*The **CREA**tion of the Department of Physical Chemistry of Biological Sys**TE**ms [CREATE]*

666295 — CREATE — H2020-WIDESPREAD-2014-2015/H2020-WIDESPREAD-2014-2

Report on the visit of prof. Pavel Jungwirth

[WP3]

Level of dissemination: PUBLIC

Warsaw, October 2016

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INTRODUCTION

The visit of Prof. Pavel Jungwirth at the Institute of Physical Chemistry of the Polish Academy of Sciences (IPC) was held under a series of cyclical lectures on interdisciplinary emerging research.

For this reason Prof. Pavel Jungwirth was invited to IPC to:

- deliver two lectures:
  - seminar on his studies,
  - seminar on education and organization reform that took place at the Czech Academy of Sciences,
- participate in meetings with synergetic teams to support mentoring activity of the ERA Chair holder,
- take part in the consultations on possible changes in IPC research/doctoral programme.

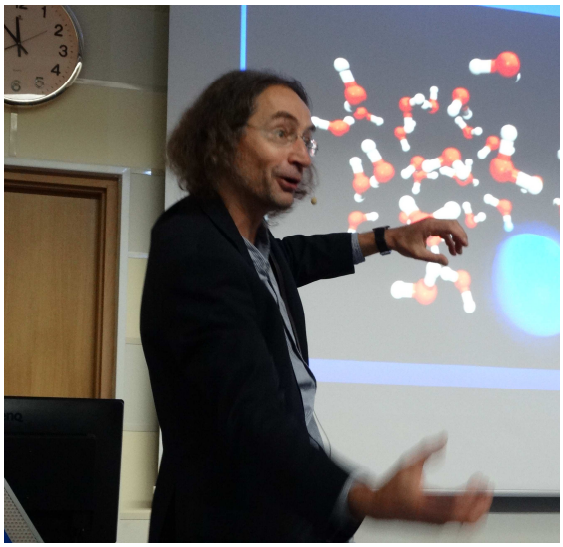
Professor Pavel Jungwirth is a physical chemist, university lecturer and popularizer of science. He studied physics at the Charles University in Prague, Faculty of Mathematics and Physics. His studies focused on chemical physics. He received his Ph.D. in computational chemistry from J. Heyrovsky Institute of Physical Chemistry, Academy of Sciences of the Czech Republic and Charles University in Prague in 1993 under supervision of Prof Rudolf Zahradník. Currently, he holds a position of the Head of research group at the Institute of Organic Chemistry and Biochemistry of the Czech Academy of Sciences in Prague.

His research interests focus on molecular simulations of ions at aqueous interfaces, including interactions of ions with proteins and membranes, chemistry of aqueous aerosols, structure and dynamics of solvated electrons. The scientific profile of Prof. Pavel Jungwirth is included in annex 1**.**

THE COURSE OF THE VISIT

The visit of Prof. Pavel Jungwirth took place on the 20th – 21th, October, 2016 [see annex 2 for agenda].

On the first day of the visit, Prof. Pavel Jungwirth delivered a seminar entitled *"Exploring Hydrated Electrons in Non-Conventional and Conventional Ways: From Alkali Metal Explosions to Non-Explosive Ways"*. The seminar was held in the assembly hall of IPC. All researchers and PhD students employed at IPC were invited to participate in this seminar.



The seminar of Prof. Pavel Jungwirth, assembly hall, the 20th October, 2016.

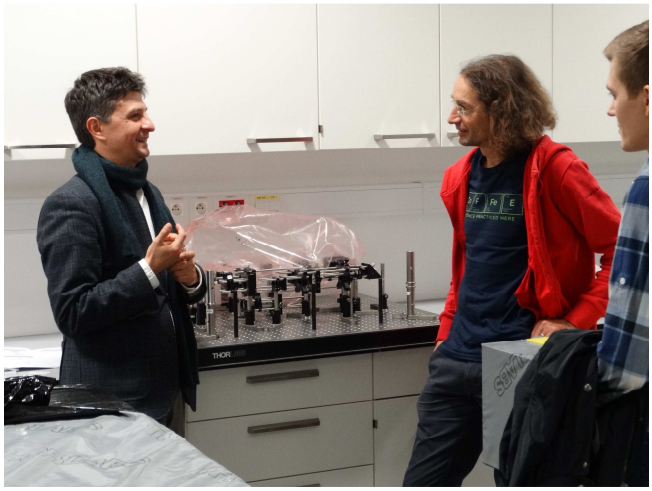
Abstract of the seminar

A dangerous – but among school kids all-time favorite – experiment demonstrating an explosive chemical reaction is throwing a piece of sodium into water. Every high school chemistry teacher knows that the explosion releases electrons from the metal to water which is accompanied by formation of steam and molecular hydrogen, which can ignite during this exoergic process. The very same gases should, however, separate the reacting metal and water and thus quench the reaction. How come that the explosion occurs anyway? Using ultrafast cameras and ab initio as well as force field molecular dynamics simulations Prof. Jungwirth and his team discovered a hitherto unknown primary mechanism of the explosive behavior of alkali metals in water. Namely, after migration of electrons from the metal to water the former acquires a huge positive charge. Thanks to mutual repulsion of these charges the metal undergoes a Coulomb explosion accompanied by ejection of metal spikes into water. This enables effective mixing of reactants, which is a necessary condition for the explosion. They also proved how blue solvate electrons formed during this reaction can be observed with a naked eye despite their sub-millisecond lifetime in water.

The seminar was aimed at encouraging scientists (in particular – junior researchers) to get inspiration for their studies from daily observations, and real life.

After the seminar, Prof. Pavel Jungwirth visited selected laboratories. The aim of this visits was to familiarize with IPC PAS, establish contacts with synergic groups supporting the ERA Chair holder and discuss possibility of future cooperation.

Meetings with the following research groups were organized:



Prof. Maciej Wojtkowski, *ERA Chair Holder, Head of the Department of Physical Chemistry of Biological Systems, Physical Optics and Biophotonics Group*

Prof. Maciej Wojtkowski is a physicist specializing in optics applications to biology and medicine. He designed and constructed the first Fourier Domain Optical Coherence Tomography instrument for in vivo retinal imaging. Currently, he holds the position of ERA Chair holder and is responsible for setting a new Department in IPC PAS.

Dr. Gonzalo Angulo, *Associate Professor, Laser Centre Group*
Dr. Yuriy Stepanenko, *Laser Centre Group*
Dr. Michal Nebauer, *Laser Centre Group*
Dr. Marcin Pastorczak, *Laser Centre Group*

Laser Centre Group is focused on development and exploration of experimental techniques to study ultrafast physical and chemical processes. The members of the Group discussed such projects as:

- chemical reactions under strong light illumination,
- designed and built by themselves a time resolved fluorescence spectrometer able to observe fluorescence emitted by molecules exited by an ultra-short pulse.

Dr. Piotr Zarzycki, *Head of the Charge transfer in biological systems and at the interfaces Group*. He studies molecular geochemistry, in particular, he develops and uses molecular modeling methods to solve geochemically relevant problems (mineral/ water interfaces, electron/ proton transfer in environmentally important settings).

Dr. Patryk Zaleski-Ejgierd, *member of the Group of Charge transfer in biological systems and at the interfaces* . He investigates hypothetic High-Pressure compounds.

Dr Adam Kubas, *member of the Modern Heterogenous Catalysis Group (MoHCa)*

His scientific interests include:

- theoretical aspects of catalysis,
- hydrogenases and FeS clusters,
- small molecules activation,
- electron transfer kinetics,
- multireference methods for electronic structure calculations.

Prof. Jacek Waluk, *Head of Photochemistry and Spectroscopy Department, head of the Group of Photophysics and spectroscopy of photoactive systems: structure and reactivity of systems with hydrogen bonds.*

His research encompasses various aspects of physical organic chemistry. A subject of particular interest is proton/hydrogen transfer, intra-molecular as well as intermolecular, occurring in the ground and excited electronic states.

Moreover prof. Pavel Jungwirth also visited very talented young researchers, among them were:

- Michał Hamkało (PhD student) who was awarded Gold Medal of Chemistry 2014 – a prestigious prize given by the Institute of Physical Chemistry of the Polish Academy of Sciences for best diploma thesis (in chemistry, physics and biology) in Poland. In October 2016 Michał joined the Department of Physical Chemistry of Biological Systems at IPC led by prof. Wojtkowski, where he works on implementing Optical Coherence Tomography (OCT) for heart imaging, and novel techniques of nanoscale bioimaging with use of ultrafast lasers.
- PhD. Krzysztof Sozański who is the post-doc affiliated with the Soft Condensed Matter Group since the 2nd year of his BSc studies. MSc received in 2013 from the University of Warsaw, Faculty of Chemistry; PhD -- from the IPC PAS in 2015 (with distinctions; at the age of 24). Currently, he deals with motion- and chemical kinetics in crowded systems, and an inclination towards biomimetic and biological systems.

The second day of Prof. Pavel Jungwirth's visit (the 21st October, 2016) was devoted to organizational reforms. In the first part of the day, Prof. Jungwirth delivered a *"Seminar on the successful reform of Czech research institutes followed by discussion on desired changes in Polish science: People first, machines and buildings later"*. The seminar was held in the assembly hall of the IPC PAS. All researchers and PhD students employed in the IPC PAS were invited to participate in this seminar. During this seminar an open discussion was provided – all participants were encouraged to participate in open discussion on the reforms in education and research institutes.

The seminar of Prof. Pavel Jungwirth, assembly hall, the 21th October, 2016.

After the seminar, the discussion on reforms was continued in a group of:

- **Professor Pavel Jungwirth** – the visiting guest
- **Professor Maciej Wojtkowski** – the ERA Chair holder, head of Department of Physical Chemistry of Biological Systems, IPC PAS
- **Professor Robert Holyst** – Project Coordinator, head of Department of Soft Condensed Matter, IPC PAS
- **Agnieszka Tadrzak –** CREATE Project Manager, Manager for R&D funding at the IPC PAS.

Discussion on educational reforms. From left: Prof. R. Holyst, A. Tadrzak, Prof. M. Wojtkowski, Prof. P. Jungwirth.

The whole discussion lasted about 2 hours. During this meeting the consultations about possible changes at IPC research and doctoral programme were carried out. Prof. Pavel Jungwirth described the changes which were launched in the Czech Academy of Sciences (mainly regarding implementation of transparent procedure for Academy members' recruitment, and resulting from law - a ban on conducting doctoral studies at institutes of the Czech Academy of Sciences). Prof. Maciej Wojtkowski mentioned that some of the changes implemented to the Czech Academy of Sciences were also introduced into IPC (like flat group structure, reduced influence of hierarchical structures, cooperation between IPC groups, putting the stress on changes in the organization and methods of management). Prof. Pavel Jungwirth suggested that it is advisable to improve the image of IPC as well as to strengthen the position of researcher in Polish society. After the meeting the ERA Chair holder made some comments and formed new recommendations aimed at IPC organizational and structural change, *inter alia* referring to:

- The potential of International Advisory Board of IPC is not fully exploited – their engagement in the process of evaluating, recruiting and building the image of IPC should be strengthened.
- It would be advisable to launch a transparent structure of internal granting system in case new funding options occur – the structure adapted to the stage of the researchers' careers as well as to specificity of work (fundamental or application research).
- Strengthening the IPC image – participation at conferences of larger groups of researchers, and in particular - participation of PhD students, and young scientists in significant national and international conferences, participation in major European consortia that enable applying for financial funds.
- Strengthening vertical integration of different research types – different evaluation criteria of leaders and members of the group, introduction of research groups categories, differentiation of team members dependent upon nature of the work performed (e.g. senior researcher, senior engineer, supporting staff etc.).

- Support in initiating and/or participation in existing large European consortia seeking funding – selection of 3-5 group leaders with the best potential and stimulate action towards creating a pan-European organization or research projects, which may as a whole to apply for funds from the European Union.
- Internationalization of the PhD programme incl. an increase of attendance of the PhD students at international significant conferences, and other events.
- Improvement of IPC image and reinforcement of PR activities.

ANNEX 1.

SCIENTIFIC PROFILE OF PROF. PAVEL JUNGWIRTH

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Prof. Pavel Jungwirth – scientific profile of the researcher

***Academic Training*:**

- PhD. in Computational Chemistry at J. Heyrovsky Institute of Physical Chemistry, Acad. Sci. of the Czech Rep. and Charles University, Prague, Czech Rep., 1993. Thesis title "Ab initio molecular dynamics: Dreams and reality"

***Academic Experience and Previous Positions*:**

- Golda Meir Postdoctoral Fellow at the Hebrew University of Jerusalem, Israel , 1994-5.
- Postdoctoral Fellow at the University of California, Irvine , 1995.
- Research group head at the J. Heyrovsky Institute of Physical Chemistry, Prague, 1995-2003.
- Visiting professor at the University of Southern California, Los Angeles, 2007.
- Visiting professor at the École Normale Superiéure, Paris, 2010.
- Visiting professor at the Rush University, Chicago, 2012.

***Present Positions*:**

- Research group head at the Institute of Organic Chemistry and Biochemistry, Acad. Sci. of the Czech Rep., Prague, Czech Republic (2003 -).
- Professor (External Faculty) at the Charles University in Prague, Faculty of Mathematics and Physics (2011 -).
- Finland Distinguished Professor at the Tampere Institute of Technology – FiDiPro program of the Academy of Finland (2013 - 2017).

***Main Scientific Awards*:**

- Annual Medal of the International Academy of Quantum Molecular Science (2001).
- Spiers Memorial Prize of the Royal Society for Chemistry (2008).
- Elected member of the Learned Society of the Czech Republic (2009).
- Praemium Academie Prize from the Czech Academy of Sciences (2010).
- Jaroslav Heyrovsky Medal of the Czech Academy of Sciences (2015).

Servis to the Scientific Community:

- Senior Editor of Journal of Physical Chemistry of the American Chemical Society (2009 -).
- Member of Editorial Board of Chemical Physics Letters (2007 -).
- Member of Editorial Board of Accounts of Chemical Research (2015 -).
- Popularizer of science – regular articles in Czech newspapers and magazines on science and society. Numerous radio and TV shows on popular science.

***Publications and presentations*:**

Around 300 research and review papers in international journals with more than 10000 citations, H-index 51.

Research funding (only current grants):

- ”Beyond the Hofmeister series: From molecular understanding of specific ion effects to their biological function” Czech Science Foundation, 2016-2018, 192,000 EUR.
- ”Interaction of ions with biomolecules in solutions: Computer simulations and experiments.” Praemium Academie of the Acad. Sci. of the Czech Rep., 2010-2016, 1.1 million EUR.
- “Translocation of molecules across cell membranes.“ FiDiPro of the Academy of Finland, 2013-2017, 1.2 million EUR.
- “Controlling structure and function of biomolecules at the molecular scale: Theory meets experiment.“ Czech Science Foundation Centers of Excellence, 2012-2018, 420,000 EUR directly to me as a Team Leader within the Center.

ANNEX 2.

Full agenda of the visit of Prof. Pavel Jungwirth

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CREATE lectures

The Institute of Physical Chemistry of the Polish Academy of Sciences

Agenda

20th October, 2016

10.30-12.00	**Pavel Jungwirth**
	„Exploring Hydratated Electrons in Non-Conventional and Conventional Ways: From Alkali Metal Explosions to Non-Explosive Ways"
12.00-13.00	**Lunch**
13.00-14.50	**lab visits**
	13.00-13.30 Prof. Maciej Wojtkowski
	13.30-13.50 dr Gonzalo Angulo
	13.50-14.10 dr Yuriy Stepanenko
	14.10-14.30 dr Piotr Zarzycki
	14.30-14.50 dr Patryk Zaleski-Ejgierd

21th October, 2016

9.40-10.10	**lab visits** - Prof. Jacek Waluk
10.30-12.00	**Pavel Jungwirth**
	„Seminar on the successful reform of Czech research institutes followed by discussion on desired changes in Polish science: People first, machines and buildings later" – with open discussion
12.00-13.00	**Lunch**
13.00-15.00	**Discussion on education reforms**
15.30	**Departure to the airport**

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