Evaluation of research and professional activity of research-oriented institutes of the Czech Academy of Sciences for the period 2015–2019

Final Report

Name of the Institute:

J. Heyrovsky Institute of Physical Chemistry of the CAS, v. v. i.

Evaluated teams and their leaders:

1. Spectroscopy (Martin Ferus)
2. Theoretical and Computational Chemistry (Jiří Pittner)
3. Biophysical Chemistry (Radek Šachl)
4. Structure and Dynamics in Catalysis (Jiří Dědeček)
5. Molecular Electrochemistry and Catalysis (Jiří Ludvík)
6. Electrochemical Materials (Ladislav Kavan)
7. Electrochemistry at the Nanoscale (Magdaléna Hromadová)
8. Chemistry of Ions in Gaseous Phase (Patrik Španěl)
9. Low-dimensional Systems (Martin Kalbáč)
10. Dynamics of Molecules and Clusters (Juraj Fedor)

Part A: Evaluation of the institute

Strengths:
High scientific reputation, recognized brand. Outstanding scientific output. Excellent equipment. Active management.

Weaknesses:
Lower salaries than peer institutions Europe-wide with which they compete for talent. Expensive maintenance of equipment park. Fewer PhD students than would be optimal.

Opportunities:
Competitive in European funding. Recruitment of both Czech and foreign talent (if the conditions are met), Career development for talented scientists.

Threats:
Fluctuations and uncertainties in Czech funding.

Main criterion: 1. Quality of results (H1.1-H1.5)

H1.1	Quality of selected outputs of Phase I
Phase I outputs clearly document high scientific quality. The Heyrovsky Institute is a jewel of the CAS. It is one of the few internationally recognized scientific brands in the Czech Republic and it competes at a top European level on the worldwide stage.	
H1.2	**Contribution of workers on the outputs reached**
Central.	
H1.3	**Quality of all outputs and results**
Outstanding.	
H1.4	**The most valuable discoveries and findings in the fields, their importance for the field**
The Heyrovsky Institute is a very large, and thematically heterogenous, institute. Please refer to the individual Department evaluations for the highlights.	
H1.5	**Contribution of the participation of the authors in large collaborations**
Please refer to the individual Department evaluations.	

Main criterion: 2. Societal relevance (H2.1-H2.5)

H2.1	Societal relevance of outputs and results pursuant to CAS and institute mission
While the principal documentation of societal relevance is in the Departmental evaluations, it should be noted that the excellent basic research in the Heyrovsky Institute leads to significant applications or potential applications.	
H2.2	**System functionality for knowledge transfer into practise, its usefulness for society. The impact of the institute´s activity on proper practice in society in the area of social sciences and humanities**

While there is some indication of Knowledge & Technology Transfer activities in some of the Departments, the efforts do not appear to be coordinated centrally. We were informed that the CAS is building up a central KTT organization, which would be very helpful in translation of the research results into applications for the benefit of society and the economy. We recommend that the CAS partner with European partners with a proven track record in KTT for policies appropriate for the organization and legal structure within an European context. American private universities would be a poor model.

H2.3	**Relation to practice**
See above.	

H2.4	**Participation in AV21 strategy**
See individual Department evaluations.	

H2.5	**Cooperation with regions of the Czech Republic**
See individual Department evaluations.	

Further criterion: 1. Position in international and national context (D1.1-D1.3)

D1.1	**Comparison of the teams and the institute with similar international and national institutes**
While there is some variation, in general, the teams at the Heyrovsky Institute are competitive with the best groups in their respective areas.	

D1.2	**Scope and quality of international and national cooperation and the role of the institute in such cooperation; engagement in broad international cooperation**
The Heyrovsky Institute is well-embedded in international cooperations with high-quality partners. Whether this is a cause or an effect of their high internal expectations, we cannot say.	

D1.3	**Participation of the workers in scientific community activities (organizing of conferences and workshops, invited lectures, awards)**
Excellent.	

Further criterion: 2. Vitality, sustainability and strategy (D2.1-D2.9)

D2.1	**Direction in line with the perspective of the planned research directions**
Excellent.	

D2.2	**Assessment of the previous research objectives and their achievement**
See individual Departments.	

D2.3	**Assessment of implementation of recommendations from past evaluation**
See individual Departments. It should be commented that many structural recommendations from the previous evaluation allowed units to more flexibly respond to the changing external scientific landscape.	

D2.4	Success in receiving grants
In general, the success in receiving grants has been good. In particular, we would comment on the very good amount of European grants coming into the Heyrovsky Institute, including the highly competitive ERC grants.	
D2.5	**Adequacy of instrumental equipment**
Excellent.	
D2.6	**Effectiveness of management**
It is difficult, given the absence of an actual site visit, to judge the effectiveness of management, although the overall success speaks well for it. We would comment that the Heyrovsky Institute was the only one of the three that we evaluated that placed an early and heavy emphasis of scientific ethics in its presentation, which we find highly praiseworthy.	
D2.7	**Assessment of professional structure, development strategy and the strategy of keeping best scientists, age structure, career and qualification growth**
In general, there seems to be a well-organized promotion path for young scientists. Many are moving into team leader roles.	
D2.8	**Creating work-life balance conditions, assessment of approach towards possible gender issues**
There are a couple of the ten Departments that we evaluated that had an adequate gender balance; most of the others had a disproportionately low number of women. There was only one woman among the ten heads of Department. The gender issue needs to be addressed.	
D2.9	**Relation of the institute with regard to the integration, development and sustainability of the research centre funded by the National Programme of Sustainability II.**
Please see individual Department evaluations.	

Further criterion: 3. Cooperation with universities and participation in education (D3.1-D3.6)

D3.1	Scope of cooperation with universities on national and international level
Very good.	
D3.2	**Effectiveness of joint research centres**
For the most part, the research did not lend itself to large, joint research centres, although there were a few instances, for example, in connection with ESA.	
D3.3	**Success rate in supervision of PhD students**
The level was uneven, with too few PhD students for an Institute of this quality, in general.	
D3.4	**Participation of PhD students in the outputs**
Good.	

D3.5	Participation of the institute in master or bachelor studies
Similar to the situation with PhDs.	
D3.6	**Assessment of cooperation intensity with universities in the form of teaching**
Generally good.	

Further criterion: 4. Outreach activities (D4.1-D4.3)

D4.1	Sufficiency of media strategy and activities in the area of research popularisation
The breadth of research areas, and the level of innovation, leads to a number of interesting avenues to address the public. The activities are fine.	
D4.2	**Publishing activities and its quality**
Outstanding.	
D4.3	**Participation in professional organisations in the area of research and development**
Good.	

Other comments of the commission:

Part B: Evaluation of teams

1. Spectroscopy

Strengths:
(1) attractive research topics, e.g. prebiotic chemistry & materials;
(2) good physical infrastructure;
(3) oriented towards EU (ERC) for quality and scientific direction;
(4) extensive international contacts and collaborations

Weaknesses:
(1) publication pressure with emphasis on numbers of outputs;
(2) low number and visibility of women in the teams

Opportunities:
(1) recruiting motivated coworkers;
(2) realistic chance to be competitive at the EU level for ERC and other top-level funding

Threats:
(1) retirement of key personnel;
(2) rising bureaucratic demands on scientists

Main criterion: 1. Quality of results (H1.1-H1.5)

H1.1	Quality of selected outputs of Phase I
The Heyrovsky Institute, in general, but the Spectroscopy group, in particular, already "looks outward" to the larger European scientific community. The quality standards they adopt internally are consistent with those at top institutions in Europe. The Spectroscopy group publishes excellent papers in high-quality journals.	
H1.2	**Contribution of workers on the outputs reached**
The co-workers are the most important resource in producing the outputs.	
H1.3	**Quality of all outputs and results**
See above.	
H1.4	**The most valuable discoveries and findings in the fields, their importance for the field**
The Spectroscopy group, with its combination of high-resolution molecular spectroscopy and plasma science provides an uncommon platform for the investigation of prebiotic chemistry. The topic is one of the very few which can command immediate attention in the lay public. Everyone is interested in the question: "From where did we come?" It provides a framework for much outreach as well. Parts of the expertise also bleed over into materials processing, which has a more immediate, practical application, and environmental monitoring, which, again, has significant impact.	
H1.5	**Contribution of the participation of the authors in large collaborations**
The Spectroscopy group is well-embedded in collaborations investigating the chemistry of exoplanets, which is an application of molecular spectroscopy that no one would have	

imagined two decades ago. It is fruitful and highly visible.

Main criterion: 2. Societal relevance (H2.1-H2.5)

H2.1	Societal relevance of outputs and results pursuant to CAS and institute mission
The materials research has immediate applications, but the societal relevance of the prebiotic chemistry and the exoplanet research is probably higher. The questions are universal questions posed by all people. "From where did we come?" and "Are we alone?"	
H2.2	**System functionality for knowledge transfer into practise, its usefulness for society. The impact of the team´s activity on proper practice in society in the area of social sciences and humanities**
NA.	
H2.3	**Relation to practice**
There are some applications in providing analytical instrumentation and new materials. The Technology Transfer activities are not prominent, though.	
H2.4	**Participation in AV21 strategy**
No comment.	
H2.5	**Cooperation with regions of the Czech Republic**
The principal cooperations appear to be outside of the Czech Republic.	

Further criterion: 1. Position in international and national context (D1.1-D1.3)

D1.1	Comparison of the team with similar international and national institutes
The Spectroscopy group ranks well in comparison with international institutes. They have already oriented themselves to the EU quality levels.	
D1.2	**Scope and quality of international and national cooperation and the role of the team in such cooperation; engagement in broad international cooperation**
See above.	
D1.3	**Participation of the workers in scientific community activities (organizing of conferences and workshops, invited lectures, awards)**
Activity at the expected level.	

Further criterion: 2. Vitality, sustainability and strategy (D2.1-D2.9)

D2.1	Direction in line with the perspective of the planned research directions
The direction of the Spectroscopy group has been moving in the direction of astrophysical and biological sciences, and in the direction of environmental analytics. They have the appropriate expertise and instrumentation, and, given the finite, but not small financial	

resources they have, they have prudently chosen to specialize in high-impact, high-visibility areas where their particular strengths make a difference.	
D2.2	**Assessment of the previous research objectives and their achievement**
No comment.	
D2.3	**Assessment of implementation of recommendations from past evaluation**
No comment.	
D2.4	**Success in receiving grants**
In the evaluation period, the Spectroscopy group received 21 grants from four different Czech funding agences. The grants are spread well over the different PIs.	
D2.5	**Adequacy of instrumental equipment**
Rather good instrument facilities.	
D2.6	**Effectiveness of management**
Difficult to evaluate. The management appears to be good.	
D2.7	**Assessment of professional structure, development strategy and the strategy of keeping best scientists, age structure, career and qualification growth**
The group has a bimodal age structure, but the bulk of the members are younger. There is a conscious career development strategy.	
D2.8	**Creating work-life balance conditions, assessment of approach towards possible gender issues**
We saw no approach to gender issues at all. The number of women was low, and they were not visible.	
D2.9	**Relation of the team with regard to the integration, development and sustainability of the research centre funded by the National Programme of Sustainability II.**
No comment.	

Further criterion: 3. Cooperation with universities and participation in education (D3.1-D3.6)

D3.1	**Scope of cooperation with universities on national and international level**
The group has extensive national and (especially) international collaborations.	
D3.2	**Effectiveness of joint research centres**
Highly effective, leverages the strengths of the Institute.	
D3.3	**Success rate in supervision of PhD students**
The numbers of Ph.D. students is low, with only 2 doctoral dissertations defended in the 2015-2019 period.	
D3.4	**Participation of PhD students in the outputs**
Good.	

D3.5	Participation of the team in master or bachelor studies
There were 6 BS and 3 MS theses defended in 2015-2019, which is an adequate number.	
D3.6	**Assessment of cooperation intensity with universities in the form of teaching**
No comment.	

Further criterion: 4. Outreach activities (D4.1-D4.3)

D4.1	Sufficiency of media strategy and activities in the area of research popularisation
With their attractive topics, the Spectroscopy group has extensive media activities. They document many appearances on Czech television, radio, and popular print media.	
D4.2	**Publishing activities and its quality**
More than 30 outputs mainly concerning research on the origin of life in PNAS. One can hardly imagine a better performance.	
D4.3	**Participation in professional organisations in the area of research and development**
No comment.	

Other comments of the commission:

2. Theoretical and Computational Chemistry

Strengths:
Wide area of topics, ranging from the theoretical development to practical applications International collaborations and visibility. Good age structure.

Weaknesses:
Difficulties in attracting young students. Low level of outreach activities.

Opportunities:
Recruiting PhD students. Competitiveness at the EU level.

Threats:
New students only from teaching collaborations with universities. Low salaries for young researchers.

Main criterion: 1. Quality of results (H1.1-H1.5)

H1.1	Quality of selected outputs of Phase I
The Theoretical and Computational Chemistry department covers a wide area of topics, ranging from the theoretical development to practical applications. The quality standards are in line with the best European institutions. The scientific productivity of the different research groups of this department publish is good and a significant part of their work has been published in high-quality journals.	
H1.2	**Contribution of workers on the outputs reached**
Most of the outputs correspond to work carried out by young members of the different teams.	
H1.3	**Quality of all outputs and results**
The scientific activities of this department range from fundamental studies addressed to the understanding of basic aspects of molecular reactivity, the early Universe chemistry, as well as areas with the potential industrial, biological and medical application.	
H1.4	**The most valuable discoveries and findings in the fields, their importance for the field**
This department studies methodological aspects of theoretical chemistry and provides theoretical support to other projects carried out in the other departments of the institute	
H1.5	**Contribution of the participation of the authors in large collaborations**
The Theoretical and Computational Chemistry department is involved in many internal and external collaborations, many of which are international.	

Main criterion: 2. Societal relevance (H2.1-H2.5)

H2.1	Societal relevance of outputs and results pursuant to CAS and institute mission
The research work carried out by this department is instrumental for the development of many other projects of the institute. Although the core projects are of fundamental nature,	

significant efforts are directed towards aspects of societal relevance. These include studies on ophthalmologic problems, investigations of pulmonary surfactants, polymeric materials for biomedical applications, and applications in the nanofabrication industry.	
H2.2	**System functionality for knowledge transfer into practise, its usefulness for society. The impact of the team´s activity on proper practice in society in the area of social sciences and humanities**
See point H2.1	
H2.3	**Relation to practice**
See point H2.1	
H2.4	**Participation in AV21 strategy**
No comment.	
H2.5	**Cooperation with regions of the Czech Republic**
No comment.	

Further criterion: 1. Position in international and national context (D1.1-D1.3)

D1.1	**Comparison of the team with similar international and national institutes**
The different groups of the Theoretical and Computational Chemistry department rank well in comparison with other international institutes.	
D1.2	**Scope and quality of international and national cooperation and the role of the team in such cooperation; engagement in broad international cooperation**
The quality of the cooperation at the international and national levels is satisfactory.	
D1.3	**Participation of the workers in scientific community activities (organizing of conferences and workshops, invited lectures, awards)**
The participation of the members of the different groups in conferences is satisfactory.	

Further criterion: 2. Vitality, sustainability and strategy (D2.1-D2.9)

D2.1	**Direction in line with the perspective of the planned research directions**
This relatively large department split in 2020 into two departments: Theoretical Chemistry and Computational Chemistry. The research objectives for 2020-2024 are essentially the same as those of the period under evaluation.	
D2.2	**Assessment of the previous research objectives and their achievement**
The previous evaluation was highly positive. Several measures have been implemented to increase the number of Master and PhD students.	
D2.3	**Assessment of implementation of recommendations from past evaluation**
Positive implementation of the recommendations from past evaluation.	

D2.4	Success in receiving grants
In the evaluation period, the Spectroscopy group received 24 grants mainly from three different Czech funding agencies. In the last year of the evaluated period (2019) was an increase in the number of grants from Czech Science Foundation (11 vs. 5-8 in each of the three previous years).	
D2.5	**Adequacy of instrumental equipment**
The Heyrovský institute has state of the art computational facilities.	
D2.6	**Effectiveness of management**
The management appears to be good.	
D2.7	**Assessment of professional structure, development strategy and the strategy of keeping best scientists, age structure, career and qualification growth**
The majority of the research members are young (good number of PhD students and postdocs). There is a clear career development strategy.	
D2.8	**Creating work-life balance conditions, assessment of approach towards possible gender issues**
The gender balance among the team leaders is low.	
D2.9	**Relation of the team with regard to the integration, development and sustainability of the research centre funded by the National Programme of Sustainability II.**
No comment.	

Further criterion: 3. Cooperation with universities and participation in education (D3.1-D3.6)

D3.1	Scope of cooperation with universities on national and international level
The different groups have many national and international collaborations.	
D3.2	**Effectiveness of joint research centres**
No comment.	
D3.3	**Success rate in supervision of PhD students**
In the period 2015-2019, 10 PhD students were supervised by the members of the department (3 Theses defended).	
D3.4	**Participation of PhD students in the outputs**
Good (see point H1.2)	
D3.5	**Participation of the team in master or bachelor studies**
Good teaching participation of the department members in advanced courses aimed for master and doctoral students. 2 Master students were supervised by the team members.	
D3.6	**Assessment of cooperation intensity with universities in the form of teaching**
No comment.	

Further criterion: 4. Outreach activities (D4.1-D4.3)

D4.1	Sufficiency of media strategy and activities in the area of research popularisation
The outreach activity refers to a training course for the International Chemistry Olympiad and the preparation for the International Young Physicists' Tournament.	
D4.2	**Publishing activities and its quality**
As indicated in point H1.1, a significant part of the work of this department has been published in high-quality journals. More than 32 of the total 150 publications correspond to D1 (i.e. J. Am. Chem. Soc. (5), Angew. Chem. Int. Ed. (3), Phys. Rev. Lett. (3))	
D4.3	**Participation in professional organisations in the area of research and development**
No comment.	

Other comments of the commission:

3. Biophysical Chemistry

Strengths:
Friendly working environment for all staff who have original ideas and are producing high quality outputs. A good age structure is in place and a multidisciplinary team ensure original ideas are developed and realised.

Weaknesses:
Limited laboratory and office space, although this is a common issue at most institutions. Perhaps some clever space sharing could be developed. Lack of ability to recruit highly qualified people – related to salary as generally it is easy to attract talent to high performing group such as this.

Opportunities:
Building upon outputs there are good opportunities to attract ERC and related funding. This in turn allows one to attract further ERCs and established researchers (if the weaknesses above are overcome).

Threats:
Funding. Always an issue. Instruments are at the heart of the group, so the institute needs to continue to support and invest. Departure of talented people in the department who are attracted to higher paid salaries, again related to weaknesses identified above.

Main criterion: 1. Quality of results (H1.1-H1.5)

H1.1	Quality of selected outputs of Phase I
41 outputs were evaluated from 21,22 FTE in phase 1. The distribution of quality is strongly focussed around 1 and 2. Over 2015-2019 the department submitted 118 papers in high quality journals of international standing, such as: Chemical Reviews, Coord. Chem. Rev, Nature Common, Methods, Protocols; Angewandte, Chemical Science, ACS Nano, Central Science, JACS, PNAS – the list goes on. In summary these are hard journals to get in and the team are doing very well to keep getting outputs accepted in these “go to“ journals.	
H1.2	**Contribution of workers on the outputs reached**
These metrics can be found from the Phase 1 evaluation report.	
H1.3	**Quality of all outputs and results**
This was evaluated in Phase 1. As summarised in H1.1, the outputs are of high quality and of international standing.	
H1.4	**The most valuable discoveries and findings in the fields, their importance for the field**
The department are making important discoveries in their field, some highlights: • *Understanding Membrane Biophysics at an Atomistic Level.* Team members have developed new approaches enabling detection and characterization of lipid nanodomains. Such work has been published in J. Phys. Chem. Lett which led to a review in a high-profile journal (Chemical Reviews). • *Elucidating relationships between dynamics/hydration/function in proteins*. Protein hydration is important in enzymatic catalysis. Team members have been able to	

develop a simple and general steady-state fluorescence spectroscopy method for site-specific analysis of protein hydration which has resulted in a two JACS papers. Again this shows a valuable discovery.

- *Relation between structure, membrane nanoscale organisation and protein function in cells and synthetic models of a cell*. The team have developed a model-free, quantitative clustering analysis to determine the distribution of membrane molecules on cellular plasma membranes. This ground-breaking work was published in Nat. Comms.

H1.5	Contribution of the participation of the authors in large collaborations

There is evidence for excellent internal collaboration with:

1. Department of Computational Chemistry: several publications with Prof. Cwiklik
2. Department of Low dimensional Systems: Kovaricek et al ACS Nano 2018, or in the framework of FET proactive ONEM).
3. Department of Chemistry and Ions in Gaseous Phase: Shestivska et al, RapidCom Mass Spect 2018;

These are good examples and should be further built upon.

In terms of international collaboration, this is very intensive, and these are evidenced by joint grants being funded.

1. GACR DFG project ” Exploring the structure function relationship of membrane pore forming FGF2 oligomers a single molecule approach” 2020 2022 , PI: R. Šachl and W.Nickel
2. Marie Skłodowska Curie ITN : Proton transport and proton coupled transport. 2019 2023, PI P. Pohl, Co PI M. Hof
3. Horizon 2020 (SUNRISE) Coordination and Support Action for the Future EmergingTechnologies 2017 2019 , PI: A. Vlček
4. COST Action CM1405 "Molecules in Motion", 2015 2018, PI: A. Vlček
5. COST Action CM1202 "Supramolecular photocatalytic water splitting", 2013 2016 .
6. FET proactive (ONEM): Optical near field electron microscopy, 2021 2024 , co PI: M.Amaro ,PI: T. Juffmann , Wien

Of course, other “informal” collaborations exist through joint publications.

Again, this is more "good practice" to build upon.

Main criterion: 2. Societal relevance (H2.1-H2.5)

H2.1	Societal relevance of outputs and results pursuant to CAS and institute mission

All research topics of the team are clearly motivated by the needs of society. Their main mission it to understand biologically relevant processes at the molecular level with primary focus on the processes taking place on cellular membranes and their synthetic models. This fits with the key mission of the institute to advance fundamental scientific research backed up by theory and experimental results, the latter the department significantly contributes to.

The main areas of scientific interest during the period 2015-2019:

1. Understanding membrane biophysics at an atomistic level by fluorescence spectroscopy and microscopy.
2. Elucidating relationships between dynamics hydration and function of proteins
3. Relation between structure, membrane nanoscale organisation and protein function in cells and synthetic models of a cell
4. Ultrafast photophysics and photoinduced electron transfer in complex systems
5. Biomimetic electrochemistry at the polarized liquid/liquid interfaces

H2.2	**System functionality for knowledge transfer into practise, its usefulness for society. The impact of the team´s activity on proper practice in society in the area of social sciences and humanities**

No patents have been submitted/filled in this period.

H2.3	**Relation to practice**

The focus of the team is on key methods and instrumentation. For example, the team are able to understand kinetics and mechanisms of photoinduced electron transfer in proteins with covalently appended organometallic photosensitizers in order to develop a comprehensive theoretical model of electron hopping processes.

H2.4	**Participation in AV21 strategy**

This was not given in the documentation nor the presentation. But it is not hard to see that this department contributes, for example in the “diagnostic methods and techniques” and many others. We do not have any concern on this issue.

H2.5	**Cooperation with regions of the Czech Republic**

No information on regional cooperation but through teaching and supervision of students, this will be actively going on.

Further criterion: 1. Position in international and national context (D1.1-D1.3)

D1.1	**Comparison of the team with similar international and national institutes**

The team can be described as internationally leading, a highly prolific and motivated team, the publication in high profile journals and the research outputs place this team as internationally standing, comparable if not better than others found in Europe. More investment, identifying the weaknesses would allow this team to grow further.

D1.2	**Scope and quality of international and national cooperation and the role of the team in such cooperation; engagement in broad international cooperation**

Extensive collaboration as evidenced by papers and funding.

D1.3	**Participation of the workers in scientific community activities (organizing of conferences and workshops, invited lectures, awards)**

The team are invited to give lectures across the globe and have delivered 26 invited lectures and 21 seminars at various institutions. This is a strong output.

Further criterion: 2. Vitality, sustainability and strategy (D2.1-D2.9)

D2.1	Direction in line with the perspective of the planned research directions

The research strategy of the department is to emphasize the physiological and medical relevance of the biomembrane studies, the planned activities build upon recent research and are wholly appropriate.

Planned departmental activities

Thematic goals set for the previous evaluation period will be continued. The activities are

currently supported by several GAČR/MEYS grants, larger EXPRO GAČR (2019 2023) and ECgrants: EU FET proactive (2021 2024), Horizon 2020 (2019 2020) and ITN (2019 2023)

Research topics planned:

1. Concert of lipids, ions and proteins in cell membrane dynamics and function.
2. Nanoscale organisation and protein function in cells
3. Photoinduced charge separation in complex systems.
4. Biomimetic electrochemistry at liquid liquid interfaces.
5. Development of new membrane supports for electron and optical microscopy ONEM and GMIET (GACR).
6. Elucidating Dynamics Function Relationships in Proteins

This is competitive and should realise new funding over the next research period (2020-2024)

D2.2	Assessment of the previous research objectives and their achievement

The last recommendations were to apply for more EU grants and two ERC proposals were diligently submitted.

D2.3	Assessment of implementation of recommendations from past evaluation

Another recommendation was to attract younger members to preserve its importance and world-recognised wealth of fundamental knowledge and experimental know-how. to solve the problems associated with the retirement of elderly team members. Success was achieved through two PhD students (H. Kvapilová, M. Pižl), one postdoc (B.R. Silver) and one young researcher (J. Heyda) joining. Of course, this is an ongoing task, which requires multiple efforts.

In summary the recommendations from the past evaluation have been met.

D2.4	Success in receiving grants

Very successful, 7 running grants and 8 new grants.

D2.5	Adequacy of instrumental equipment

Noting that the focus of the team is on key methods and instruments, a suite of home-made equipment is available:

- Time resolved fluorescence spectroscopy and Fluorescence Lifetime Imaging (FLIM)
- Fluorescence Correlation and Cross Correlation Spectroscopy (FCS and FCCS)
- 3D nanoscope with photoactivated localization microscopy (PALM)
- Basic molecular biology approaches
- Fast transient electrochemical techniques for the polarization of liquid/liquid interfaces
- Dynamic interfacial tension measurements using video image pendant drop method

More investment should be considered to be given to the department from the institute to ensure upkeep and new equipment to be built. The assessment is incomplete as it was not possible to visit the Institute due to the pandemic problems.

D2.6	Effectiveness of management

Hard to access due to not visiting and being able to speak to people nor anything mentioned in the report.

That said, the success of the department can be attributed to effective management.

D2.7	Assessment of professional structure, development strategy and the strategy of keeping best scientists, age structure, career and qualification growth

No comment.

D2.8	Creating work-life balance conditions, assessment of approach towards possible gender issues

No data was provided to allow the assessment of work-life balance. The age of the team is good with a strong cohort of 35-40 coming through to lead the department in the future. Gender statistics were given in neither the presentation nor the report.

D2.9	Relation of the team with regard to the integration, development and sustainability of the research centre funded by the National Programme of Sustainability II.

No evidence/data was provided to assess this.

Further criterion: 3. Cooperation with universities and participation in education (D3.1-D3.6)

D3.1	Scope of cooperation with universities on national and international level

There is good evidence of national and international level collaboration in grants and outputs plus invitations to lectures and seminars.

D3.2	Effectiveness of joint research centres
The available documents do not contain data on the participation of team in joint research centres.	

D3.3	Success rate in supervision of PhD students

The department has 10 PHD students currently being supervised.

Data for success rate:

Type of study	No. of supervisors	No. of consultants	Theses defended 2015-2019
Bachelor	2	1	7
Master	2	2	4
Doctoral	8	11	6

D3.4	Participation of PhD students in the outputs
Yes, the PhDs students participate in the outputs.	

D3.5	Participation of the team in master or bachelor studies
Yes, the team supervises MS and BS students, as can be seen in the table above**.**	

D3.6	Assessment of cooperation intensity with universities in the form of teaching
The team deliver lectures and seminars and Charles' University, UPOL, Uni of South Bohemia in CB and UCT Prague.	

Further criterion: 4. Outreach activities (D4.1-D4.3)

D4.1	Sufficiency of media strategy and activities in the area of research popularisation

Very active.

National media

•Czech Television, 2016: GM $_1$ ganglioside inhibits β amyloid oligomerization induced by sphingomyelin

•Czech Television , 2017: Quantifying protein densities on cell membranes using super resolution optical fluctuation imaging.

•Czech Television , 2018: Molecular Gating of an Engineered Enzyme Captured in Real Time

D4.2	Publishing activities and its quality
Very active, 118 papers in high impact journals.	

D4.3	Participation in professional organisations in the area of research and development
There were no data concerning this activity.	

Other comments of the commission:

4. Structure and Dynamics in Catalysis

Strengths:
- Optimum age structure of the team with young talented scientists and senior researches
- Good gender balance
- Adequate instrumental equipment for research development
- Good balance between the different stages of research in the field of catalysis

Weaknesses:
- Relatively low number of team members
- Very low number of PhD students
- Low effectivity in grants acquisition for research and update of equipments

Opportunities:
- Recruiting PhD students
- Acquisition of an industrial partner
- Obtaining long-term funding
- Competitive at the international/EU level

Threats:
- Poor stability of the team, many members on short-term contracts
- Insufficient funding, funding in short-term scale

Main criterion: 1. Quality of results (H1.1-H1.5)

H1.1	Quality of selected outputs of Phase I
Most of publications correspond to D1, Q1 and Q2, including some top chemistry journals	
H1.2	**Contribution of workers on the outputs reached**
Participation of team members is evident in most of the outputs, and it is essential.	
H1.3	**Quality of all outputs and results**
Very high. As mentioned above, that includes top chemistry journals (Nature Chemistry, Angew. Chemie, ACS Catalysis, etc.)	
H1.4	**The most valuable discoveries and findings in the fields, their importance for the field**
The group has developed some interesting methodologies for the synthesis of tailored micro and mesoporous solids. This has yielded many new zeolite materials with potential applications in new catalytic processes.	
H1.5	**Contribution of the participation of the authors in large collaborations**
The group is a member of ERIC (European Research Institute for Catalysis), together with other major European catalytic research centres.	

Main criterion: 2. Societal relevance (H2.1-H2.5)

H2.1	Societal relevance of outputs and results pursuant to CAS and institute mission
The impact on society of the research carried out by the catalysis group is unquestionable. Important and relevant hot topics are addressed by the group.	
H2.2	**System functionality for knowledge transfer into practise, its usefulness for society. The impact of the team´s activity on proper practice in society in the area of social sciences and humanities**
No comment.	
H2.3	**Relation to practice**
Some collaborations with national industrial partners exist. In any case, it is not the essential part of its activity.	
H2.4	**Participation in AV21 strategy**
The group participates in AV21, although not as a leader.	
H2.5	**Cooperation with regions of the Czech Republic**
No comment.	

Further criterion: 1. Position in international and national context (D1.1-D1.3)

D1.1	Comparison of the team with similar international and national institutes
The group is very well positioned internationally. It competes in quality with the best centres in the world in the area of catalysis.	
D1.2	**Scope and quality of international and national cooperation and the role of the team in such cooperation; engagement in broad international cooperation**
As mentioned above, the participation in ERIC is evidence of a great engagement in the cooperation worldwide.	
D1.3	**Participation of the workers in scientific community activities (organizing of conferences and workshops, invited lectures, awards)**
The group maintains a certain level of activity by participating in courses, congresses, etc.	

Further criterion: 2. Vitality, sustainability and strategy (D2.1-D2.9)

D2.1	Direction in line with the perspective of the planned research directions
The core of the group is well oriented towards the research on zeolites. As stated before, they are in a very good position to develop good science. It is not clear how the planned splitting of the team will improve the perspective.	

D2.2	Assessment of the previous research objectives and their achievement
The evolution of the team has been very positive, significantly increasing the quality of the outputs.	
D2.3	**Assessment of implementation of recommendations from past evaluation**
No comment.	
D2.4	**Success in receiving grants**
Considering the size of the team, there is a relatively low success in obtaining grants.	
D2.5	**Adequacy of instrumental equipment**
The team has the necessary equipment for its research. Its updating and renewal must be ensured.	
D2.6	**Effectiveness of management**
It appears to be suitable for the development of its activities.	
D2.7	**Assessment of professional structure, development strategy and the strategy of keeping best scientists, age structure, career and qualification growth**
The structure and distribution of the team is good. The number of members in the 30-45 year age group demonstrates a good recruitment policy and ensures continuity in the coming years. The number of students, however, is very low.	
D2.8	**Creating work-life balance conditions, assessment of approach towards possible gender issues**
The number of women (>65%) is unusually high. Shows a non-discriminatory gender policy.	
D2.9	**Relation of the team with regard to the integration, development and sustainability of the research centre funded by the National Programme of Sustainability II.**
No comment.	

Further criterion: 3. Cooperation with universities and participation in education (D3.1-D3.6)

D3.1	Scope of cooperation with universities on national and international level
The group has relevant participations with national universities. Occasional participation in the international field (University of Palermo).	
D3.2	**Effectiveness of joint research centres**
Not reported.	
D3.3	**Success rate in supervision of PhD students**
Considering the number of researchers in the group (FTE), the number of PhD students is very low.	

D3.4	Participation of PhD students in the outputs
Appropiate.	
D3.5	**Participation of the team in master or bachelor studies**
Once again, and considering the FTE, the number of students is very low.	
D3.6	**Assessment of cooperation intensity with universities in the form of teaching**
As indicated above, the team participates in a significant number of courses at national universities, mainly related to the topics in which they have expertise.	

Further criterion: 4. Outreach activities (D4.1-D4.3)

D4.1	Sufficiency of media strategy and activities in the area of research popularisation
The outreach activity, specially in relation to photocatalysis, is very relevant. There is no evidence of activities in other areas.	
D4.2	**Publishing activities and its quality**
Appropriate publishing activity in the field of photocatalysis.	
D4.3	**Participation in professional organisations in the area of research and development**
No comment.	

Other comments of the commission:

5. Molecular Electrochemistry and Catalysis

Strengths:
Good representation of young workers. Well-designed, vertically integrated research programs. Student participation in research programs. International collaborations and visibility.

Weaknesses:
Instrumentation needs replacement. No large EU or other international grants to support research. Few mid-range (40-50 year old) staff. Gender balance of staff.

Opportunities:
International collaborations ripe to be strengthened. European research council funding to be pursued. Funding for new NMR instrumentation, replacement of other failing instrumentation.

Threats:
Low salaries make it difficult to retain top young talent. Old instrumentation may fail.

Main criterion: 1. Quality of results (H1.1-H1.5)

H1.1	Quality of selected outputs of Phase I
Of the 19 outputs evaluated in phase 1 from this group, 12 were published in journals from the 1st quality quartile of journals in the area of organometallic and electrochemistry. Two more were published in quartile one journals in the areas of organic and physical chemistry. The overall quality of the outputs selected for evaluation in Phase 1 was high.	
H1.2	**Contribution of workers on the outputs reached**
The research outputs were principally contributed by workers from the Institute. In particular the electrochemistry studies were carried out entirely in this group, along with most of the synthesis and computational work. Collaborations contributed some synthetic work and some computational work. The Molecular Electrochemistry and Catalysis group contributed the majority of the work described.	
H1.3	**Quality of all outputs and results**
Over the course of the evaluation period, a total of 87 journal articles were published by the group. 17 of these papers were published in journals of Quartile 1, and 6 in journals of Quartile 2. The remaining 64 publications were in 3rd and 4th quartile journals. Efforts should be continued to publish a larger fraction of the growing output of the group in higher impact journals.	
H1.4	**The most valuable discoveries and findings in the fields, their importance for the field**
Many important discoveries and findings resulted from the work of this group over the reporting period. We can mention two examples and their importance to the field here. The first is recent work on singlet fission, the preparation of new molecules that can enhance the photon to electron yield of organic solar cell systems. Synthesis and characterization of promising fluorinated 1,3-diphenylisobenzofurans was recently accomplished. These sorts of molecular synthetic studies will impact renewable energy production. The second example is the development of hydrosilane-$B(C_6F_5)_3$ adducts used as activators in zirconocene based ethylene polymerization catalysis. This sort of work to improve catalytic activity of molecular catalysis by obtaining an understanding of the	

detailed mechanism of catalytic action, will have enormous economic impact given the amount of ethylene polymerization that is carried out worldwide.

H1.5	Contribution of the participation of the authors in large collaborations
The group has no current participation in large collaborations. They are indeed active in a number of smaller collaborations, involving one or two additional researchers or groups from international institutes.	

Main criterion: 2. Societal relevance (H2.1-H2.5)

H2.1	Societal relevance of outputs and results pursuant to CAS and institute mission
Much of the work of this group has significant societal relevance. Examples are the many research studies impacting on the details of molecular catalysis, with direct relevance to large scale chemical manufacture. In addition, electrochemical studies have led to the development of unique and highly sensitive electrochemical detectors and sensors. Also, molecular synthesis of cancer therapeutics has resulted from studies by this group.	
H2.2	**System functionality for knowledge transfer into practise, its usefulness for society. The impact of the team´s activity on proper practice in society in the area of social sciences and humanities**
In so far as a robust chemical industry affects the social sciences through a strong economy and a stable political system, the work of this group is very useful for society.	
H2.3	**Relation to practice**
No Comment	
H2.4	**Participation in AV21 strategy**
No comment	
H2.5	**Cooperation with regions of the Czech Republic**
Many instances of cooperation with various universities and institutes in the Czech Republic. Collaboration with students and faculty at the Charles University in Prague, with the Masaryk University and the Masaryk Cancer Institute in Brno, and with the University of Chemistry and Technology in Prague.	

Further criterion: 1. Position in international and national context (D1.1-D1.3)

D1.1	Comparison of the team with similar international and national institutes
This is a strong internationally recognized team.	
D1.2	**Scope and quality of international and national cooperation and the role of the team in such cooperation; engagement in broad international cooperation**
There are a number of international collaborations, with workers in the USA (University of Colorado, Brookhaven National Laboratory) as well as in Europe, Africa, and Asia (TU Graz, University Rey Juan Carlos, Madrid, University of Gujarat, India, and University of Ngauoundere in Cameroon). The group has a broad and high quality engagement with	

international partners.	
D1.3	**Participation of the workers in scientific community activities (organizing of conferences and workshops, invited lectures, awards)**
A long list of participation of group members in the organization of conferences and workshops, and scientific community activities in general. Several invited lectures were given, and Jiri Ludvik was awarded the Silver Medal of the Faculty of Sciences by the Charles University, Prague. This is to be expected for an active, well regarded research group.	

Further criterion: 2. Vitality, sustainability and strategy (D2.1-D2.9)

D2.1	**Direction in line with the perspective of the planned research directions**
The group has followed well along the line of the planned research directions, appropriately modifying goals and directions as the science develops.	
D2.2	**Assessment of the previous research objectives and their achievement**
The research objectives planned at the close of the last review were appropriate and provided a reasonable challenge for the group. They have successfully achieved their goals for the most part.	
D2.3	**Assessment of implementation of recommendations from past evaluation**
The team management and the staff have successfully addressed the recommendations of the past evaluation. They have worked to replace (and shift workload) of senior scientists with younger researchers to address the age distribution of the team. The introduction of new research themes, such as the singlet fission work, and the active effort to publish the work of the group in more visible and higher impact journals is to be commended. The shift in emphasis of the molecular catalysis work from fine chemical synthetic routes to catalysis more relevant to high volume polymer production has been effective. The effort to shift the balance between permanent staff and staff supported on research grants is ongoing.	
D2.4	**Success in receiving grants**
Ten grants were active during the review period, with six of these awarded during the last part of the review period. This bodes well for continued success in attracting grants going forward, and also supports the shift in scientific focus signaled by the introduction of new areas of research, as noted above.	
D2.5	**Adequacy of instrumental equipment**
It is clear that instrumentation must be continuously upgraded. This will become an urgent problem in the near future, if funds are not made available to address this threat.	
D2.6	**Effectiveness of management**
The management has been effective in the face of difficult budgetary constraints, and the challenge to attract and retain young researchers who have better prospects in other parts of Europe and overseas.	
D2.7	**Assessment of professional structure, development strategy and the strategy of keeping best scientists, age structure, career and qualification growth**
The structure is improving, but there are still challenges in retaining and developing the best young talent.	

D2.8	Creating work-life balance conditions, assessment of approach towards possible gender issues
Further work can be done to address the gender imbalance in the team. This is a difficult problem, but can be addressed by making sure that all staff are supported to be successful in their work, and have a welcoming and supportive workplace environment. Progress has been made.	
D2.9	**Relation of the team with regard to the integration, development and sustainability of the research centre funded by the National Programme of Sustainability II.**
No comment.	

Further criterion: 3. Cooperation with universities and participation in education (D3.1-D3.6)

D3.1	Scope of cooperation with universities on national and international level
Good cooperation with universities on the national level. Teaching and research mentorship arrangements with Charles University, Masaryk University in Brno, and the University of Chemistry and Technology in Prague.	
D3.2	**Effectiveness of joint research centres**
No active joint research centres.	
D3.3	**Success rate in supervision of PhD students**
Six PhD dissertations were successfully defended during the period of the review.	
D3.4	**Participation of PhD students in the outputs**
A large majority of the work of the group involves PhD students. Their contributions and participation in the research outputs of the group are substantial, many being first authors on the research publications of the group. This is as it should be in an academic research group.	
D3.5	**Participation of the team in master or bachelor studies**
A total of ten masters and bachelor's theses were defended during the review period. Members of the team participated as both supervisors and consultants (co-supervisors) for these BSc and MSc students.	
D3.6	**Assessment of cooperation intensity with universities in the form of teaching**
Significant cooperation in teaching with Charles University and the University of Chemistry and Technology in Prague.	

Further criterion: 4. Outreach activities (D4.1-D4.3)

D4.1	Sufficiency of media strategy and activities in the area of research popularization
Significant participation in educational outreach activities targeted to high school students and teachers, and to the general public.	

Media interviews with radio, television, and print media regarding the work of the institute.	
D4.2	**Publishing activities and its quality**
Materials for preparation for International Chemistry Olympiad, and materials for electrochemistry summer camp were published. Useful and of high quality.	
D4.3	**Participation in professional organizations in the area of research and development**
Active in organizing and in attendance at conferences and workshops relevant to the research efforts of the laboratory. Including conferences with a focus on graduate student participation and recognition.	

Other comments of the commission:

6. Electrochemical Materials

Strengths:
Good scientific level of outputs, good external funding, important societal impact of research themes and good international contacts

Weaknesses:
Limited institutional subsidy, lack of administrative and technical positions putting non-productive burden on scientists, aging of some key instruments.

Opportunities:
Recruit motivated new collaborators, find adequate replacement of colleagues after their retirement, receive support for new experimental infrastructure from CAS, JHIPC and external resources.

Threats:
Problems in attracting excellent students from universities, risk of team shrinkage, if new grants and/or adequate institutional funding were not available, difficult access to students at universities, departure of talented people abroad.

Main criterion: 1. Quality of results (H1.1-H1.5)

H1.1	Quality of selected outputs of Phase I
Most outputs (62%) are located in the first and second quartile of all published articles. However, only 8 were in the first Decile. It must be emphasized, however, that it was also known to articles published in leading magazines such as: Energy Environ. Sci. (IF = 30.29), Accounts Chem. Res. (IF = 20.83), Nature Astronomy (IF = 11.52), and J. Am. Chem. Soc. (IF = 14.61). These are not specialized magazines in the field of electrochemistry, but the other outputs were in such periodicals as Electrochim. Acta (13 items), Carbon (12 Items) And J. Phys. Chem. C (10 items). Note that more than half of the outputs are included in the 3 quartiles.	
H1.2	**Contribution of workers on the outputs reached**
Exactly half of the authors outputs from first quartile comes from the team. This is evidenced by the Team's involvement in the conducted research, as well as about cooperation with other research groups.	
H1.3	**Quality of all outputs and results**
The scientific activities of the Department are devoted to fundamental studies and applied research in the field of solar cells, Li-ion batteries and pollution control. The quality of outputs is high and the published results make a significant contribution to the development of solar cells and optoelectronics.	
H1.4	**The most valuable discoveries and findings in the fields, their importance for the field**
To the most important results that can find practical application I would like to find the discovery of protective coating based on thin and electrically conductive nanocrystalline Boron-Doped Diamond (BDD) layers deposited on Si photo electrodes over a wide pH	

range (1-14) in aqueous electrolyte solutions. The protecting layer maintains an efficient charge carrier transfer from the underlying silicon to the electron solution. (ACS Applied Materials & Interfaces, 10, 2019, 29552-29564). This is important from the point of view of fabricating cheap photo-cells.

Second important achievement applies to the production of new structures of Perovskite Quantum Dots (PQDS) and graphene, which allowed light-emissive, ultrasensitive, ultrafast, and broadband vertical phototransistor that can simultaneously act as an efficient photodetector and light emitter within a single device. The phototransistor was moisture - insensitive, environmentally stable, light-emissive, ultrafast, and ultrasensitive (ACS Nano, 2019, 13, 12540-12552). This can be a useful route for dual-functional optoelectronic devices.

H1.5	Contribution of the participation of the authors in large collaborations

The cooperation of the group with national and foreign scientific centers was very intense and efficient. Significant part of outputs resulted from joint research, and for noteworthy, the fact that both of the publications mentioned above containing the most important achievements are the result. It deserves to be emphasized by the fact of cooperation with an excellent EPF-Lausanne scientific center, CH managed by Prof. M. Grätzel, with 10 joint publications, including 2 publication where the group members were the first and corresponding authors. The key responsibility of the team was application of graphene as cathode catalyst in dye-sensitized solar cells. They participated in other international programs like: COST Action CM1104 “Reducible oxide chemistry, structure and functions”; EU-Asia cooperation in 3 different international consortia carrying out research activities aimed at solving the task of photocatalysis (4G PHOTOCAT), batteries (AdOX) and perovskite solar cells (PPL).

Main criterion: 2. Societal relevance (H2.1-H2.5)

H2.1	Societal relevance of outputs and results pursuant to CAS and institute mission

The key mission of the institute is thus largely to advance fundamental scientific research involving original ideas that are tested by state-of-the-art theoretical and experimental methods with the aim to reach conclusions based on reliable data, observation and inference. The Department mainly deals with basic research, however, aimed at the possibility of implementing them to industry. The team fulfils this role well. It participated in two AV21 strategy programs: "Efficient Energy Conversion and Storage" and "Molecules and Materials for Life". Published results on increase of efficiency of photocatalytic processes, new materials for photovoltaic paints and functional surfaces for environmental protection, Li-Ion and Na-Ion batteries, development of hybrid materials and thin films for direct solar splitting of water, dye-sensitized and perovskite solar cells are fit well into both programs.

H2.2	System functionality for knowledge transfer into practise, its usefulness for society. The impact of the team´s activity on proper practice in society in the area of social sciences and humanities

The Institute does not have the possibility of technological research, however, the members of the team patent useful results in the country and cooperate with relevant scientific and industrial units that may be interested in their research results. The aim of their research is to improve human life related to the transition to green energy sources related to the use of solar energy.

H2.3	Relation to practice
The research subject of the team is to solve significant problems related to the processing and storage of solar energy as it concerns dye-sensitized and perovskite solar cells and lithium-ion or sodium-ion battery. A proof of concept of a 4V cell with capacity of 80-100 Wh was developed in collaboration with an industrial partner, which is a component of the 48V Li accumulator. As part of multilateral international cooperation, a floating photocatalyst was obtained with sorption for solar cleaning of water in Vietnam which is contaminated with the remains of post-war pollution, including dioxin or DDT. Solar self-cleaning facade paint has also been developed, which has been tested in the humid climate of Vietnam. Group members obtained 10 patents and 7 utility models, and was awarded by Czech Intellect for the Invention Category.	
H2.4	**Participation in AV21 strategy**
The research subject of the team fits well in AV21 strategy. You can list here at least 2 programs launched in 2015 "Efficient Energy Conversion and Storage" and "Molecules and Materials for Life", which cover their research topics. It should also be added that some of the tasks carried out by the team in 2015-19 fit well in the new subject of the AV21 Strategy program, which was launched in 2020, called "Water for Life".	
H2.5	**Cooperation with regions of the Czech Republic**
No information on regional cooperation, but the research group works intensively with the Charles University in Prague and with other national universities for example UCT Prague and Palacky University in Olomouc. Members of group often give lectures and use contacts to recruit PhD students.	

Further criterion: 1. Position in international and national context (D1.1-D1.3)

D1.1	Comparison of the team with similar international and national institutes
The scientific level of the research group is comparable to the best units with the same research subject, from neighbouring countries with a similar level of development, such as Poland, Hungary or Lithuania. The comparison to similar units in countries such as Germany, France or Great Britain is a bit worse. This is mainly due to the difference in the level of funding, which allows to recruit the best scientists around the world, including from the Czech Republic.	
D1.2	**Scope and quality of international and national cooperation and the role of the team in such cooperation; engagement in broad international cooperation**
The international cooperation of the group is very wide and basically covers the entire research field. In the years 2015-19, they obtained 5 international grants, the scope of which was related to: Dye-sensitized and perovskite photovoltaics, EPF-Lausanne, CH (M. Grätzel); Nanodiamond, University of Hasselt, BE; Mechanical deformation in 2D materials, FORTH / ICE-HT Patras, GR; Electron Injection into Ti (IV) Oxides, Uni Vienna, AT; Nano-pillar arrays; wrinkling in 2D materials, IPHT Jena, DE; Li-batteries, SAS Bratislava, Uni Warsaw, Uni Shiuzoka, JP; Perovskite photovoltaics, SAS Bratislava, SK, Wigner Institute, Budapest, HU, Military Inst. of Technology, PL Wroclaw, Uni Korea, Seoul, KR. The collaboration turned out to be fruitful as 28 outputs were obtained. Cooperation with local Universities is wide and it should be emphasized that Prof. Kavan is the member of Scientific Council of Charles University.	

D1.3	Participation of the workers in scientific community activities (organizing of conferences and workshops, invited lectures, awards)

The members of the group organized and participated in organization of 15 international icoferences like: 49th Heyrovský Discussion on Electrochemical Interfaces at the Nanoscale, 29 May - 2 June 2016; 11 CEMME 2019 Chemnitz, 17– 19 November 2019, Chemnitz, Germany; The 66th Annual Meeting of International Society of Electrochemistry (ISE), Taipei, Taiwan, October 2015; The 22nd International Conference on Semiconductor Photocatalysis and Solar Energy Conversion, Clearwater Beach, Florida November 13-16, 2017; Semiconductor Photocatalysis & Solar Energy Conversion SPASEC-20 San Diego, USA 15-19.11.2015 or Visegrad-4/Japan Workshop on Electrochemical properties of advanced materials for next generation batteries, 5-6 October 2018, Košice, Slovakia. They participated in Workshop of Senate Parliament of the Czech Republic on “Potential of Lithium Mining and Applications in Advanced Technologies”. They have been invited to give 14 invited lectures at international conferences and university seminars for examples: “Graphene and its interfaces” The Nanosci. Summer School, 2018, Yachay, Equador; “Multi-modal in-situ Raman spectroscopy of 2D materials”, Raman Fest 2019, Oxford; “Wrinkle patterns at conformal graphene-polymer interfaces”, 30th Int. Conf. on Diamond and Carbon Materials 2019, Seville, Spain; “Deformation in 2D materials” NanoNet Int. Conference 2019, Dresden, Germany; “Quasi-2D liquid nanofoams on water-immersed solid surface” Nanobubble 2018, Suzhou, China; Nanomaterials based on Ti(IV) Oxides: Applications for Electrochemical Energy Conversion and Storage”, ISNT, Tainan, Taiwan, 2016; “Engineering of oxide semiconductors: Solar fuel and perovskite photovoltaics”, E-MRS-Fall Meeting, Warsaw, Poland, 2018; “Conduction band in semiconducting oxides: Applications in perovskite photovoltaics and beyond”, 10th SPEA, Almeria, Spain, 2018; “Perovskite and dye-sensitized solar cells: What can we learn from electrochemistry?” 23rd SPASEC, Shanghai, China, 2018; “Titania Single-Crystal Electrode: Energy Conversion and Storage Fundamentals”, NPM-4, Antwerp, Belgium, 2018; “Electrochemical performance of sol-gel TiO2 based ternary oxides for Na ion batteries” E-MRS-Fall Meeting, Warsaw, Poland, 2018.

Three workers was awarded: Ladislav Kavan (2017): Frantisek Behounek Prize for promoting Czech Republic in European research area (2019); Silver medal of Faculty of Science, Charles University Prague; J. Jirkovský (2016): Innovation of the Year, Association of Innovative Entrepreneur and O. Frank (2016): Neuron Impulse for Physics.

Further criterion: 2. Vitality, sustainability and strategy (D2.1-D2.9)

D2.1	Direction in line with the perspective of the planned research directions

The group's research plans are mainly a continuation of the subject matter carried out in the assessed period, especially under the AV21 Strategy. These include, among others, Li-sulfur batteries, nano-Si, Si/graphene anodes for Li/Na-ion, mechanism of photo-degradation of pollutants, focus on harmful intermediates; new photocatalysts, nano-sized domains controlling the electrochemical gas evolution kinetics and solar fuel by photo-assisted electrolysis of water.

D2.2	Assessment of the previous research objectives and their achievement

In the previous period, the research subject was similar and conducted correctly, and the scientific achievements were sufficient. They provided a good basis for the development of research conducted in the reporting period.

D2.3	Assessment of implementation of recommendations from past evaluation

The main recommendation of the Committee in the previous evaluation, was that the

Institute should find means of funding the new advanced instrumentation, which the group depend critically for its further development. The recommendation concerned not the team, but the entire Institute. The group obtained a new instrument for atomic layer deposition and the advanced setup for tip-enhanced spectroscopy, which greatly improved the experimental possibilities.	
D2.4	**Success in receiving grants**
The team received 20 grants from national and international agencies. In each reporting year, there were from 8 to 10 grants, which ensured the continuity of financing research, and the possibility of employing additional staff and doctoral students. The ability of the group's employees to obtain financing from foreign sources is noteworthy, including participation in the very prestigious European program WP11, which concerns the implementation of solar and fuel energy generation devices based on graphene and 2D crystals and hybrid systems.	
D2.5	**Adequacy of instrumental equipment**
Laboratory equipment is adapted to the research subject matter. It consists of the following apparatus: - Syntheses: glove boxes, vacuum lines, ALD set up. - Electrochemistry, impedance spectroscopy, battery testing. - Raman spectroscopy and spectroelectrochemistry. - AFM / STM in liquids (electrolyte sol.) & Photoexcitation - AFM with quantitative nanomechanical mapping and coupled AFM -Raman (TERS, photocurrent mapping). - Ellipsometry with μm resolution and Photoelectrochemistry, solar simulator, IPCE/QE/IV. Such a set of apparatus is sufficient for the implementation of further research plans, but the assessment of this fact is incomplete as it was not possible to visit the Institute due to the pandemic problems.	
D2.6	**Effectiveness of management**
Scientific effects, the development of young staff and the awards obtained prove the good management of the research group. This fact may be confirmed by the ability of the group's members to obtain and correctly implement national and international grants.	
D2.7	**Assessment of professional structure, development strategy and the strategy of keeping best scientists, age structure, career and qualification growth**
Comparing the two periods of assessment of the group, it can be seen that it is able to adapt to the changing conditions in which it operates. It is a good sign that the planned strategy will be properly implemented. Maintaining the research potential, staff development and the ability to acquire outstanding scientists depends mainly on financial conditions. Seeing the group's ability to obtain national and international grants we assess their possibilities positively.	
D2.8	**Creating work-life balance conditions, assessment of approach towards possible gender issues**
The gender issue has already been met as approximately 54% of the group are women.	
D2.9	**Relation of the team with regard to the integration, development and sustainability of the research centre funded by the National Programme of Sustainability II.**
Research on new energy sources (solar energy) and photocatalysts (water purification and	

the extraction of hydrogen from water decomposition) correlate well with two of the four main tasks of the National Program of Sustainability II. These are Air Protection and Water Protection.

Further criterion: 3. Cooperation with universities and participation in education (D3.1-D3.6)

D3.1	Scope of cooperation with universities on national and international level
The team actively collaborates with several national universities, including the (best in Czech Republic) Charles University in Prague. Collaboration is mainly based on joint research, which allows better use of the research infrastructure. In addition, several employees give lectures on Nanomaterials, Microscopic and spectroscopic methods and Environmental photochemistry for students of this University. During the reporting period, the group's employees gave a close to 500 lectures or seminars at 7 Czech Universities and the University of Dresden. 50 early stage researchers and 9 master students from Universities participated in the research conducted as part of the group's scientific work.	
D3.2	**Effectiveness of joint research centres**
The available documents do not contain data on the participation of team in joint research centres.	
D3.3	**Success rate in supervision of PhD students**
In the period under review, 4 PhD thesis were defended, in which supervisor or consultant was a member of team. It is not much, and such an experienced research group could promote more doctorates. The problem is that the group depends on being able to get good candidates from universities.	
D3.4	**Participation of PhD students in the outputs**
PhD students participating in the research, regardless of whether they were group members or coming from universities, were always cited as co-authors of joint publications. They contributed significantly to the scientific outputs generated by the team.	
D3.5	**Participation of the team in master or bachelor studies**
In the period under review, 2 Bachelor and 1 Master thesis were defended, in which supervisor or consultant was a member of team. It is not much, and such experienced research group could promote more. The problem is that the individual depends on the possibility of getting good candidates from the universities.	
D3.6	**Assessment of cooperation intensity with universities in the form of teaching**
The members of the department: Kavan, Janda and Jirkovský delivered 6 different courses on Nanomaterials, Microscopic and spectroscopic methods and environmental photochemistry tought at Charles University, UCT Prague and Palacký University in Olomouc.	

Further criterion: 4. Outreach activities (D4.1-D4.3)

D4.1	Sufficiency of media strategy and activities in the area of research popularisation
The team was active in National Media, presenting 6 programs on radio and TV stations such as Czech Radio, Czech Radio Plus, Czech TV and CT 24, presenting information on Graphene and Lithium batteries. Interesting results are also continuously shared on social networks.	
D4.2	**Publishing activities and its quality**
Publishing activity is very good. During the reporting period, they published 126, including several review articles, of which a publication in the popular journal Accounts of Chemical Research should be mentioned.	
D4.3	**Participation in professional organisations in the area of research and development**
There were no data concerning this activity.	

Other comments of the commission:

7. Electrochemistry at the Nanoscale

Strengths:
Good international standing and contacts, age structure of the team, unique instrumentation development, multidisciplinary research, focus on original ideas.

Weaknesses:
Lack of laboratory and office space, difficulties in recruiting highly qualified people, dependence on organic synthesis outside the Institute.

Opportunities:
Recruiting motivated people, carrier growth encouraging new directions, larger collaborations.

Threats:
Insufficient funding, irreparable failure of the instruments, difficult access to students at universities, departure of talented people abroad.

Main criterion: 1. Quality of results (H1.1-H1.5)

H1.1	Quality of selected outputs of Phase I
The group focused its research to the fundamental understanding of charge transfer and transport processes at the interface of designed and tailored molecular systems and electrode materials down to the nanoscale level. The in-depth characterization of molecular systems allows developing building blocks for molecular electronic devices, electrochemical sensors or electrocatalysts. During the evaluation period, the Department of Electrochemistry at the Nanoscale published 155 papers in impacted scientific journals. Approximately 1/3 outputs (38%) are located in the first and second quartile of all published articles. Moreover, 11 were in the first Decile. It must be emphasized, however, that there were numerous publications in leading journals such as: J. Am. Chem. Soc. (IF = 14.61), Angew. Chem. Int. Ed. (IF = 12,959), Nanoscale (IF = 6,895). These are not specialized magazines in the field of electrochemistry, but the other outputs were in such leading periodicals as Electrochim. Acta, ChemElectroChem (15 items), Sensorsand Actuators B, Electroanalysis, J. Electroanal. Chem. (28 Items) and Chem. Comm., Chem. Eur. J. (5 items).	
H1.2	**Contribution of workers on the outputs reached**
Exactly a quarter of the authors outputs from first quartile comes from the team. This proves the commitment of the group's employees to large research teams, necessary in the case of solving multidisciplinary scientific problems.	
H1.3	**Quality of all outputs and results**
The scientific activities of the team are devoted to the fundamental understanding of charge transfer and transport processes and related phenomena at the interface of newly designed and tailored molecular systems and novel electrode materials down to the nanoscale level. The quality of outputs is high and the published results make a significant contribution to the development of molecular electronics and sensors.	
H1.4	**The most valuable discoveries and findings in the fields, their importance for the field**
Research group members conducted research to understand the electron transfer –	

initiated processes at molecular level with focus on the systems important in catalysis, electrosynthesis, molecular electronics and biology. Among the published 155 papers, 2 book chapters and 2 patents, the following results deserve attention:

- Discovery of the promising group of molecules, based on extended viologens, serving as conducting wires in future molecular electronic devices (*J. Phys. Chem. C* 2015, 119, 32, 18056–18065).

- The conductivity of molecular wires terminated with fullerene anchors has been shown to be dependent on the pressure exerted on the junction, which paves the way for reversibility of mechanically controlled molecular switches (*J. Am. Chem. Soc.* 2015, 137, 6, 2318–2327).

- discovery of novel tripodal anchoring groups, based on 9,9´-spirobifluorene and tetraphenylmethane, implemented into structures of molecular wires (*Chem. Eur. J. 22 (2016) 13218*-13235; *Nanoscale, 2019, 11, 12959-12964; Chem. Commun. 55 (2019) 3351*-3354*)*.

- discovery of the two-electron activation mechanism of bipyridine complexes with dipyridylamine ligand with an uncommon one electron activation and higher catalytic efficiency towards electrochemical reduction of CO_2 (*ChemElectroChem, 2 (2015) 1372-1379; Chem. Eur., J. 23 (2017) 4782-4793*).

- the implementation of boron doped diamond electrodes, carbon screen printed electrodes and carbon and metal based conductive composites processable by 3D printing electrode to multipulse amperometric detectors for biologically and environmentally important substances, including genotoxic derivatives and tumor markers (*Sens. Actuators B Chem. 227 (2016) 263-270; Analytica Chimica Acta 2019, 1087, 44-50*).

H1.5	Contribution of the participation of the authors in large collaborations

The cooperation of the group with national and foreign scientific centres was very broad and efficient. Significant part of outputs resulted from joint research, and for noteworthy, the fact that some of the publications mentioned above containing the most important achievements are the result. It deserves to be emphasized by the fact of cooperation with excellent universities as Karlsruhe Institute of Technology (Germany), Universities of Basel and Bern (Switzerland), University Turin and University of Pisa (Italy), University Stuttgart, University of Regensburg and Freie Universität Berlin (Germany), Université de Paris (France) and University of Porto and University of Coimbra (Portugal). This collaboration resulted in 51 joint publications. At the national level the group members collaborated with Charles University in Prague, University of Chemistry and Technology Prague, Palacký University in Olomouc, University of Pardubice and research institutes of the Czech Academy of Sciences like Institute of Organic Chemistry and Biochemistry, Biophysical Institute, Institute of Physics and Institute of Microbiology.

Main criterion: 2. Societal relevance (H2.1-H2.5)

H2.1	Societal relevance of outputs and results pursuant to CAS and institute mission

The key mission of the institute is thus largely to advance fundamental scientific research involving original ideas that are tested by state-of-the-art theoretical and experimental methods with the aim to reach conclusions based on reliable data, observation and inference. The Department mainly deals with basic research on charge transfer and transport processes and related phenomena at the interface electrode solution. These studies may be relevant for future molecular electronic devices (molecular conductors and switches) as well as electrocatalysts to tackle challenges of the

anthropogenic climate change (production of hydrogen as a sustainable fuel, mitigation of global warming by the reduction of atmospheric carbon dioxide). Their research may be utilized in electrochemical sensing of environmentally relevant substances like pollution markers and genotoxic compounds and fully fit into the implementation of the mission of the CAS and Institute.

H2.2	System functionality for knowledge transfer into practise, its usefulness for society. The impact of the team´s activity on proper practice in society in the area of social sciences and humanities

The Institute does not have the possibility of technological research, however, the members of the team patent useful results in the country and cooperate with relevant scientific and industrial units that may be interested in their research results. The aim of their research is to improve human life related to the transition to green energy sources related to the use of solar energy.

H2.3	Relation to practice

An increased productivity of realized electrochemical experiments and increased amount of information gained within one measurement by applying an automatic device constructed according to their invention, which can be used in industry was developed.

H2.4	Participation in AV21 strategy

The research subject of the Department fits well in AV21 strategy. You can list here at least 2 programs; "Molecules and Materials for Life" and “Land Save and Recovery”, which cover their research topics, where you can find research on new catalysts for electrochemical reduction of CO_2 or new materials for sensors of broad range of biologically and environmentally important substances.

H2.5	Cooperation with regions of the Czech Republic

No information on regional cooperation, but the research group works intensively with the Charles University in Prague and with other national universities and Institutes, for example UCT Prague, Palacky University in Olomouc and Institute of Physics.

Further criterion: 1. Position in international and national context (D1.1-D1.3)

D1.1	Comparison of the team with similar international and national institutes

The scientific level of the research group is comparable to the best units with the same research subject, from neighbouring countries with a similar level of development, such as Poland, Hungary or Slovakia. The comparison to similar units in countries such as Germany, France or Great Britain is a bit worse. This is mainly due to the difference in the level of funding, which allows to recruit the best scientists around the world, including from the Czech Republic.

D1.2	Scope and quality of international and national cooperation and the role of the team in such cooperation; engagement in broad international cooperation

The international cooperation of the team is very wide and basically covers almost the entire research field. In the years 2015-19, they obtained 5 international grants, the scope of which was related to: the development of new molecular conductors and switches for molecular electronics (Karlsruhe Institute of Technology, Universities of Basel and Bern, Université de Paris and Research Centre for Natural Sciences of the Hungarian Academy

of Sciences); the design of new electrocatalysts (Sorbonne University, University Turin, Indian Institute of Technology Bombay, University Stuttgart and Freie Universität Berlin); charge transfer processes in biologically and environmentally important molecules (University of Pisa and Institute of Chemistry of Organometallic Compounds CNR Pisa, Slovak University of Technology, University of Silesia and University of Ioannina); the development of new electrochemical (bio)sensors for analytical applications (National and Kapodistrian University of Athens, University of Porto, University of Coimbra and University of Regensburg). The cooperation consisted mainly in using the competences of the group's employees in the field of electrochemical and spectroelectrochemical measurements and the construction of electrochemical sensors.

D1.3	Participation of the workers in scientific community activities (organizing of conferences and workshops, invited lectures, awards)
The team members were very active in this area. They organize or participated in organization of several international conferences as: an international electrochemical conference Heyrovský Discussions, the international conference Modern Electrochemical Methods, Heyrovský Memorial lecture, the Congress of the Czech and Slovak Chemical Societies, the Regional Symposium on Electrochemistry, South-East Europe, the International Symposium on Electrochemical Impedance Analysis the 70th Annual Meeting of the International Society of Electrochemistry. They had 21 invited lectures at different international and national conferences, workshops and at the universities during the evaluation period. The team members obtained several awards as: Otto Wichterle Award (V. Kolivoška); Metrohm Achievement Award (L. Pospíšil); Metrohm Young Chemist Award (T. Sebechlebská); International Society of Electrochemistry Award (Š. Lachmanová); J. Heyrovský Young Scientist position (V. Kolivoška); Metrohm Young Chemist Award (J. Kocábová).	

Further criterion: 2. Vitality, sustainability and strategy (D2.1-D2.9)

D2.1	Direction in line with the perspective of the planned research directions
The group's research plans are mainly a continuation of the subject matter carried out in the assessed period. These include, among others, the research on the preparation, properties and applications of porphene in a form of a two-dimensional polymer, application of derivatives of 4,4`-bipyridines as electron reservoirs for solar energy harvesting systems, investigation of molecular electronic components employing conventional metallic and novel 3D printed carbon-based composite electrodes, the research of rationally designed model complexes for the development of catalysts for the removal of NO_x pollutants, the investigation of copper(oxide)-based catalysts for the electrochemical reduction of carbon dioxide, the development and detailed electrochemical and spectroscopic characterization of artificial enzymes, the development of chemical sensors for biologically active compounds involving drugs, phytohormones, pesticides and biomarkers.	

D2.2	Assessment of the previous research objectives and their achievement
In the previous period, the research subject was similar and conducted correctly, and the scientific achievements were sufficient. They provided a good basis for the development of research conducted in the reporting period.	

D2.3	Assessment of implementation of recommendations from past evaluation
During the previous evaluation period there was a redefinition of the research scope aimed towards important areas involving molecular control of electron transfer activation and	

transport. The only recommendation is that the group must pursue its reorientation and implement with success its planned research. Transformation of the Department of Molecular Electrochemistry to Department of Electrochemistry at the Nanoscale reinforced the research aims towards electroactive molecular systems from the perspective of nanoscale dimensions. Recommendations concerning the visibility of group on the international scene and the participation of the younger scientists in high-level international conferences have been fulfilled.

D2.4	**Success in receiving grants**
The team received 18 grants from national (12 grants) and international (6 grants) agencies. In each reporting year, there were from 4 to 9 grants, which ensured the continuity of financing research, and the possibility of employing additional staff and doctoral students. The members of the group were not coordinators of the European grant from Horizon'2020 funding.	

D2.5	**Adequacy of instrumental equipment**
The group has the following instrumentation and methodology: advanced electrochemical instrumentation, in-situ spectroscopic techniques (UV-Vis, FTIR and fluorescence), Analytical separation/detection platforms, scanning probe microscopies, diverse break-junction techniques, density functional theory based computational approaches, 3D printing and computer assisted design. Such a set of apparatus is sufficient for the implementation of further research plans, but the assessment of this fact is incomplete as it was not possible to visit the Institute due to the pandemic problems.	

D2.6	**Effectiveness of management**
Scientific effects, the development of young staff and the awards obtained prove the good management of the research group. This fact may be confirmed by the ability of the group's members to obtain and correctly implement national and international grants.	

D2.7	**Assessment of professional structure, development strategy and the strategy of keeping best scientists, age structure, career and qualification growth**
Comparing the two periods of assessment of the group, it can be seen that it is able to adapt to the changing conditions in which it operates. It is a good sign that the planned strategy will be properly implemented. Maintaining the research potential, staff development and the ability to acquire outstanding scientists depends mainly on financial conditions. Seeing the group's ability to obtain national and international grants we assess their possibilities positively.	

D2.8	**Creating work-life balance conditions, assessment of approach towards possible gender issues**
The gender issue has already been met as approximately 53% of the group are women.	

D2.9	**Relation of the team with regard to the integration, development and sustainability of the research centre funded by the National Programme of Sustainability II.**
Research on electroactive systems for molecular catalysis for CO_2 reduction and the elaboration of electrochemical methodology to the analysis of broad range of biologically and environmentally important substances correlate well with two of the four main tasks of the National Program of Sustainability II. These are Air Protection and Water Protection.	

Further criterion: 3. Cooperation with universities and participation in education (D3.1-D3.6)

D3.1	Scope of cooperation with universities on national and international level
Members of the team participated in the education process at the Charles University, University of Chemistry and Technology Prague, Palacký University Olomouc and Masaryk University. They conducted lectures and other activities for bachelor, master and PhD. students in diverse fields of electrochemistry. There is no educational activity at foreign universities.	
D3.2	**Effectiveness of joint research centres**
The team was not involved in the education process within the framework of the joint research centres.	
D3.3	**Success rate in supervision of PhD students**
In the period under review, 7 PhD thesis were defended, in which supervisor or consultant was a member of team. This is a reasonable amount considering the number of academics working in the group.	
D3.4	**Participation of PhD students in the outputs**
During the reporting period, 17 PhD students worked in the group (7 theses were defended). Participation of PhD students in the outputs of the team was mainly through publications either as first authors (involving major experimental work related to their thesis) or as co-authors according to the degree of their contribution. They were also involved in the organization of conferences and of outreach activities including science popularization among the high school students and teachers. All students were encouraged to present their work at the national and international conferences.	
D3.5	**Participation of the team in master or bachelor studies**
In the period under review, 2 Bachelor and 3 Master theses were defended, in which supervisor or consultant was a member of team. It is not much, and such experienced research group could promote more. The problem is that the individual depends on the possibility of getting good candidates from the universities.	
D3.6	**Assessment of cooperation intensity with universities in the form of teaching**
The members of the department: Hromadová, Navrátil, and Sokolová delivered 16 different courses on Physical Chemistry, Electrochemistry, Applied Voltammetry, Electrode Kinetics, Experimental Methods in Physical and Macromolecular Chemistry, Fundamentals of Medicinal Chemistry and Biochemistry and Pathobiochemistry, taught at Charles University, UCT Prague, Masaryk University and Palacký University in Olomouc.	

Further criterion: 4. Outreach activities (D4.1-D4.3)

D4.1	Sufficiency of media strategy and activities in the area of research popularisation
The members from the team took active part as lecturers in Popularization Experimental Education project and served as supervisors of high school students involved in the Student's Professional Activity projects. They also participated in the project Open Science, where they conducted workshops for primary and high school students and their teachers	

and gave a number of interviews in the Czech media.	
D4.2	**Publishing activities and its quality**
Publishing activity is very good. During the reporting period, they published 155 articles. It should be noted, however, that only some of them have been published in reputable journals in the field chemistry and electrochemistry, while a large part was in mid-range or national magazines of local importance.	
D4.3	**Participation in professional organisations in the area of research and development**
The members of the team were very active in the International Society of Electrochemistry where team leader Magdaléna Hromadová was Vice-Chair and Chair Elect of Division 6: Molecular Electrochemistry and regional representative of ISE for the Czech Republic. Prof. Navrátil was member of the Presidium, scientific chair of Analytical Chemistry and Toxicology Divisions of Czech Chemical Society and scientific secretary of UNESCO Laboratory of Environmental Electrochemistry at Charles University. Researchers from the team served also as members of the evaluation panels (of the Czech Science Foundation (GAČR), as subject-area board experts of the Charles University Grant Agency (GAUK) and evaluated proposals from different grant agencies including National Science Foundation USA, Swiss National Science Foundation, European Cooperation in Science and Technology (COST), Scientific Grant Agency (VEGA) and Slovak Research and Development Agency (APVV) Slovakia.	

Other comments of the commission:

8. Chemistry of Ions in Gaseous Phase

Strengths:
Strong team with good instrumentation, diversified funding with good access to competitive European grants, interesting applications

Weaknesses:
The instrumentation is not necessarily unique, innovation not on the instrument, despite some efforts in miniaturization which can be important

Opportunities:
Improve international networks, competitive for ERC, competitive for new instrumentation

Threats:
Irreparable failure of older instruments before replacements, recruitment of young talent

Main criterion: 1. Quality of results (H1.1-H1.5)

H1.1	Quality of selected outputs of Phase I
The quality and quantity of outputs is good. There is some work on basic ion-molecule chemistry, which is necessary to do, but which is not unique—other places may be as well situated. It should be noted that this particular area is one for which the Heyrovsky Institute has historically been well-known and visible. The applications in a variety of analytical settings is newer, and more diverse. These applications result in outputs of high visibility and significant innovation, where the Institute, by being an early mover, can gain an advantage internationally. Examples on the basic side are the spectrometers for space missions, e.g. Titan, and the breath analysis for medical diagnosis.	
H1.2	**Contribution of workers on the outputs reached**
The contribution comes from the workers.	
H1.3	**Quality of all outputs and results**
See above.	
H1.4	**The most valuable discoveries and findings in the fields, their importance for the field**
As mentioned above, the field of ion-molecule chemistry is by itself, a mature field in which many Institutes worldwide are excellent. The innovation, and hence the value, in the efforts in the Prague derive from novel applications of ion-molecule chemistry. For example, SIFT-MS was exploited extensively in the US from the 1970s to the 1990s, with many of the instruments going offline since 2000. The Prague group, however, has managed to use the advantages of the SIFT-MS to solve problems in environmental, food safety, semiconductor manufacturing, etc., which is development which did not happen in the US. Similarly, the group has designed and manufactured a miniaturized SIFT-MS whose portability opens more applications. This is an interesting positioning of the group scientifically, and it could provide the opportunity to raise the group's profile further.	
H1.5	**Contribution of the participation of the authors in large collaborations**
The group is part of a large European consortium project for ion-molecule relations in analytical chemistry. Another part of the group works with the Synchrotron Soleil in Paris on chemical reactions in the atmosphere of Titan, which is inherently a large collaboration,	

given the extensive large-scale infrastructure. The group is part of a large collaboration with a CNRS lab within the context of the European Space Agency.

Main criterion: 2. Societal relevance (H2.1-H2.5)

H2.1	Societal relevance of outputs and results pursuant to CAS and institute mission
The analytical applications have direct societal relevance. I mention especially the MS-based breath analysis for non-invasive medical diagnostics. Only a few groups engage in this kind of work, since the original discovery of the phenomenon by R.G. Cooks at Purdue University. The group in Prague is one of the best, and it should be noted that they pursued the project against previous recommendations. The basic research and the instrument design activities support the applications, and need to be continued.	
H2.2	**System functionality for knowledge transfer into practise, its usefulness for society. The impact of the team´s activity on proper practice in society in the area of social sciences and humanities**
We received insufficient information to judge the effectiveness of the knowledge transfer.	
H2.3	**Relation to practice**
NA	
H2.4	**Participation in AV21 strategy**
NA	
H2.5	**Cooperation with regions of the Czech Republic**
NA	

Further criterion: 1. Position in international and national context (D1.1-D1.3)

D1.1	Comparison of the team with similar international and national institutes
The group is world-class in applications of mass spectrometry to a variety of interesting analytical applications.	
D1.2	**Scope and quality of international and national cooperation and the role of the team in such cooperation; engagement in broad international cooperation**
See comments above.	
D1.3	**Participation of the workers in scientific community activities (organizing of conferences and workshops, invited lectures, awards)**
The group leaders have a good list of invited and keynote lectures at the best meetings in the field.	

Further criterion: 2. Vitality, sustainability and strategy (D2.1-D2.9)

D2.1	**Direction in line with the perspective of the planned research directions**
Good, they should keep doing what they are doing.	
D2.2	**Assessment of the previous research objectives and their achievement**
NA	
D2.3	**Assessment of implementation of recommendations from past evaluation**
NA	
D2.4	**Success in receiving grants**
Track record on grants is exemplary.	
D2.5	**Adequacy of instrumental equipment**
Instrumentation is very good.	
D2.6	**Effectiveness of management**
Management appears to be fine.	
D2.7	**Assessment of professional structure, development strategy and the strategy of keeping best scientists, age structure, career and qualification growth**
Age distribution is bimodal, with a good pipeline of young scientists.	
D2.8	**Creating work-life balance conditions, assessment of approach towards possible gender issues**
There are a number of women, but evidently not yet in senior positions.	
2.9	**Relation of the team with regard to the integration, development and sustainability of the research centre funded by the National Programme of Sustainability II.**
We cannot judge this in detail, but the environmental analytical activities would fit well.	

Further criterion: 3. Cooperation with universities and participation in education (D3.1-D3.6)

D3.1	**Scope of cooperation with universities on national and international level**
The collaborations, at least those that we can see, are mostly international, and these are exemplary.	
D3.2	**Effectiveness of joint research centres**
NA	
D3.3	**Success rate in supervision of PhD students**
There were only two Ph.D. dissertations defended in the 2015-2019 period.	
D3.4	**Participation of PhD students in the outputs**
Students were fully integrated, but it would be beneficial if there were more of them.	

D3.5	Participation of the team in master or bachelor studies
There were only two M.S. theses defended in the 2015-2019 period.	
D3.6	**Assessment of cooperation intensity with universities in the form of teaching**
The level does not appear to be high. The group leader, Patrik Spanel, cites 30 hours per year for teaching.	

Further criterion: 4. Outreach activities (D4.1-D4.3)

D4.1	Sufficiency of media strategy and activities in the area of research popularisation
Many of the projects are well-suited for outreach and media dissemination. The group documents multiple instances in Czech radio, television, and print media.	
D4.2	**Publishing activities and its quality**
Publication activity is good.	
D4.3	**Participation in professional organisations in the area of research and development**
NA	

Other comments of the commission:

9. Low-dimensional Systems

Strengths:
Unique instrumentation for study of 2-D materials. Generous funding. Young age distribution. International reputation.

Weaknesses:
Not enough permanent positions. Cramped laboratory and office space.

Opportunities:
Developing new collaborations. Acquiring new expertise with young people coming in.

Threats:
Administrative overload. Loss of expertise as established investigators retire or are moved to different groups.

Main criterion: 1. Quality of results (H1.1-H1.5)

H1.1	Quality of selected outputs of Phase I
25 outputs were selected for evaluation during Phase 1. Most of these papers were published in top quartile journals relevant for the area of study (Carbon, ACS Applied Materials and Interfaces, Angewandte Chemie, ACS Nano, Nature Communications).	
H1.2	**Contribution of workers on the outputs reached**
Members of the group were principal contributors to the evaluated work. Ranging from 100% of the authors as members of the research group, down to situations where 40 % of the work was done by the research group (preparation of samples, initial characterization, analysis of the data). Clearly the driving force in the work reported.	
H1.3	**Quality of all outputs and results**
135 publications resulted from work of this group over the review period. A significant fraction (100 outputs) published in Decile 1, Quartile 1 and Quartile 2 journals for the field of 2-Dimensional materials, chemical physics and nanomaterials. A very strong publication record across the areas of 2D materials, and nanostructured catalysis.	
H1.4	**The most valuable discoveries and findings in the fields, their importance for the field**
Studies of graphene stacking and property tuning, use of graphene in field effect transistors, graphene functionalization, nanoscale design and synthesis of MnO_2 oxygen reduction reaction catalyst, and developments of methods for the spectroscopic characterization of graphene and other 2D materials under stress and in the presence of impurities are all significant contributions from this group. Many have significant impact on technology (catalysis, fuel cells, sensor systems, developing quantum technologies).	
H1.5	**Contribution of the participation of the authors in large collaborations**
Members of this team participate in large international collaborations, and they are primary contributors to the design and execution of the work in these collaborations.	

Main criterion: 2. Societal relevance (H2.1-H2.5)

H2.1	Societal relevance of outputs and results pursuant to CAS and institute mission
The fundamental science carried out in this group has multiple future applications, in emerging technologies such as quantum computing, electronic sensors, and alternative energy.	
H2.2	**System functionality for knowledge transfer into practise, its usefulness for society. The impact of the team´s activity on proper practice in society in the area of social sciences and humanities**
Fundamental science done here contributes significantly to the society, both in terms of future applications, and in the construction of the edifice of knowledge that is crucial for human society.	
H2.3	**Relation to practice**
Several of the various projects have clear connections to technological developments. These range from actual nanodiamond manufacture to development of active catalysts for fuel cell applications to strategies for control of properties of 2D materials for use in quantum electronics applications. Very clear connections between the fundamental science of this group and patentable intellectual property that will underlie industries of the future.	
H2.4	**Participation in AV21 strategy**
No comment	
H2.5	**Cooperation with regions of the Czech Republic**
The group is involved in significant cooperative programs with institutes and organizations in the Czech Republic. Cooperation on carbon nanostructures for sensors with TESLA BLATNA a.s. and University of West Bohemia is an example. Other institutions involved in cooperation with the group include Charles University, Technical University of Liberec, University J.E. Purkyne in Usti Nad Labem, and Palacky University Olomouc. The level of cooperation with institutes and organizations across the Czech Republic is extensive and impressive, both currently and planned for the future.	

Further criterion: 1. Position in international and national context (D1.1-D1.3)

D1.1	Comparison of the team with similar international and national institutes
The Low Dimensional Materials program of the Heyrovsky Institute operates at an international level of recognition. They are comparable in both quantity and quality of research in this area to other internationally well-known research centres focused on the study of 2D materials and quantum engineering. They have enjoyed fruitful collaborations with groups at MIT in the USA, Cambridge in the UK, Dresden, Köln, Madrid and Strasbourg in Europe, as well as initiation of recent collaborations with the CA2DM at the National University of Singapore.	

D1.2	Scope and quality of international and national cooperation and the role of the team in such cooperation; engagement in broad international cooperation
The team is engaged in significant international and national cooperation, and they play a leading role in these collaborations. Their unique abilities in sample preparation and graphene functionalization, detailed X-ray and Raman spectroscopic characterization, and efforts in hybrid 2-D materials device applications have led to this level of recognition.	
D1.3	**Participation of the workers in scientific community activities (organizing of conferences and workshops, invited lectures, awards)**
The team is very active in national and international conference organization and attendance. Many members of the team have given invited lectures around the US, Europe and Asia. CAS sponsored awards for both junior scientists (Kovaricek) and more established scientists (Kalbac) have been awarded to team members during the period of the review.	

Further criterion: 2. Vitality, sustainability and strategy (D2.1-D2.9)

D2.1	Direction in line with the perspective of the planned research directions
Management of the team is clearly aligned with the research directions planned for the future. The management structure is very well designed and effective in promoting flexibility to address new leads in research. The management structure is also well set up to help develop the careers of junior colleagues, as well as to support those in mid-career and improve efforts to identify, hire and retain the best talent. More long-term support from the CAS in the form of full-time research appointments would support these efforts.	
D2.2	**Assessment of the previous research objectives and their achievement**
The previous ambitious and well-planned research objectives were achieved for the most part during the time of the evaluation. In addition, the group was adept at shifting directions and seizing on breakthroughs in the planned research and exhibited an ability to change directions to follow these opportunities.	
D2.3	**Assessment of implementation of recommendations from past evaluation**
Reorganization of the team structure, as recommended by the previous review panel, has been carried out by splitting the department into two teams, Low Dimensional systems, and Nanocatalysis. This appears to be working to the benefit of the entire department, and certainly still results in a good deal of interdepartmental collaboration.	
D2.4	**Success in receiving grants**
The group has experienced remarkable success in proposing research projects at the cutting edge, and receiving the funding to support these ideas. There have been 24 grants active during the time of the review, with a total funding amount of greater than 12 million Euros. These included national grants from the Czech science foundation, CAS awards, direct support from industry, and two significant ERC grants, a consolidator grant and a starting grant. The group has been very successful in this regard.	
D2.5	**Adequacy of instrumental equipment**
The instrumental equipment is very unique in many instances, and for the present time is adequate for the needs of the group. This is not likely to continue however, as many of these unique pieces of instrumentation are aging and will be difficult to adequately maintain	

soon. Plans must be in place to replace and upgrade this instrumentation if the group expects to maintain its international prominence in the quality of their research.

D2.6	Effectiveness of management
The management structure is very well designed and effective in promoting flexibility to address new leads in research. The management structure is also well set up to help develop the careers of junior colleagues, as well as to support those in mid-career and improve efforts to identify, hire and retain the best talent. More long-term support from the CAS in the form of full-time research appointments would support these efforts. The management structures are very well thought out, and appear to work effectively to develop a spirit of collaboration and cooperation among the researchers in the department.	

D2.7	Assessment of professional structure, development strategy and the strategy of keeping best scientists, age structure, career and qualification growth
The age distribution is on the young side. In order to maintain an influx of new talent, and strengthen the leadership cadre in the mid-career ranks of the group, the answer is more competitive salaries across the board. This coupled with generous start up packages for the best young scientists that are attracted to the Heyrovsky Institute will lead to a sustainable research team that will continue to be a leader in the field of 2-D materials internationally.	

D2.8	Creating work-life balance conditions, assessment of approach towards possible gender issues
As with many physical science research teams, the gender imbalance is obvious (6 female of 27 research scientists). Policies to support family leave, international efforts to attract researchers to the institute, and support with appropriate salary levels will all help with this problem.	

D2.9	Relation of the team with regard to the integration, development and sustainability of the research centre funded by the National Programme of Sustainability II.
No comment.	

Further criterion: 3. Cooperation with universities and participation in education (D3.1-D3.6)

D3.1	Scope of cooperation with universities on national and international level
A very significant level of cooperation with universities on the national and international level in the area of education. Teaching at Master's level at TU Dresden, UCT Prague, Czech Technical University Prague, Charles University, and Palacky University Olomuc, have all been provided by members of the team.	

D3.2	Effectiveness of joint research centres
No joint research centres to assess.	

D3.3	Success rate in supervision of PhD students
Ten doctoral students were supervised during the review period, and 7 have defended their dissertations.	

D3.4	Participation of PhD students in the outputs
PhD students are directly involved in publications, as co-authors and often first authors on	

the research articles published by the research team.	
D3.5	**Participation of the team in master or bachelor studies**
Direct master's level teaching in a number of universities, as well as master and bachelor student researchers participating in the research of the institute.	
D3.6	**Assessment of cooperation intensity with universities in the form of teaching**
A very significant level of cooperation with universities on the national and international level in the area of education. Teaching at Master's level at TU Dresden, UCT Prague, Czech Technical University Prague, Charles University, and Palacky University Olomuc, have all been provided by members of the team.	

Further criterion: 4. Outreach activities (D4.1-D4.3)

D4.1	**Sufficiency of media strategy and activities in the area of research popularisation**
Good media strategy in place. Several radio interviews, print articles, and television stories about the work of the research group. Summer school for nanomaterials targeted at university students is an example of outreach activities.	
D4.2	**Publishing activities and its quality**
Print articles regarding the outreach activities have been published. Hard to judge the quality.	
D4.3	**Participation in professional organisations in the area of research and development**
Members of the group participate in professional organizations focused on the area of research.	

Other comments of the commission:

10. Dynamics of Molecules and Clusters

Strengths:
Strong instrument park with unique spectrometers, often home-built, core team maintains expertise, very strong grant financing and international collaboration

Weaknesses:
The field is difficult to explain to the lay public, student recruitment could be better.

Opportunities:
Competitive for EU funding based on excellence

Threats:
Administrative overload

Main criterion: 1. Quality of results (H1.1-H1.5)

H1.1	Quality of selected outputs of Phase I
The group was split off from the Department of Chemistry of Ions and Clusters in 2017. The latter retained the primarily analytical directions, whereas the Molecules and Clusters group moved out with the much more physics-based experiments. The outputs in the evaluation period, in terms of publications and external lectures, is outstanding. Even though the group sees itself in an exotic field, the quality of the work makes the group visible internationally.	
H1.2	**Contribution of workers on the outputs reached**
The workers were central to the outputs.	
H1.3	**Quality of all outputs and results**
See above.	
H1.4	**The most valuable discoveries and findings in the fields, their importance for the field**
The group has built superb instrumentation which cannot be purchased commercially. With the instruments, they have conducted basic research on photodissociation dynamics and dissociative attachment reactions. The molecules are usually small, but the group has recently moved into larger, biologically relevant molecules. This transition should be encouraged. They are also moving into new technologies, such as the liquid jet spectroscopy, which will open further opportunities.	
H1.5	**Contribution of the participation of the authors in large collaborations**
The group participates in a number of large collaborations, but their contributions are still primarily individual.	

Main criterion: 2. Societal relevance (H2.1-H2.5)

H2.1	Societal relevance of outputs and results pursuant to CAS and institute mission
Whereas the cluster work is primarily basic research, the group has leveraged their	

expertise into some industrially relevant areas, for example, nanofabrication. In principle, they can investigate some of the chemistry underlying the technology of electron beam line writers, which is poorly understood despite being widely used.	
H2.2	**System functionality for knowledge transfer into practise, its usefulness for society. The impact of the team´s activity on proper practice in society in the area of social sciences and humanities**
We were unable to assess the effectiveness of knowledge transfer. The industry contracts documented by the group speak for themselves, though.	
H2.3	**Relation to practice**
See above.	
H2.4	**Participation in AV21 strategy**
NA	
H2.5	**Cooperation with regions of the Czech Republic**
NA	

Further criterion: 1. Position in international and national context (D1.1-D1.3)

D1.1	**Comparison of the team with similar international and national institutes**
With regard to their core areas of expertise, dissociative attachment and photodissociation dynamics, the group is competitive with the best groups worldwide, not just in Europe.	
D1.2	**Scope and quality of international and national cooperation and the role of the team in such cooperation; engagement in broad international cooperation**
The scope and quality of international collaborations is excellent. The group documents collaborations with the ETH Zürich, the University of Innsbruck, the University of Southern California, as well as more local collaborations with Bratislava and Belgrade. They are members of an EU COST action, and have further projects with LBNL in Berkeley.	
D1.3	**Participation of the workers in scientific community activities (organizing of conferences and workshops, invited lectures, awards)**
The group has a large number of high-profile lectures and has organized an international conference on dissociative attachment.	

Further criterion: 2. Vitality, sustainability and strategy (D2.1-D2.9)

D2.1	**Direction in line with the perspective of the planned research directions**
Good.	
D2.2	**Assessment of the previous research objectives and their achievement**
The group is independent only since 2017. The separation from the analytical group allowed the Molecules and Cluster group to engage in its own strategy.	
D2.3	**Assessment of implementation of recommendations from past evaluation**

See above.	
D2.4	**Success in receiving grants**
Outstanding.	
D2.5	**Adequacy of instrumental equipment**
Outstanding.	
D2.6	**Effectiveness of management**
Management appears fine.	
D2.7	**Assessment of professional structure, development strategy and the strategy of keeping best scientists, age structure, career and qualification growth**
Demographics of the group strongly tilted towards younger scientists.	
D2.8	**Creating work-life balance conditions, assessment of approach towards possible gender issues**
Insufficient information.	
D2.9	**Relation of the team with regard to the integration, development and sustainability of the research centre funded by the National Programme of Sustainability II.**
NA	

Further criterion: 3. Cooperation with universities and participation in education (D3.1-D3.6)

D3.1	**Scope of cooperation with universities on national and international level**
The group seeks more cooperation with universities. Teaching activities by the senior members is fine.	
D3.2	**Effectiveness of joint research centres**
NA	
D3.3	**Success rate in supervision of PhD students**
There were only two dissertations defended in the evaluation period.	
D3.4	**Participation of PhD students in the outputs**
Fully integrated.	
D3.5	**Participation of the team in master or bachelor studies**
Five M.S. students defended their theses in the evaluation period, which is good for a small group.	
D3.6	**Assessment of cooperation intensity with universities in the form of teaching**
See above.	

Further criterion: 4. Outreach activities (D4.1-D4.3)

D4.1	Sufficiency of media strategy and activities in the area of research popularisation
Activities are at the usual level, which is very good considering the research topic.	
D4.2	**Publishing activities and its quality**
Outstanding.	
D4.3	**Participation in professional organisations in the area of research and development**
Good.	

Other comments of the commission:

Final report was elaborated by:

Commission 3.1 - Chemical sciences
Evaluated teams No.: 1, 2, 3, 4, 5, 6, 7, 8, 9, 10

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