

Evaluation of the Research and Professional Activity of the Institutes of the Czech Academy of Sciences (CAS) for the period 2010–2014

Final Report on the Evaluation of the Institute

Name of the Institute: J. Heyrovsky Institute of Physical Chemistry of the CAS

Fields, in which the Institute registered its teams:

Chemical sciences

Observer representing the Academy Council of the CAS: Jiri Ctyroky

Observer representing the Institute: Petr Carsky

Commission No. 4: Chemical sciences

Chair: Dr Habil, Academician Christian Amatore

Date(s) of the visit of the Institute: November 30 - December 4, 2015

Programme of the visit of the Institute: see attached Minutes from the visit

Evaluated research teams (in the order of the Director's presentation):

- **Department of Biomimetic Electrochemistry**
- **Department of Electrochemical Materials**
- **Department of Chemistry of Ions and Clusters**
- **Department of Molecular Electrochemistry**
- **Department of Low-dimensional Systems**
- **Department of Spectroscopy**
- **Department of Structure and Dynamics in Catalysis**
- **Department of Synthesis and Catalysis**
- **Department of Theoretical Chemistry**

A. Evaluation of the Institute as a whole

1. Introduction

In his general report about the institute, its director, Prof. Zdeněk Samec, provided an exhaustive overview of the scientific accomplishments and strategies of the Institute over the evaluation period, and discussed its organizational structure, age composition of the institute, *etc.*

The J. Heyrovsky Institute is one of the world-wide best known scientific institutes. Its mission is clear and convincing. The organizational structure recently achieved involves 9 departments that overall encompass chemical physics, catalysis, and electrochemistry. It corresponds to what is expected for a modern institute of physical chemistry of international stature in order to achieve excellence in contemporary physical chemistry (including new materials for catalysis) through advanced experimental and theoretical (including computational chemistry and code-writing) avenues. In this respect, it is noted with pleasure that the number of foreign visitors at the institute has always been high, and it is still growing since this is one of the clearest indicators of scientific excellence.

Although the number of young scientists hired is high (though, with a rather heterogeneous distribution among the departments), the number of mid-career scientist is too low. Conversely, the number of scientists above 65 years of age is high. Therefore, altogether this makes the age distribution of the PIs problematic. In this respect, the Committee welcomes the adopted strategy aiming to the creation of new groups with young leaders. However, a similar effort should be performed to hire (or promote) younger scientists in the department headed by the oldest PIs in order to avoid their disappearance for lack of sufficient programming. This is not a singularity in this Institute since the same problem exists in several other ones evaluated by this Committee, but may result drastically deleterious for the J. Heyrovsky Institute. In this respect, the Committee recognizes with satisfaction the successful number of applications for the J. E. Purkyně Fellowship since this provides an important mechanism to attract young scientists in the Institute. Indeed, three high-level foreign scientists younger than 40-year (from Imperial College London, Stanford University, University of Fribourg) joined the Institute during the last five years through these fellowships to expand the Institute research fields.

The number of international contacts and collaborations is impressive especially in view that they involve numerous world-wide leading groups and excellent institutions. In this context, founding the “Center for innovations in the field of nanomaterials and nanotechnologies”, equipped with high-performance experimental techniques for syntheses and functional characterizations of nanomaterials, is remarkable. Besides servicing the need of many teams in the Institute, its presence has allowed creating a network of collaborations with domestic and foreign institutions, thus increasing the visibility of the Institute.

The output of scientific publications is high and often published in high-ranked journals (*ACS Nano*, *Advanced Functional Materials*, *Advanced Materials*, *Angew. Chem.*, *J. Cell Biol.*, *JACS*, *Nano Lett.*, *Nature Chem. Biol.*, *Nature Chem.*, *Phys. Rev. Lett.*, *PNAS*, etc.). Accordingly, the average IF of publications has been growing steadily in the 2010-2014 period. For example, within the Czech Republic, this CAS Institute is the one that has the largest score in term of its IF/FTE ratio (its score results nearly twice that of most other Institutes evaluated by this Committee). This shows that when compared to other institutes (undeniably within the Czech Republic but even also international ones), the Institute is doing extremely well with lesser funds and lesser personnel.

Based on the excellence of most of its researches, the institute has a high grant success at national and international (EC) grant agencies: This is certainly commendable and greatly helps but simultaneously present a significant danger if the amount of national grant calls decreases since ca. 60% of its FTE involved in research are financed by external funding resources. Therefore, insufficient financial and human resources remain the biggest problems of the institute and condition its future. It is thus hoped that the present trend in decrease of the total number of national grant calls can be reversed.

The many cross-links established between the Institute and several CAS institutes or Czech universities through scientific collaborations and teaching activities form an adequate mean for attracting undergraduate and graduate students who participate in the research effort of the institute (presently 69 graduates and undergraduates). The ensuing student fluxes are quantitatively high and clearly bring strength to the Institute, especially considering that there are many foreign students involved.

However, the student flux is rather heterogeneous among the teams and the Institute should benefit of finding adequate means for increasing them.

2. Strength and opportunities

Almost all the strong points and corresponding opportunities are already identified in the above section and are thus not repeated here. It is sufficient to recognize here that the Institute has been able to gather a number of excellent and enthusiastic scientists and have them working in good synergy.

This contributes to its national and international visibility and to its attractiveness for talented national and foreign young scientists, including Czech ones who started their careers abroad thanks to the J. E. Purkyně Fellowship.

3. Weaknesses and threats

The main danger that the Institute is facing is related to the unfavorable age distribution in many of its teams. Great care has to be taken in planning the consequence of the predictable retirement of some of the Institute most prominent leaders. This has been done satisfactorily in a few teams and allowed their rejuvenation in the process, but this may not always be possible if actions are not taken sufficiently in advance.

As for all other Institutes evaluated by the Committee the state-funded salaries are lower than expected based on the excellent value of several scientists. This may create a potential danger for the positive politics of recruiting young scientists from abroad when they may be financed only/mainly from the Institute's state resources.

The Institute has been extremely successful despite the fact that its competition with equivalent top world research institutions is intrinsically biased owing to the lack of comparable financial and human resources. This is particularly critical for the salaries, as noted above, but also for the maintenance and operation of several of the Institute state-of-the-art equipment. Wagering that this may continue forever based on the Institute success would be misleading; CAS should consider this point seriously and find the mean of increasing the subsidies allocated to its best Institutes such as the present one.

Finally, albeit there is a relatively high number of Ph.D. students and undergraduates in the Institute, a lack of them is apparent in a few departments.

4. Recommendations

The plans presented by the Institute Director are sound should the Institute has the financial means of implementing them to continue its present successful researches, so no specific recommendation needs to be made except on one important point detailed below.

The replacement of Department Leaders having reached the age of retirement by younger scientists with outstanding research performance based on the Institute Board approval is a wise plan. However, its proper application pre-supposes the existence of such younger talented colleagues already in the Department. In the case the Board foresees that this should not be ultimately feasible, alternative decisions have to be taken well in advance of the senior scientist departure: hiring a distinguished young person from outside the Institute; closing or fusing the team with another one. However, great care has to be taken when the decision is made of fusing teams since this may create an artificial structure that eventually needs to be split later, or “sterilizing” some very good components among those fused together. During the evaluations of the individual teams, the Committee has spotted some cases in which such dangers may already exist even if the fused team still performs excellently.

5. Detailed evaluation

Several detailed remarks have been provided in §1 and will thus not be stated again hereafter. Furthermore, the detailed evaluation of the scientific research accomplishments is performed through the evaluations of its individual teams. Therefore, the following is mostly concerned with some of the strategies and management issues.

The Fellowship J. E. Purkyně granted by the Academy of Sciences provides an excellent and valuable opportunity to attract high-level scientists complementing the new research interests of the Institute.

Though the Institute has a “flat” structure, the Committee appreciates that the departments heads have a decision-making power as concerns the personnel promotion and their hiring (on available positions) based on transparent selection procedures that are finally supervised at the Institute Board level. This is a strong guarantee of maintaining equivalent scientific level of recruitments in all Departments.

The Committee also welcomes the quinquennial evaluation of researchers performance based on detailed analyses of individual scientific outcomes, followed by decision on their promotion or the prolongation of their new contract.

Finally, although the Institute scope and orientation are highly focused on basic sciences and the fact that most of the Institute teams are highly successful in this direction, the Committee members think that in some cases, noted in the individual evaluations, practical issues should be also considered.

B. Evaluation of the individual teams

Evaluation of the Team: Department of Biomimetic Electrochemistry

1. Introduction

The Team was formed in 2013 by merging of two electrochemical groups. The main scientific activities of the team focus on the properties of systems designed to be biomimetic models of living systems (polarized interfaces between liquids as such or as models of biological interfaces, ion transport across membranes, role of amino acids in biological electron transfer, photo-induced process in biomimetic metal complexes) with fundamental (modeling) and applied outcomes (biosensors based on solid amalgam electrodes and polarized interfaces).

The group's research directions are based on the long tradition of careful electrochemical investigations that prevails at the Institute. So, the Team explores modern issues of electrochemical sciences, the historical experience being transferred and adapted to allow investigating modern subjects. When this matters, the Team's experience is adequately complemented thanks to several fruitful collaborations.

The development of the field of liquid-liquid interfaces across the world owes greatly to the sound contributions of this team following bright decisions made by its former Director, Prof. Vladimir Marecek with the precious help of the present Team Leader. Since then, many teams across the world have understood theoretically these systems, thus recognizing the importance of this field either in rationalizing natural systems or in adapting the liquid-liquid interface concepts to investigate or promote many research avenues (e.g., thanks to the development of nano-pipettes). Following this trend, the main achievements of the team during the evaluated period involve an interesting application of the liquid-liquid interfaces to describe new (and unexpected!) mechanisms of oxygen reduction, as well as electrocatalysis of electron transfer. This is worth mentioning since this work established concretely that usual views rooted on homogenous phase concepts may be highly misleading in the presence of liquid-liquid interfaces explaining why nature frequently implements such situations.

The other main original research avenue investigated concerns the use of solid amalgam electrodes for very sensitive amperometric sensors of bioactive materials.

This is an important specialty of the team (and of a related one in Prague at Charles University) which has been developed in Prague because of historical reasons (J. Heyrovsky's polarography involved mercury) to overcome the present restrictions on the use of mercury. It is absolutely undeniable that these sensors present high electroanalytical qualities for cathodic detection in water-based media precisely due to the mercury presence. However, it is as clear that the spreading of their use unfortunately faces the consequences of the general ban of mercury and mercury salts in most laboratories across the world.

This team has presently an aggregate number of 11 researchers (3 senior scientists, 9 scientists; yet, about half of them are partly employed) and 1.43 FTE for its support members. The age distribution of its staff is somewhat preoccupying with half of its members above 65 years and 3 between 55 and 60. It involves 3 graduate students.

The Team's member strong teaching commitment helps attracting students to work on their projects. Still, the number of students might be higher but it is clear that this reflects a general disaffection for physical chemistry among university students across the occidental world.

2. Strengths and Opportunities

The main strength of the Team is inherent in its high expertise in theoretical description of electrochemical phenomena coupled with important experimental skills. Both are rooted in the Team historical role in development of electrochemistry of interface between phases, and of solid amalgams substitute to Hg-electrodes.

The vigor of this team is exemplified by its success in obtaining grants (5 from Czech SF, 7 from Ministry of Education, and 1 from CAS) and by publications in high-level international journals of the fields covered.

The team has a recognized international position in the electrochemical community, and a major one for what concerns liquid-liquid interface systems due to its seminal and historical role in this important field.

Its scientific outputs are often published in high-ranging journals, as well as in specialized and multidisciplinary ones according to the topics and the publication aim.

3. Weaknesses and Threats

The main threat is related to the age of the prominent scientists of the team. Several

of them already devote only fraction of their times to the team and its Director will reach soon an emeritus status. It is essential that the team attracts several new members to replace them. However, these new scientists need to be selected with great care to maintain the high-level standing of the group while building new research axes based on the wealth of knowledge presently gathered in the team.

The Team expertise should move soundly towards “real” (biological) liquid-liquid interfaces and complicated matrices to explore novel applications of its considerable theoretical and experimental understanding of these issues.

4. Recommendations

The main recommendation of the Committee is that the group should find ways to attract younger members in order to preserve its important and world-recognized wealth of fundamental knowledge and experimental know-how. This only may solve the problems associated to the retirement of elderly team members. This process may probably also bring new research axes, thus great care should be taken to maintain a scientific coherence in the process to capitalize on the present know-how and avoid scientific dispersion.

Future research plans were well communicated during the on-site presentation by the Team Leader. They seem reasonable and were positively welcomed by the Committee.

Yet, it is clear that the group is torn between continuing investigations of model systems (in which all aspects can be mastered experimentally and theoretically) and its aspiration to attack real systems (as is already clearly stressed in the Team’s name). Nature offers a wide variety of important systems amenable to biomimetic modeling in which a proper scientific understanding is necessary.

For example, micro- and nano-liquid-liquid interfacial systems are present in many crucial systems for oceans’ life (i.e., CO₂ and O₂ exchanges at sea-salted water micro-drops foams, etc.). The same is true in key biological ones albeit their macroscopic (e.g., roots, sap, lungs, etc.) or microscopic (ion channels, brain-blood barriers, vesicular release of bioactive molecules and ions, etc.) dimensions. This offers a wealth of tantalizing research avenues in which the team could find important lead-problems in which it could contribute with excellence and high visibility by expanding its “biomimetic” components well beyond their present status.

Evaluation of the Team: Department of Electrochemical Materials

1. Introduction

The main activities of the Department of Electrochemical Materials focus on the synthesis, characterization and applications of advanced electrode materials, with special emphasis on carbon-based nanomaterials and oxide semiconductors. The department possesses state-of-the-art synthesis and characterization equipment including XRD, SEM, AFM/STM, UV-Vis spectroscopy, HPLC, TOC-analyzer, IR/Raman and thermal analysis. The group developed advanced unique in-situ spectro-electrochemical methods (visible and Raman).

The scientific activities of the Department are synergistically balanced between fundamental studies and applied research in the field of solar cells, Li-ion batteries and pollution control. Studies are closely offering bases for cooperation with industry. Recently, the group produced one groundbreaking research by evidencing the feasibility of spectral sensitization of boron-doped diamond to visible light. This opens new horizons for future development of photocathodes in dye-sensitized solar cells.

The group scientific outputs are of high level. In fact, the Committee was very impressed by the results presented. Altogether, they shape an ensemble of cutting edge researches aimed to important fields of modern science. The projects are innovative, as e.g. shown by the interesting new developments in photocatalysis (a project that is also of importance for practical solutions in, e.g., water purification).

The team has presently an aggregate number of 10.05 researchers and 5.69 other members. The age and gender composition are also very favorable at the moment: the Department has 12 women (55%) vs. 10 men (45%) with, altogether, an average age of 43.

2. Strengths and Opportunities

The strength of the team is well demonstrated by its success in obtaining grants (5 from Czech Science Foundation, 2 from Ministry of Education, 7 from EU FP7, 2 from Czech Technological Agency and 2 from CAS) and by numerous publications in high-level international journals.

The team belongs to the worldwide recognized leading groups in several of its research areas: electrode materials for dye-sensitized and perovskite solar cells,

electrode materials for advanced Li-ion batteries, nanocarbons (nanotubes, graphene, nanodiamond) and photocatalysis for environmental protection and remediation.

3. Weaknesses and Threats

No noticeable weaknesses could be detected, yet further development of the group is required to reach an international level. Unfortunately, this is limited not by the intrinsic value of the group scientists but by the relatively low funding, especially that necessary for renewing and up-grading of the group equipment.

4. Recommendations

The group is dynamic, productive and relatively young with a very good potential for further developments. The main recommendation of the Committee is that the Institute should find means of funding the new advanced instruments on which the group depend critically for its further development.

Evaluation of the Team: Department of Chemistry of Ions and Clusters

Important Caveat: *The Commission lacked a proper scientific expertise on most of the topics developed in this team, especially those that have a strong “chemical physics” character. This was indicated to the CAS Administration by the Chair before Phase II began but unfortunately no appropriate remedy could be offered. We therefore apologize if some of the comments made hereafter may result inadequate or even wrong. If so, we urge CAS to look for an adequate expertise to correct any wrong statement.*

1. Introduction

During the evaluated period, the former Department of Photochemistry, Spectroscopy and Ion Chemistry has been split up into two new departments, the Department of Spectroscopy and the Department of Chemistry of Ions and Clusters. Each of these teams is nevertheless evaluated independently following the CAS recommendation.

The department consists of two groups: Chemistry of Ions in the Gaseous Phase Group and Molecular and Cluster Dynamics Group.

The study of ions and clusters in the gas phase has become an increasingly important field during the last decades. This is not surprising since the problems investigated span a very broad spectrum, ranging from ion-molecule reactions for trace gas analysis to clusters of biological importance and studies concerning analytical problems from space chemistry and physics. Accordingly, the work of this Department focuses on the chemistry and structure of molecular ions and clusters in the gas phase with the announced scope of understanding their reactions and implement them for practical use.

Albeit this unitary principle the research activities of the department within the period of evaluation involve eight rather unrelated research directions. This seems to be a too broad research scope even taking into account that two groups are fused in the Department, though the Molecular and Cluster Dynamics Group seems to be more focused and investigates several important and topical issues related to fundamental processes: clusters *per se*, clusters important for atmospheric chemistry, or having biological relevance.

One of the projects underway in the Department uses trace gas analyses by mass spectrometry and ion spectroscopies for the detection of marker molecules that may be of interest in breath analysis for diagnosis and therapeutic monitoring. This was published in the *Journal of Breath Research*, nonetheless, there was some concern among the Committee members that this area is very active worldwide, and may be well ahead of what is being done in this department when an international context is considered rather than a national one. However, in this respect, it is noted with interest that the project is a clever repurposing of instrumentation previously used for more basic studies of small molecular ion spectroscopies.

More basic studies are directed toward understanding of atmospheres of planetary satellites (that of Titan, for example). This might be a more significant project to address with these powerful methods.

In addition, some of the performed cluster chemistry (including structure and analysis of small inorganic or organic clusters) may be of relevance to terrestrial atmospheric chemistry, and may develop into a project area of expanding interest owing of the growing importance recognized nowadays to such clusters.

Overall, the department has defined a good mix of basic and more applied research, with contributions to the basic research area having often a high impact internationally within their community. This is also evidenced by the number of national and international collaborations underway in this department; they are encouraged since they enhance the impact of the work.

The publications (130 publications were published during the evaluation period) of this department have a high international impact (several with IF > 6). A significant number of other publications were published in high-impact international journals of physical chemistry such as *J. Phys. Chem.*, *PhysChemChemPhys*, and *Anal. Chem.* The group also publishes frequently in more specialized journals such as *J. Mass Spectrom.*, *J. Am. Soc. Mass Spectrom.*

The department consists of 9 key scientists and 9 postdocs, one technician, and some students. The age structure of the team at present is quite good with a peak around the 45-50 age cohort. The team is well-balanced with a reasonable number of young graduate students who seem to be quite pleased with their research works and the group ambiance.

2. Strengths and Opportunities

This is a very good multidisciplinary team gathering a set of excellent scientists (former and current Purkynje fellows, l'Oreal prize for young women in science, etc.) with complementary skills and knowledge with good international collaborations.

The members of the department are active in their research fields, with several serving on editorial boards, and are also serving as PI's and co-PI's of collaborative projects.

The department is well equipped with mass spectrometry, cluster-formation means and ion spectroscopy facilities.

The grants come primarily from public sources, mostly from the Grant Agency of the Czech Republic. However, especially in view of the topics covered, the success seems to be stable and fair.

The involvement in teaching at universities is very good. There is also a significant public outreach for the work of the team. That and the intellectual attraction of the topics covered in the Team may explain why there is a reasonable number of young graduate students working its laboratories.

3. Weaknesses and Threats

The team may be engaged into a too broad range of topics. This may limit its capacity in exploring each of them up to the desired level owing to the international standards in these fields.

There is almost no overlap between the two groups (why they coexist within one department?).

Operational costs and those for maintenance and further development of expensive instruments present a financial risk owing to the limited funding from institutional sources.

4. Recommendations

Focus the Team efforts onto a smaller number of research topics. Splitting into two smaller but scientifically more homogenous departments might be a reasonable option owing to the two sub-groups interests.

Even if this adds a new topic to the present ones, the new one aimed to investigate

the influence of free electrons on chemical processes is welcomed. This is an area that could also be of importance in developing more intense industrial contacts.

This is an internationally excellent Team in terms of the originality, significance and rigor but which falls short of the highest standards of excellence owing to its too broad scopes in view of its task-force size.

Evaluation of the Team: Department of Molecular Electrochemistry

1. Introduction

Electron transfer activation of molecules and ensuing processes, i.e., redox-reactions in general, are of very high importance in all branches of chemistry and biochemistry. The group enjoys a high international reputation for its seminal contributions to the area of molecular electrochemistry, ranging from electron transfer processes in single molecules to practical applications of new molecules with interesting electrochemical properties.

During the present period, thanks to its new Director, the group has undergone a profound reorganization of its research scopes. Indeed, previously, despite its rare and world-recognized knowledge about molecular electrochemistry and fine investigations into electron-transfer activation of molecules coupled to group or atom transfers, the group has been trying with pain to redefine its competencies towards modern problems that impact issues of general chemical interest, i.e., well beyond strict molecular electrochemistry. Indeed, owing to the prevalence of reaction mechanisms involving intra- and intermolecular electron transfer steps in chemistry, molecular electrochemical concepts may often provide exceptional entries not available by other methods, even when these entries are not directly related to electrochemistry.

It is clear that the present research directions (electron transfer induced reorganization and intramolecular cross-talk at the single molecule level; design of new multi-redox-active molecules for specific electronic communication; molecular switching and oscillating phenomena; push-pull electronics and 2D-architectures for molecular sensors and electronic gating; etc.) decided by the group show that it has successfully performed its mutation. It is excellent and has already (or, undoubtedly, will rapidly, according to the topics) received high recognition.

This remarkable mutation is also favored by collaborations with excellent international groups which provide the PIs with interesting and important molecules in win-win cooperation that include common publications, student exchange, and funding. Examples for these high-impact collaborations are the study of electron transfer processes in extended viologen molecules (“molecular wires”), the investigation of redox switching in chiral heliquats, and the so-called ‘configurational gating’ that is

observed during reduction reactions of several investigated systems. These studies are sound and of high interest in their own right, but also attract the attention of scientists from other fields (e.g. preparative organic chemists).

The group publication record is excellent with several publications in the world-leading chemical journals (*Angew. Chem.*, *JACS*, *Chem. Eur. J.*), but also in more specialized excellent journals such as *Organometallics*, etc.

This team involves 12 scientists (one is in maternity leave), 1 research assistant and 5 students with, at present, an aggregate number of 7.44 researchers with only 3 of its 16 members above 65 years but 5 young ones. This composition looks adequate to sustain the important reorganization achieved by the group.

2. Strengths and Opportunities

The generational age change that occurred over the evaluated period has thoroughly created new scientific boundary conditions to the group while keeping its traditional strengths brought by its most senior members who still participate in several works.

The vigor of this team is exemplified by its high success in obtaining grants (3 from the CAS, 6 from the Czech Grant Agency, and 2 from the Ministry of Education, as well as 4 grants within international programs) and by 115 publications in high-level international journals of the fields covered. This provides the group with a favorable grant situation that is expected to extend into the future.

The team has a recognized and highly respected international position based on the high expertise of most of its members in molecular electrochemistry as is apparent from the dense research networking of collaborations across Europe and USA.

The ability of the group in redefining its research goals towards excellent domains and to initiate new fields illustrates how this rare knowledge can be adapted to the undertaking of new fundamental researches with potentially applied targets.

3. Weaknesses and Threats

Though several leading members of the group are in a favorable age range, a main threat is related to the age of some of the prominent scientists of the team. The presence of several of these older but highly experienced scientists is an important advantage for the group. It is then essential that several new members may replace them through processes allowing an appropriate transfer of knowledge. This will

preserve the know-how and the enthusiasm for pursuing the recent opening to modern problems.

4. Recommendations

As stated above, over the evaluated period, the group has taken important decision in redefining its research scopes aimed towards important areas involving molecular control of electron transfer activation and transport. The Committee has appreciated all the efforts performed up to now, but insists in affirming that if the present achievements are remarkable, the efforts should be continued and reinforced to reach the high international visibility deserved by the group. This has to proceed not only by publications in top-level journals but also by the participation of the younger scientists to high-level international conferences whose scope goes well beyond strict electrochemistry.

Altogether, this is a strong department working in many different areas both of fundamental and applied importance, so the only recommendation is that the group must pursue its mutation and implement with success its planned researches.

Evaluation of the Team: Department of Low-dimensional Systems

1. Introduction

This Team was established in 2014 as a result of the rebuilding of two former departments of the Institute by integrating the groups of three principal investigators (Dr. Kalbac, the present group Leader, Dr. Bastl and Dr. Krtil). Dr. Bastl is reaching the retirement age, but Drs. Kalbac and Krtil have undoubtedly reached the high scientific levels required to lead the team onto important future research avenues. Researches of the principal investigators have been reported independently in the written documents and during the on-site presentation. This clearly signaled to the Committee that each PI's achievements are worth pursuing, so that care must be taken to avoid weakening some by improper management considerations.

Owing to its three components, the Team forms a well-established group in nanoscience/material research by exploring innovative avenues and producing important fundamental results and applications for nanoelectronics, electrochemical storage and electrocatalysis for fuel cells. Accordingly, the group covers a wide range of fundamental research on carbon nanotubes, fullerenes, graphene and graphene-like materials or nanocrystalline metal nanoalloys and oxides. These materials are prepared and characterized in brand-new electronic-standard clean rooms equipped with lithography and similar microfabrication techniques. Their characterization involves advanced techniques (Raman spectroscopy/microscopy, XPS, spectroelectro-chemistry, surface characterization). In this context, altogether, these laboratories and their researches unified in a single entity form a unique center in the Czech Republic.

The Committee particularly noted the work aimed to “greener” transistors using a graphene basis since, beyond the interesting concept involved, the first results point out to an energy consumption being ca. 1000-times less than for MOSFETs. Also important from fundamental and practical viewpoints is the development of new electrocatalysts for selective sea water splitting through partial replacement of RuO₂ moieties by Zn atoms.

Generally, the Team is very young (with an average age of less than 35 years) and this is especially true for its three PIs. The principal investigators of the Team have independently gained their own international reputation. The team is truly

international (about half of its members came from abroad) and has a good balance between permanent staff and students (10.57 FTE for researchers and 5.08 FTE for other members).

In the recent past, the Team members have secured a number of national and international grants and, currently, it has very reasonable financial support. It benefits from the awarding of one ERC-CZ grant and hired several young foreign postdocs with a positive effects on its personal structure. More precisely, during the last 5 years, members of the Department acted as principal investigators of 13 projects funded by different funding agencies; presently 5 projects are funded (2 from Czech Science Foundation, 1 from Ministry of Education, 1 from EU ITN, 1 from Czech Technological Agency) in addition the above mentioned ERC-CZ grant.

The Team members are also involved in a number of very good international collaborations (e.g., MIT, Boston; Univ. Colorado, Boulder; University of Ulm; IFW Dresden, etc.) and they publish in top-ranked journals (*Angew. Chem.*, *JACS*, *Nano*, etc.), or in material or interdisciplinary journals. Over the period 2010-2014, the members of the Department of Low-Dimensional Systems have thus published (as authors or co-authors) a total of 112 papers in impacted journals.

2. Strengths and Opportunities

Establishing the Department of Low-Dimensional Systems was an excellent opportunity to combine expertise and collaboration between formerly separated groups (however, gaining a full future benefit of this clusterization requires avoiding an important danger, see below §3).

The Team carries out topical research in (nano)material sciences based on the high expertise of each of its PI and its enthusiastic other members, and from very good equipment with their new adequate clean labs (this appears to be truly unique in the Czech Republic).

The Team has been able to attract talented young people from the Czech Republic and from abroad.

Its financial position is expected to remain good during the following years (however, see below §3). The Team has been (or is) involved in several European projects.

3. Weaknesses and Threats

At least in a close future, financing is certain. However, maintenance of the Team infrastructure might result expensive, so means of accessing external and/or internal financial sources should be ensured in the longer term. The same is true for staff and student salaries/stipends that seem to be mostly based on external sources – however, this is a recurrent problem for most chemical institutions in the Czech Republic.

The largest real problem that the group is facing concerns the possible “sterilization” of some of its component(s) to the benefit of other(s) or of other Department(s) from the Institute. The rationale behind the “fusion” is certainly good, but this group’s Leader and the Institute should define conditions prone to preserve the individual competencies of its three PIs and let them to develop. Evidently, this should not prevent productive collaborations between the three PIs on selected targets.

4. Recommendations

The Institute and CAS should clearly decide how the Team and its people/ space/ equipment can be preserved if a problem arises with external financing. Indeed, the Team development should be further cultivated and further consolidated since most of its own research axes are expected to lead to new groundbreaking results by each of its sub-groups, which will benefit to the whole Team and to the Institute. This also involves supporting ALL three groups by providing them with adequate staff structures.

The Team, i.e., including all its scientific components, was considered as one of the best teams evaluated by this Panel, and is undoubtedly the best young group over all CAS chemical Institutes examined by this Committee.

5. Detailed evaluations

The Team members have proven to be able to carry out exceptional researches and to publish in top journals. The area of nanoscience is boosting worldwide and the Team is on the same level as other labs working on similar topics anywhere.

There is an international group of students and postdocs involved in the projects and substantial part of the Team’s work is carried out by students. The Team members are involved in educational activities and scientific boards of universities.

The Team projects deal with fundamental researches comparable to what is ongoing in top-laboratories of advanced countries relying on science and technology as the basis for society development.

The Team is unique in the national context and is fully competitive on the international scene, with already a very good international outreach and visibility. It has already built fruitful collaborations with academic and industrial partners in the Czech Republic, a fact that is important for transferring its knowledge into future technologies.

The Team is very young and motivated and its perspective is rather bright. Their works are also important for education of young people in nanoscience.

Research plans are clearly stated and welcomed by the Committee; fortunately, at least for the next years, the financing seems to be secured.

Evaluation of the Team: Department of Spectroscopy

1. Introduction

During the evaluated period, the former Department of Photochemistry, Spectroscopy and Ion Chemistry has been split up into two new departments, the Department of Spectroscopy and the Department of Chemistry of Ions and Clusters. Each of these teams is nevertheless evaluated independently following the CAS recommendation.

The main scientific activities of the Department of Spectroscopy can be characterized by the development of new types of lasers and photonic materials, the chemistry induced by extremely large laser sparks (used for investigating a hypothesis on origin of life, see below), as well as time-resolved spectroscopy of atoms and reactive intermediates thus created. This led to novel techniques in UV/Vis, infrared and microwave spectroscopies with applications in astrophysics, material sciences and biology.

The research activities of the department over the period of evaluation were distributed over four main interesting research directions: 1) Origin of life; 2) UV/Vis and IR spectroscopy of photoactive molecules and materials; 3) Time-resolved spectroscopy of radicals and molecular ions and 4) Development of new types of lasers for applications in industry. The results concerning the origin of life are certainly very spectacular and have even quickly found their way into the popular press. However, what they really mean about the origin of primal biomolecules is a different question.

Among the several remarkable Team's equipment, the Committee noted the unique high-energy laser facility available to the department for spectroscopic investigations of highly excited metal atoms in relevance to the assignment of spectral lines recorded in astrophysical observations.

The team consists of 5 key scientists, 1 technician, 4 PhD students and several MSc and BSc students, so this is the smallest department in the Institute. The age structure of the team seems favorable at present but the four scientists in the oldest cohort (55-60) could be retiring over the next five to ten years. That calls for plans for bringing younger leadership on board over the next few years.

Overall, this department is doing excellent basic science in the area of molecular and atomic spectroscopy. It publishes regularly in high-impact international journals,

(*Phys. Rev.*, *J. Phys. Chem.*, *Anal. Chem.*, *PhysChemChemPhys*), as well as in more specialized journals such as *J. Mol. Spectroscopy* and *J. Mol. Struct.* The international impact of the work of this department is high, in consonance with the overall impact of the Heyrovsky Institute in the field of physical chemistry.

2. Strengths and Opportunities

The focus on hot topics such as chemical evolution of biomolecules (origin of life) on early Earth, addressing the possibility of spark-source generation of biotic precursor molecules in the pre-biotic environment, provides a high visibility to the Team and to the Institute and Science in general (even if validating this hypothesis is not necessary demonstrating that it has happened).

International and national collaborations with world recognized experts (e.g., for theoretical calculations, and industrial cooperation).

Good involvement in teaching. Ability to attract BSc MSc and PhD students.

Access to large research infrastructures such as PALS and, in future, ELI.

3. Weaknesses and Threats

Limited funding from institutional sources creates a potential risk since the Team's works highly rely on its specific equipment. Additional support from the CAS would be useful, in particular for the appointment of a qualified electronics technician for the laboratories of this Department.

(The inability of the head of the department to present all achievements within his allocated presentation time, led to an unstoppable declination of details and more than doubled his time before he was strongly summoned to stop by the Chair. This was highly embarrassing. Fortunately, this was the only case the whole on-site evaluation of the Institute).

4. Recommendations

The Committee has appreciated all the efforts performed up to now but insists in stating that the present achievements should be continued and reinforced to reach higher international visibility deserved by the group. This has to proceed not only through publications in top-level journals but also through the participation of the younger scientists to high-level international conferences.

A number of important research projects are underway, and should be continued through maintaining strong basic science. This includes the work on pre-biotic origin of life as stated above but also other ones such as the development of vertical cavity surface-emitting lasers for HF detection, and IR-detection of iso-topologues of CO₂, or the time resolved spectroscopy of atoms, radicals and ions in space using deep IR spectroscopy expected to be implemented on the Webb satellite telescope which will be launched in 2019.

Evaluation of the Team: Department of Structure and Dynamics in Catalysis

1. Introduction

The scientific activities of this team focus on the study of the structure (by solid-state NMR) and design of catalytic centers on a sub-nanometer (atomic) scale in crystalline matrices and the synthesis of nanostructured oxidic materials. Future developments include the study of applications in redox-, acid-base- and photo-catalysis.

The strength of the department consists its ability to prepare and characterize novel catalytic materials. Accordingly, the outcomes of the works of this department are highly regarded at the international level. High-impact journals such as *JACS*, *Appl. Phys. Lett.*, *Topics in Catalysis*, and *Inorg. Chem.*, are common places for the publication of the results established in this department.

A number of patents have also resulted from these works. However, industrial collaborations and intellectual property agreements may have limited the visibility of some of the works and may create difficulties to students (Ph.D.s, post-doctoral fellows) in developing their careers, due to restrictions on publication for their work.

An additional strength of the department is its very good age structure. There are a number of young researchers involved in the work, as well as a reasonable distribution of mid-career scientists and older leaders in the group.

2. Strengths and Opportunities

The productivity and publication record of this group is very good, with a significant number of publications in the best journals. The balance between applied and basic research is also satisfactory: the group has already several patents and has applied for other patents.

The number of international collaborations, mainly with other groups in Europe, is also very significant.

The team has a favorable age structure and a good international membership (two out of the six key scientists are from other European countries).

3. Weaknesses and Threats

One important weakness of the department is the phenomenological approach of

most of its development work in catalysis. Although the title of the department is Structure and Dynamics in Catalysis, there does not appear to be much work performed on the mechanistic/dynamic aspects of catalytic research. A focus on more basic science could improve the overall quality of the research outcomes, and lead to further advances for developing new catalysts by implementation of mechanistic results.

It was not clear how well differentiated the work of this department is from the work of the Department of Synthesis and Catalysis.

An important weakness of this group is its low number of Ph.D. students; even if this is also the case with other groups in the Institute, this is highly surprising for this one owing to its large applicative goals. Indeed, such researches should certainly benefit to students interested by industrial careers.

4. Recommendations

Some consideration should be given to the consolidation (or redefinition of roles) of this department vis-à-vis the Department of Synthesis and Catalysis.

The financial support of this group involves a good mix of direct funding by the CAS and industrial collaborations. This enables interesting applications of the materials synthesized in the department. This should continue, though without neglecting the importance of introducing more basic science that should perhaps enable new avenues and novel supports.

Overall, the research plans are very strong and prone to pursue the present aspects of the works performed in the Team. The proposed future focus on the development of nanomaterials and nanotechnologies aimed to impact environmental questions is a good plan.

Evaluation of the Team: Department of Synthesis and Catalysis

1. Introduction

The scientific activities of the team are broad and include the development of novel microporous materials and organometallic complexes as well as their applications in adsorption and catalysis or in medicine. Of particular note is this team's strength on zeolite chemistry, since it has developed new syntheses of 2D-zeolites following original bottom-up approaches using quaternary ammonium salts as templates and by the disassembly of zeolites and their reassembly into new types of zeolites (two papers in *Nature Chemistry* have been published on this topic). Zeolites and conceptually related metal-organic frameworks (MOFs) are also being developed in this team for their applications in adsorption of gases (such as CO₂) and in catalysis.

The activities on metallocene chemistry are more conventional and focus on basic organometallic Ziegler-Natta-type reactivity of titanocene complexes and on the heterogenization of metallocenes and ruthenium metathesis catalysts. Based on their expertise on metallocenes, the team also participates in the development of new anti-cancer drugs based on bio-organo-organometallic concepts.

The work on the influence of zeolites on classical organic transformations such as oxidations (epoxidation, Baeyer-Villiger oxidation) rearrangements (Beckmann), condensation reactions (Knoevenagel, Friedländer) and transformations of aromatic substrates (substitution, isomerization) was very impressive. It is hoped that these very useful processes become popular in organic synthesis soon.

Similarly, the preparation of new zeolites by the so-called 'ADOR' method is of extreme interest, since it should allow the preparation of zeolites with a continuously tunable porosity. This discovery could have a very strong influence on the practical use of zeolite catalysts in industry.

This team is one of the largest of the J. Heyrovsky Institute, with presently an aggregate number of 11.2 researchers and 6.51 other members. Additionally, most of its members are young (7 PhD students) with only 4 senior scientists being above 60 years and 3 between 55 and 60. It is important to note that this team has been able to attract many foreign Ph.D. graduate students from other European countries.

Many publications have an excellent quality and appeared in the very best journals (*Nature Chemistry*, *JACS*, *Chem. Rev.*, *Angew. Chem.*) or in very good more specialized ones.

2. Strengths and Opportunities

The vigor of this team is exemplified by its highly original contributions on zeolite chemistry and by its publications in the top journals of chemistry (*Nature Chemistry*, *Angew. Chem.*, *J. Am. Chem. Soc.*, *Chem. Rev.*) as well as by its overall publication record (154) in journals with significant impact factors or by many awards and invited lectures in major conferences.

Noteworthy, the group has developed several collaborations with very good international partners that appear to be based on win-win mutual cooperation.

The balance between applied and basic research is also satisfactory: the group has also several patents and has issued several patent applications.

Though this is not easily found in the written report, the group seems to have a high success rates in obtaining national or international grants relative to all fields covered in the team.

The group important recent changes provide great perspectives for the future, especially considering the team favorable age structure.

3. Weaknesses and Threats

The only weakness detected concerns the approaches pursued on metallocene chemistry, which are mostly rather conventional. However, the activation of H₂S coupled with the preparation of titanocene sulfide complexes is interesting from a mechanistic and structural viewpoint; as far as one can tell this is a new way of preparing dimeric titanocene sulfides.

The present large unbalance between permanent staff and non-permanent ones (i.e., whose salaries are, at least in part, paid from grants) may create a difficulty since the stability of the group is relying on a continuous success of its applications to grants calls (note that even if this is the normal way in US, here the situation is changed in that it involves professional experienced scientists beyond the Department Director).

4. Recommendations

The research directions appear of high interest and perfectly compatible with the impressive knowledge and savoir-faire gathered in the group.

CAS should clearly decide how to remediate the financial threat in §3 to allow the team to successfully pursue its excellent researches by keeping its experienced scientists.

Hydrogenation of double and triple bond systems with H_2 and various titanocene complexes have been studied comprehensively. Though these reactions are probably of little importance in organic synthesis (viz., for the preparation of fine chemicals) they may be useful for other industrial applications. The group is encouraged to investigate such avenues.

Evaluation of the Team: Department of Theoretical Chemistry

1. Introduction

This team dates back to its creation by Professor Rudolf Zahradnik, who played a crucial role for the permanence of Quantum Chemistry in Czech Republic. After 1968, when several important Czech quantum chemists left the country, R. Zahradnik was virtually the only professor to stay on place. His influence extended not only to the former Czechoslovakia, but also to East Germany.

The team headed now by Dr. Jiří Pittner currently consists now (i.e., in 2015) of ten scientists and six Ph.D. students, and has a favorable age distribution exhibiting a maximum around 35-40 years.

The group has an excellent international reputation, and participates in several national and international collaborations involving very good foreign teams.

The Committee was impressed by the breadth of the methods developed in this group to better understand important problems from a theoretical viewpoint. Methodological developments extend from new ‘Coupled Cluster’ methods, to new DFT and the so-called quantum chemical Density Matrix Renormalization Group (DMRG) methods. Among the “practical” problems studied, the work on zeolites needs to be mentioned as well as the molecular dynamics (MD) simulations of photochemical processes.

The team published 96 scientific papers and 9 chapters in books over the period evaluated (2010-2014). These papers have been published in international journals, most typically in high-quality ones for the field (e.g. *J. Chem. Phys.*).

2. Strengths and opportunities

To the best of knowledge of the Committee, this group is only one among the theoretical teams of the CAS, which develops essentially new quantum-theories. In short, it may be said that its scientific output certainly belongs to the frontiers of quantum chemistry.

The team successfully applies its expertise to several problems of important practical character such as the molecular dynamics of lipid layers, and chemical catalysis in zeolites.

The funding situation (grants from various sources) seems to be stable (but see below §3).

3. Weaknesses and threats

No essential threat was identified except for those that typically burden most CAS chemical institutes, i.e., the difficulties in attracting young students, particularly from abroad. Though, it is noted that the department is heavily involved in various teaching projects at Charles University.

Similarly, continuous financial support for (foreign) researchers remains a permanent problem as in most other groups

4. Recommendations

The planned researches seem sound and should help the Department to further increase its scientific outreaches and international visibility.

The reasons underlying the low student flux should be clearly analyzed. However, this is valid for most of the Teams and Institutes evaluated by this Committee.

5. Detailed evaluation

The group scientific impact and reputation are linked to the creation of chemical theories and computer programs (codes) based on them.

The theory preferred (correctly) is the known Coupled Cluster method, currently the best one in quantum chemistry (that, by the way was introduced in quantum chemistry by Jiri Cizek, a former member of the Heyrovsky Institute). The method is based on postulating the so called wave operator that transforms a starting wave function into the exact one (ground-state). In this scientific direction, the team attacks a very difficult problem of quasi-degeneracy of the lowest-lying states in the energy scale. In other words, these are highly-correlated systems, which are sensitive to even small external interactions. The 'Coupled Cluster' method is a good basis for finding the wave operator, provided that the starting wave function is already good. This is precisely what the team ensures by carefully choosing starting wave functions as linear combination of several electronic configurations (Multi-Reference, MR).

The same problem is attacked in parallel by the team using a novel method called DMRG (Density Matrix Renormalization Group). Though this method is not yet an established theoretical tool, it is apparently particularly useful for such quasi-

degenerate problems.

Another avenue investigated by the team relies on the use of the Localized Pair Natural Orbitals. The goal is to increase the numerical efficiency of quantum calculations; this is indeed possible by profiting of the concept of localized electronic orbitals (instead of usual delocalized ones). The ultimate goal – which seems theoretically possible based on these approaches - is to achieve a linear scaling of the computation times with the molecules sizes, i.e., to afford a considerable gain that should enable the computation of much larger systems than feasible today.

Finally, the group investigates and, in several aspects, pioneers a very important problem, viz., electron-molecule collision. There, the key states are electronic resonances, i.e., states that are quasi-stable. These states thus require special care since they are not stationary solutions of the Schrodinger equation.

Date: December 31, 2015

Commission Chair: Dr Habil, Academician Christian Amatore