

### J. Heyrovský Institute of Physical Chemistry





# **Continuing the legacy of Prof. Jaroslav Heyrovský**

• Scientific Excellence

- Scientific Ethics and Integrity
- International Openness

 Giving Opportunities to Perspective Scientists



### **Organization Structure since 1/2019**





### **Employees 2019 (head counts)**



\*Senior scientists, scientists, research assistants, postdoctoral fellows, Early Stage Researchers (PhD students)



### **Age profile of Researchers** (Total headcounts 2019)



- 50 Early Stage Researchers and 9 Students; highly international (49 % non Czechs) Students (MSc, PhD) have minimum 0.1 FTE + addition to stipend
- Retirement policy: "Age 66" and "Age 70" : 0.5 and 0.05 FTE from Institutional Resources
- 72 Post-Docs, 6 Heyrovský Young Scientists and 6 Department's (Deputy) Heads (33 % non Czechs)

### **Subsidies in millions CZK/€ (% from Total)**

Year	2015	2016	2017	2018	2019
Total budget*	280/10.8	282/10.8	267/10.3	315/12.1	360/13.8
Institutional	93/3.6	127/4.9	124/4.8	127/4.9	131/5.0
	33 %	45 %	46 %	40 %	36 %
Personnel	124/4.8	135/5.2	138/5.3	161/6.2	183/7.0
	44 %	48 %	52 %	51 %	51 %

2019: 8.8 Mio Euro from external sources

Institutional budget is 40% of the overall budget; 60% gained by external sources
50% of the overall budget is used for salaries

\*including institutional subsidies and grant agencies; including investment money

On-site evaluation



### **Projects funded by various grant agencies**

Year	Czech Science Foundation	Technology Agency CZ	Ministry of Education, Youth and Sport CR	Ministry of Industry and Trade CR	<b>Others</b> <sup>+</sup>	European Commission
2015	53	6	17	1	11	10
2016	49	6	15	0	9	10
2017	46	4	16	2	16	10
2018	48	5	19	2	14	9
2019	56	7	21	3	18	8

+ Czech Academy of Science, Prague City Hall grants, Foundation Neuron, Ministry of Culture CZ, Ministry of the Interior CZ



# International Openness > 1/3 scientists are foreigners

• Bilingual environment, manuals and guidelines



# **Scientific Ethics and Integrity**



# In January 2019 the J. Heyrovský Institute as the first Institute of the CAS obtained the

### "Human Resources Excellence in Research Award"

The **HR Award is** awarded by the European Commission to research institutions that implement a personnel strategy based on the 40 principles of the **European Charter for Researchers** and the **Code of Conduct for the Recruitment of Researchers**.

#### Supported by the Ministry of Education, Youth and Sport

- Capacity Development of ÚFCH JH, v.v.i. for Research and Development (CZ.02.2.69/0.0/0.0/16\_028/0006251) obtained in 2017
- Capacity Development of ÚFCH JH, v.v.i. for Research and Development II- obtained in 2019



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





# **Scientific Ethics and Integrity**



- Female and Male Ombudspersons
- Committee for Scientific Work Ethics
- German Ombudsman for Ethics in Science is Member of our International Advisory Board
- Guidance on Authorship in Scientific Publications

# Giving Opportunities to Perspective Scientists A. J. Heyrovský Young Scientist Position

"Carreer development scheme towards heading a department"

- Scientific excellence (assessed by international reviewers)
- Younger than 35 years
- Extensive experience from aboard

After 5 years evaluation resulting in carrier recommendation

On-site evaluation



### J. Heyrovský Young Scientists



Stochkolm

head/vice-head of departments

Berlin

Caen

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### Development of single-molecule fluorescence methods for applications in membrane biophysics

**ACS** Publications



**Dr. Radek Šachl**, Ph.D. Umeå University in 2012, Post-Doc at Royal Institute of Technology (Stockholm) in 2014.Since 2020 Head of department of Biophysical Chemistry; Heyrovský Young Scientist Position 2017, *Otto Wichterle Award* 2017

#### Very recent paper:

<u>Šachl\*</u>, <u>S. Čujová, V. Singh, P. Riegerová, P.</u> <u>Kapusta, H. Müller, J. Steringer, M. Hof</u>, W. Nickel

Functional Assay to Correlate Protein Oligomerization States with Membrane Pore Formation Analytical Chemistry Nov. 2020



www.acs.org

Identifying functional pores formed by protein oligomers by single molecule based approaches

...with applications for cellular apoptosis and protein translocation across the plasma membrane

### J. Heyrovský Institute

### Development of functional circuit elements for singlemolecule electronic devices



**Dr. Viliam Kolivoška**, Ph.D. UCT Prague 2011; Post-Doc, University of Bern till 2013. Since 2018 Vice-head of department of Electrochemistry at the Nanoscale; Heyrovský Young Scientist Position 2017, *Otto Wichterle Award 2019* 

#### Very recent paper:

<u>S. Novakova Lachmanova</u>, **V. Kolivoska**, J. <u>Sebera</u>, J. Gasior, G. Meszaros, G. Dupeyre, P. P. Laine<sup>\*</sup>, <u>M. Hromadova<sup>\*</sup></u>

Environmental Control of Single-Molecule Junction Evolution and Conductance: A Case Study of Expanded Pyridinium Wiring Angewandte Chemie Jan. 2021





Conductance tuning via molecule-electrode interactions in solvent-controlled single molecule junctions

... with applications as switches in molecular electronic devices

# **Giving Opportunities to Perspective Scientists**

### **B. Purkyně Fellowship (from 2018 Lumina Quaeruntur)**

"Competition on the level of the CAS for attracting incoming scientists providing over-average salary"

- Martin Srnec, Stanford with Edward Solomon, 2014/18, since 2019 heading Computational Chemistry Dept.
- Juraj Fedor, Fribourg with Michael Allan, 2015/19, since 2020 heading Dynamics of Molecules and Clusters Dept.

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- Vladimira Petrakova, FU Berlin with Stephanie Reich, awarded in 2020
- Matej Velicky, Manchester with Kostya Novoselov, application approved by Institute's Board 16. March 2021 On-site evaluation



### **Research Departments and their Heads**













### **Research Departments and their Heads**

Structure and Dynamics in Catalysis Mgr. Jiří Dědeček, CSc.,DSc. FTE 27,4 Molecular Electrochemistry and Catalysis Mgr. Michal Horáček, Ph.D. *FTE 10,5*  Electrochemical Materials Prof. RNDr. Ladislav Kavan, CSc., DSc. FTE 16,8 Electrochemistry at the Nanoscale Mgr. Magdaléna Hromadová, CSc. FTE 12,2



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On-site evaluation



### **Research Departments and their Heads**







### **Inter-Departmental Collaborations**



### **Two new Departments established in 1/2019**

**Computational Chemistry** RNDr. Martin Srnec, Ph.D.



2011-13 Postdoctoral Stay – Stanford University 2010 PhD – Charles University, Prague joint 2014 the Institute via Purkyně Fellowship Nanocatalysis RNDr. Štefan Vajda, CSc., Dr. habil.



2002-2018 Senior Scientist at Argonne National Lab 1995-2002 Freie Universität Berlin; Habilitation 1990/91 Fellowship – Fulbright University of Chicago 1990 PhD – Charles University, Prague joint 2019 the Institute via Horizon 2020 ERA chair

### Department of Computational Chemistry (Head: Dr. Srnec)

"Computational modeling of complex systems including studies of practical catalytic and biochemical processes."

**Very recent papers:** 

Chalupský J., <u>Srnec M.\*</u>, Yanai, T. Interpretation of Exchange Interaction through Orbital Entanglement J. Phys. Chem. Lett 2021

#### Maldonado-Domiguez M., Srnec M.\*

Understanding and Predicting Post H-Atom Abstraction Selectivity through Reactive Mode Composition Factor Analysis **JACS** 2020

Bím D., Chalupský J., Culka M., Solomon E. I., Rulíšek L., <u>Srnec M.\*</u> Proton-Electron Transfer to the Active Site Is Essential for the Reaction Mechanism of Soluble  $\Delta 9$  Desaturase JACS 2020







#### Martin Srnec – prizes and awards

Werner von Siemens Award 2020 for the most significant result in fundamental research

#### **Quantum Bio-Inorganic Chemistry Society Award 2020**

The award recognizes the outstanding contributions of Dr. Srnec to the theoretical treatment of chemical reactivity.

**Prize of Learned Society of Czech Republic 2020** 

**Otto Wichterle Award 2015** 

Fellowship J. E. Purkyně 2013-2018













### Department of Nanocatalysis (Head: Prof. Vajda)

"Catalysis and Electrocatalysis at the (sub)nanometer Scale"





This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 810310

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### **Department of Nanocatalysis**

Design of catalysts atom-by-atom





### **Department of Nanocatalysis**

November 2019 Inauguration of the newly renovated labs







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### **Department of Nanocatalysis**

### **JUNE 2020**

#### **CLUSTER LAB**



#### TEST LAB I – gas chromatography



TEST LAB II – mass spectrometry





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### **Department of Nanocatalysis** (Head: Prof. Vajda)

"Catalysis and Electrocatalysis at the (sub)nanometer Scale"

B. Yang, XI. Yu, A. Halder, XI. Zhang, XI. Zhou, G. J. A. Mannie, E. Tyo, M. J. Pellin, S. Seifert, D. Su, **S. Vajda**: Dynamic Interplay between Copper tetramers and Iron Oxide Boosting CO<sub>2</sub> Conversion to Methanol and Hydrocarbons under Mild Conditions, **ACS Sustain Chem Eng** 2019

S. Lee, A. Halder, G. A. Ferguson, S. Seifert, R. E. Winans, D. Teschner, R. Schlögl, V. Papaefthimiou, J. Greeley, L. A. Curtiss, **S. Vajda**: Subnanometer Cobalt Oxide Clusters as Selective Low Temperature Oxidative Dehydrogenation Catalysts, **Nat Commun** 2019

Y. Lei, F. Mehmood, S. Lee, J. P. Greeley, B. Lee, S. Seifert, R. E. Winans, J. W. Elam, R. J. Meyer, P. C. Redfern, D. Teschner, R. Schlögl, M. J. Pellin, L. C. Curtiss, **S. Vajda**, Increased Silver Activity for Direct Propylene Epoxidation via Subnanometer Size Effects, **Science** 2010

16. March 2021







# Number of outputs in selected years in first decile and quartiles



On-site evaluation

# **Quality of Science: National Standing**

"Evaluation of Research Organisations by the Czech Government in the years 2015-2019"

• (Numerical) Evaluation organized by the government till <u>2016</u> resulting in **one number** ("**RIV points**") was criticized that it supports to much quantity to quality

•From <u>2017</u> so-called "Metodika 17+" based on **"D1 and Q1" classification**. Evaluators used that to compare the Czech Research Organization among each other but also with EU15 standards



# **RIV points 2015 / CZK Institutional Support**

#### Heyrovský Institute has been repeatedly the most efficient CAS Institute according RIV points



#### CZK Institutional support 2016 from CAS in thousand CZK



### Evaluation of Research Organisations by the Czech Government – "The M17+" for 2016-2018

#### 1.4 Chemical Sciences (2016-2018, database WoS)

Order	Research organization	Share in the field in D1	The number of results of the organization in D1
1	Charles University	21%	121
2	Palacký University in Olomouc	19%	114
3	University of Chemistry and Technology in Prague	16%	96
4	Institute of Organic Chemistry and Biochemistry of the CAS	15%	86
5	J. Heyrovský Institute of Physical Chemistry of the CAS	12%	71
6	Institute of Physics of the CAS	9%	52
7	Masaryk University	8%	44
8	Brno University of Technology	6%	33
9	Institute of Macromolecular Chemistry of CAS	5%	28
10	Institute of Biophysics of the CAS	4%	26



### **Evaluation of Research Organisations by the Czech Government – "The M17+" for 2016-2018**

How is the bibliometric profile of the Czech research organizations (RO) compared to world / EU15 level?

"The **bibliometric profiles of large universities** are mostly at the global (national) level, however, compared to the EU15, the shares of publications are significantly lower for D1 and Q1. However, J. Heyrovsky Institute was pointed out as an exception: excellent research organization, at the top on a national scale in its main fields. It is significantly better compared to EU15 in chemical sciences, very high share of publications in D1 with corresponding author from the institute indicating that the know-how originates from the institute."

If one takes the size of the RO's into account, are there smaller RO's that exceed the performance of larger institutions in terms of quality

"Yes, the J. Heyrovsky Institute stands out amongst other Institutes of the CAS, having compared to their FTE a higher number of publications in D1 with corresponding author from the institutes compared to other Institutes of the CAS." 32



## **Quality of Science: National Standing**

• Numerical Evaluation ("RIV" points) done till 2015 has seen the J. Heyrovský <u>Institute is the most effective Institute of the CAS</u>

• "Metodika 17+" based on "D1 and Q1"classification as well as sees the J. Heyrovský <u>Institute as the most effective Research</u> <u>Organisation in Chemical Sciences</u>



### Selected Awards confirm highest national standing

Awards of the Academy of Sciences of the Czech Republic:

- A) Praemium Academiae M. Fárník (2017), M. Kalbáč (2019)
- B) The J. Heyrovský Honorary Medal for Merit in Chemical Sciences
   Z. Samec (2018)
- C) Otto Wichterle Award J. Kočišek (2018), V. Kolivoška, P. Kovařiček,
  - E. Krupičková Pluhařová (2019)
- D) Purkyně Fellowship (Lumina Quaeruntur) J. Fedor (2019),
  - Vladimira Petrakova (2020)
- The Josef Hlávka Award: A. Melcrová (2019)
- Prize of the Learned Society of the Czech Republic for young scientists

J. Fedor (2019)

Awards of MEYS - František Běhounek Award: L. Kavan (2017)

Czech Intelect for Doctorandus in Natural Science:

D. Bím (2019)

<u>Czech Intelect for the Invention Category:</u> J. Dědeček, E. Tabor, Š. Sklenák (2020)



Otto Wichterle Award 2019 V. Kolivoška, P. Kovařiček, and E. Krupičková Pluhařová

### **Quality of Science: International Standing**

# Comparison with



### FRITZ-HABER-INSTITUT MAX-PLANCK-GESELLSCHAFT



### Heyrovský Inst. vs. Fritz-Haber-Institute MPG

Heyrovský Inst (2015): 244 employees - 182 scientists (FTE including 40 PGS), budget ca. Mio ca 10 EUR

FHI MPG (2015): 400 employees – 192 scientists (38 senior, 92 PGS, 62 postdocs), budget ca Mio 28 EUR





### **International Standing**

•Comparison with Fritz-Haber-Institute (Berlin) of the Max-Planck-Gesellschaft:

- The number of full time employees is smaller, but somewhat comparable
- Budget of FHI is 3 times higher
- Publication profiles of both institutions are comparable in quantitative and qualitative means
- Number of citations at Fritz-Haber-Institute is higher

Fritz-Haber-Institute is better integrated into the European research landscape than the J. Heyrovsky institute



### **EC Projects as an Indicator for Excellence**

Acronym	Title	Funding scheme	EU contribution (thousand €)	years
J. Heyrovský Chair	The ERA-Chair at J. Heyrovský Institute - The institutional approach towards ERA	Widening	2 483	2018-23
ONEM	Optical Near-field Electron Microscopy	FET Proactive	885	2021-24
TSuNAMI	Trans-Spin NanoArchitectures: from birth to functionalities in magnetic field	ERC-STG	486	2017-22
ELCOREL	Electrochemical Conversion of Renewable Electricity into Fuels and Chemicals	MSCA-ITN	465	2017-21
StR-ESFRI2	Support to Reinforce the European Strategy Forum on Research Infrastructures	CSA	283	2019-22
PROTON	Proton transport and proton-coupled transport	MSCA-ITN	235	2019-23
TAGGED	Graphene light emitting hybrid MOEMS Device	ERA-NET	233	2021-24
IMPACT	Ion-Molecule Processes for Analytical Chemical Technologies	MSCA-ITN	232	2016-19
ShaleXenvironmen T	Maximizing the EU shale gas potential by minimizing its environmental footprint	RIA	210	2015-18
GrapheneCore1	Graphene-based disruptive technologies	RIA	207	2016-18
GRAPHENE	Graphene-Based Revolutions in ICT And Beyond / Flagship	CP-CSA	90	2013-16
InRoad	Research Infrastructures Beyond National Relevance	CSA	78	2017-19
ENERGY-X	ENERGY-X: Transformative chemistry for a sustainable energy future / Flagship		41	2019-20
SUNRISE	Solar Energy for a Circular Economy / Flagship	CSA	11	2019-20

CP- CSA Collaborative projects - The Coordination and Support Action MSCA-ITN Marie Skłodowska-Curie Actions - The Innovative Training Networks ERC-STG European Research Council: Starting Grants FET Proactive The Future Emerging Technologies programme On-site evaluation RIA Research and Innovation Action 38 ERA-NET Horizon 2020 ERA-NET COFUND



### **EC Projects as an Indicator for Excellence**

•Compared to other Institutes of CAS the Heyrovský Inst. is one of the most successful Institutes in obtaining EC funding

- •Success in EU Horizon 2020 programs, e.g.:
- Coordinating / participating in three Marie Curie Initial Training Networks (ITN)
- Involvement in three Flagship actions
- Co-PI of ERC starting grant
- ERA Chair (Widening)
- Very Recent: FET Proactive: Emerging Paradigms and Communities



- Even several applications were submitted, no ERC Advanced / Consolidator Grant was yet awarded to the Institute

J. Heyrovský Inst. has to be better integrated into the European research landscape

On-site evaluation



# Strategy for better integrating into the European research landscape

Formulated with three **objectives**:

- **1. Establishing a consolidated inter-institutional international network** allowing cooperation among various scientific lines, but also including science training aspects. Using EC funding schemes like Twinning for that.
- 2. Closely collaborate with international partners in sharing unique scientific infrastructure, equipment and related services.
- **3.** Attract talented students and early stage researchers and provide together with international partners high-quality training in sophisticated scientific techniques in the broader field of physical chemistry. The mid-term perspective of this objective is to intensify the scientific cooperation with a <u>foreign university working towards a jointly awarded doctorate</u>.



# Strategy for better integrating into the European research landscape

### Collaboration with a Strong Partner on the Institutional Level Helmholtz-Zentrum Dresden- Rossendorf (HZDR)



Signing Memorandum of Understanding with the Director of HZDR Prof. Roland Sauerbrey

16. March 2021



## **Knowledge Transfer into Practice Patents and utility models**

Jirkovsky, Rathousky et al. Self cleaning paint, BETOSAN, sro, Advanced Materials-JTJ



Year	Voor	Pate	ents	Utility models		
	applied	granted	applied	registered		
	2015	3	7	0	0	
	2016	1	5	4	3	
	2017	4	1	0	0	
	2018	1	4	0	1	
	2019	1	2	3	1	

Dědeček et al. 2020 Direct methane ( $CH_4$ ) to methanol ( $CH_3OH$ ) oxidation by molecular oxygen ( $O_2$ )



<u>Awarded by Czech Intelect for the</u> <u>Invention Category:</u> J. Dědeček, E. Tabor, Š. Sklenák (2020)



# Joint projects with partners from industry

- 1. Carbon nanostructures for sensor applications (M. Kalbáč, 2013-16)
- 2. Research for the production of multifunctional photoactive nanocomposite for use in construction and paints (J.Jirkovský, 2013-16)
- 3. Use of photoactive nano-surfaces to solve current problems of air and water purification (J. Jirkovský, 2013-16)
- 4. Advanced phosphor for high power LEDs and laser diodes (S. Civiš, 2014-17)
- 5. Catalytic process for complete elimination of nitrogen oxide emissions for nitric acid production technology (P. Sazama, 2015-17)
- 6. Progressive materials for protection against serious environmental damage (J. Dědeček, 2018-21)
- 7. Replacement of SF6 gas in switchboards (J. Fedor, 2017-20)
- 8. Development of high-performance alkylation and isomerization catalysts (P. Sazama, 2018-20)
- 9. Powerful light sources (S. Civiš, 2018 19)
- 10. SEPIOT Gas sensors based on hybrid nanostructures for IoT applications (M. Kalbáč, 2019-22)
- 11. Photoactive nanocomposite systems for environmental improvement (J. Jirkovský, 2019-21)
- 12. National Competence Center for Materials, Advanced Technologies, Coating and Their Applications (M. Kalbáč, 2019-22)
- 13. Research and Construction Design of 48V Lithium Accumulators for New Generation of Automobiles (Zukalová, 2017-2020)

Year	Projects	Contractual research
2015	7	12
2016	6	7
2017	6	9
2018	7	9
2019	10	8

# **Cooperation with Universities and Participation in Education**

- 50 Early Stage Researchers in common PhD programs with Universities; 9 Master Students
- Close to 500 lectures or seminars / year by 40 scientists are given at 7 Czech Universities (more than half at Charles University Prague) and the University of Dresden (i.e. Privat-Dozent P. Krtil)
- 17 of running grants do have the co-PI located at the Universities (2019)



Year	Total number of realized programs ***	Lectures for secondary and basic school students (hours)	Stays of second. school students	Number of visitors of Open Days	Exhibitions organized by institute	_
2015	78	55	32	230	6	
2016	85	77	42	210	6	
2017	90	84	53	210	8	
2018	117	87	77	355	7	
2019	115	50	80	360	10	





\*\*\* programs: e.g. lectures for students, educative seminars for teachers, practices in laboratories and stays in laboratories; chemical performances for children from kinder garden, workshops for basic school pupils or secondary school students, summer school for secondary school students, exhibitions, stands with experiments on yearly science fair. Web page of Heyrovsky educative team PEXED (Popularization Experimental Eduction) http://www.3nastroje.cz



# **Organization of conferences and festive lectures (2015-2019)**



#### Organised by the institute :

- R. Brdička Memorial lecture (annually since 1991)
- Heyrovský Discussion (Castle Třešť, annually, c.a. 50 participants)
- Seminar of students of the Heyrovský Institute (Liblice, annually, ca. 60 participants)
- The scientists of the institute organised **over 40 conferences and workshops** in the period 2015-2019 including



### **Other Outreach Activities**

We have professionalised our Outreach Activities within the last 3 years. As a results the Institute presents the results of its activities in the media and on social networks continuously year-round.

For more details, see https://web.jh-inst.cas.cz/press-releases and https://web.jh-inst.cas.cz/media













#### The institute is internationally respected for the quality of scientific research

- The research program at the institute is well balanced in the field of contemporary physical chemistry
- Highly qualified senior research staff with a good or excellent international reputation
- Leading scientists are invited as plenary speakers at international conferences and to evaluate science on the European level

### The institute is one of the best research Institutions within the Czech Republic

### The institute is well-equipped by instrumentation and expertise

• Unique instrumentation and expertise located at one place, which was further extended by Nanocatalysis lab

### The institute is internally well-balanced

- A comparable level of the scientific performance in all research departments of the institute.
- Well-balanced personnel structure.
- The number of Non-Czech scientists has increased to 38%, which is well above the national standards.

### The institute is active in education and popularization

### The institute has established European standards in research management







#### Lower impact and limited visibility of the research performed in the institute compared to top Western Research Organizations

- Some research strategies are determined by evolution from traditional directions of electrochem., catalysis and chemical physics
- Difficulties to compete with top world research institutions in some areas of the material and methodological research
- Attempts to obtain ERC consolidator / advanced grants have not yet been successful.

#### **Financial weaknesses**

- Salary level of the institute is substantially lower not only when compared to western research institutes, but also when compared to certain Czech research units. Recruitment of prospective young scientists is difficult.
- Expensive maintenance and operation of sophisticated research instruments
- Presently 60% of the FTE in research is financed by external funding resources.

#### **Organizational weaknesses**

- The majority of the leading scientists has Czech citizenship, and have spent the largest part of their scientific career in the CR.
- A lack of PhD students is felt in several departments.
- Absence of administrative and technical staff within the individual departments.



# **SWOT** analysis

### **Opportunities**

- Better integrate the Institute into the European research landscape and increase overall visibility
- Developing and implementing strategies to make the institute more attractive to ESR and Post-Doc's
- Increasing the success rate in EC funding
- Continuing supporting the best young scientists by selecting more J. Heyrovský Young Scientists
- Promoting them to department head / vice-heads



### Threats

- The biggest threat is the omnipresent underfunding of research in the Czech Republic and fluctuations of funding based on political interventions
- The financial instability may, despite successfully introduced structural changes at the institute, cause lag of institutional funding sufficient for following the world trends in science.
- Low success rates grant funding would threaten the balanced budget of the institute.
- The reluctance of the Czech Scientific decisionmakers to establish European standards regarding continuity and transparency in the management of science.



# Thank you for your attention!

