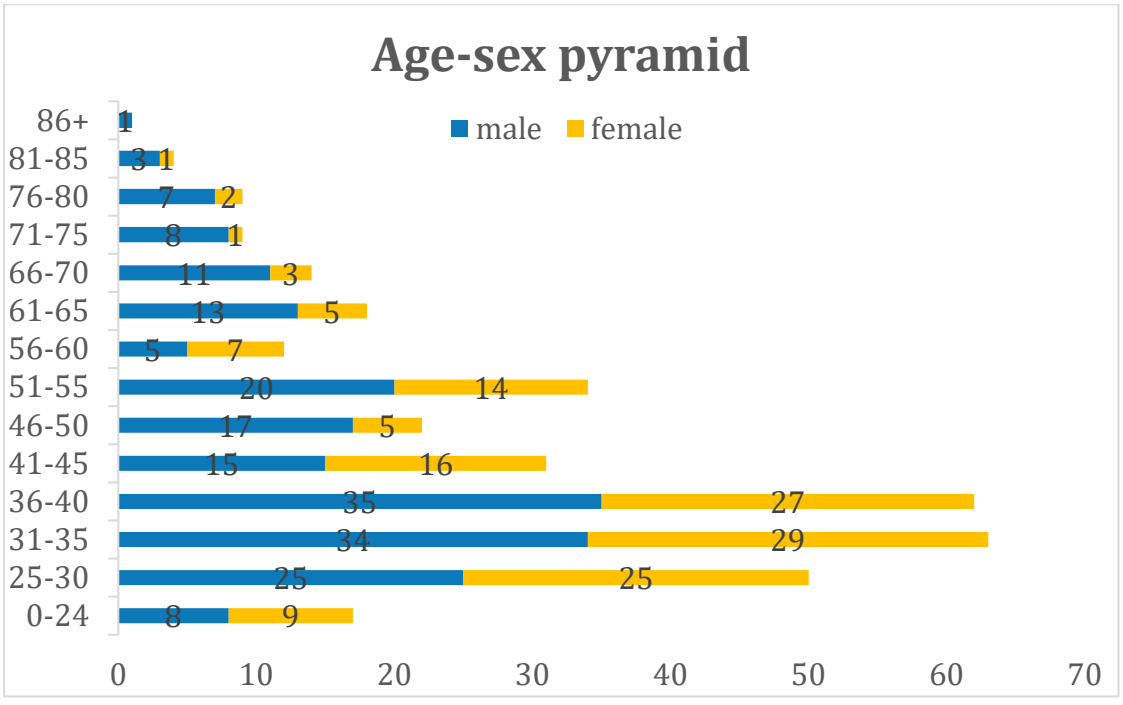
in cooperation with the city district office. The JHIPC also sorts the waste produced, namely glass, paper, plastics, batteries and accumulators.

IX. Activities in the field of labour 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 31 December 2021 was 346, the average recalculated number for 2021 was 262. The classification of the JHIPC's employees into the categories of professionals and researchers based on the updated internal salary regulations and career rules of the CAS is built upon the evaluation of scientific work by heads of departments and evaluation commissions based on specific criteria.

NUMBER OF EMPLOYEES AS OF 31. 12. 2020

TOTAL NUMBER OF EMPLOYEES	346
AVERAGE RECALCULATED NUMBER OF EMPLOYEES	262
NUMBER OF EMPLOYEES (scientific positions)	198
PhD STUDENTS	69
N. OF FOREIGN SCIENTISTS (scientific positions)	78 (39 %)
N. OF WOMEN (scientific positions)	53



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

In 2021, no request for information was submitted under Act No. 106/1999 Coll., On Free Access to information.

Stamp

Czech Academy of Sciences
J. Heyrovský Institute of Physical Chemistry
Dolejškova 2155/3, 182 23 Prague 8
Czech Republic ①

signature of the director of the JHIPC

This document was translated 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.

EVROPSKÁ UNIE
Evropské strukturální a investiční fondy
Operační program Výzkum, vývoj a vzdělávání

MINISTERSTVO ŠKOLSTVÍ, MLÁDEŽE A TĚLOVÝCHOVY