*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. Jochen Blumberger

[WP3]

Level of dissemination: PUBLIC

Warsaw, February 2018

This project has received funding from the *European Union's Horizon 2020 research and innovation programme* under grant agreement No 666295

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INTRODUCTION

The visit of Prof. dr Jochen Blumberger 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. Prof. Jochen Blumberger was invited to IPC to:

- deliver seminar composed of two parts:
  - current studies of Prof. Blumberger and his group,
  - the art of leading a research group,
- participate in meetings with synergetic teams to support mentoring activity of the ERA Chair holder,
- take part in the consultations on required changes at IPC to improve our performance.

Professor Jochen Blumberger obtained a Master degree in Interdisciplinary Natural Sciences from ETH Zurich (2001) and a PhD degree in Theoretical Chemistry from Cambridge University (2005). During his PhD he worked on density functional based molecular dynamics simulation of redox reactions, under the supervision of Professor Michiel Sprik. After a 2-year post-doctoral stay with Professor Michael L. Klein at the University of Pennsylvania he returned to Cambridge on a Royal Society University Research Fellowship (2006). In 2009 he moved to University College London (UCL), Department of Physics and Astronomy, where he was appointed University Lecturer (2009), Reader (2013), and Professor of Chemical Physics (2015). In 2016 Professor Jochen Blumberger have been awarded **ERC Consolidator Award** to develop a novel computational method for the simulation of charge carrier transport in organic semiconducting materials and proteins that find applications in organic photovoltaic cells and nanobioelectronic devices.

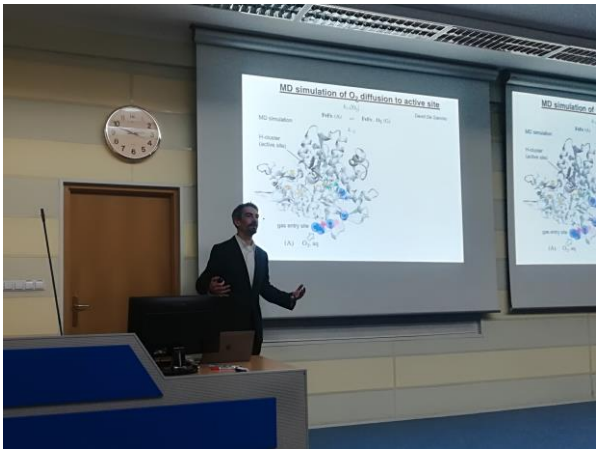
THE COURSE OF THE VISIT

The visit of Prof. dr. Jochen Blumberger took place on the 22 – 23, February, 2018 [see annex 1 for agenda]. On the first day of the visit, Prof. Blumbereger delivered seminar composed of 2 parts:

- **“Inorganic Interfaces, Organic Materials and Energy Converting Enzymes: The Power of Computational Chemistry”**
- **“The Art of Leading a Research Group”**

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 [see annex 2 for poster promoting the seminar] – the seminar was attended by approx. 70 people.



The seminar of Prof. dr Jochen Blumberger, assembly hall, the 22nd February, 2018.

Abstract of the seminar

Inorganic Interfaces, Organic Materials and Energy Converting Enzymes:
The Power of Computational Chemistry

In the last few decades we have witnessed tremendous progress in Computational Chemistry and Physics due to more refined and efficient theoretical algorithms that enabled us to solve, albeit still approximately, some of the most fundamental equations that govern chemical and physical processes. As a result, Computational Chemistry has penetrated many sub-disciplines of the Natural Sciences in the last thirty years, from Astrochemistry to Material Science and Biological Physics as a complementary tool that aids our interpretation and understanding of Chemistry and Physics at the molecular level. In his talk, Prof. Blumberger surveyed a number of studies where his group used modern electronic structure calculations as well as state-of-the-art molecular dynamics simulations to gain mechanistic insight into a diverse range of chemical and physical processes. He presented results on the atomistic structure and dynamics of transition metal oxide/liquid water interfaces relevant for electrochemical water splitting. Prof. Blumberger also explained challenges one faces when it comes to describing charge transport processes in organic materials that form the active layers of organic light emitting diodes and organic solar cells, and simulations of electron flow in some of the most intriguing enzymes that have evolved to export electrons from the inside of the cell to extracellular space. Finally, Professor described how small inhibitor molecules diffuse to active sites of hydrogen-converting enzymes (hydrogenases) and the theoretical method they have put forward for prediction of mutations that could interfere with ligand diffusion and binding.

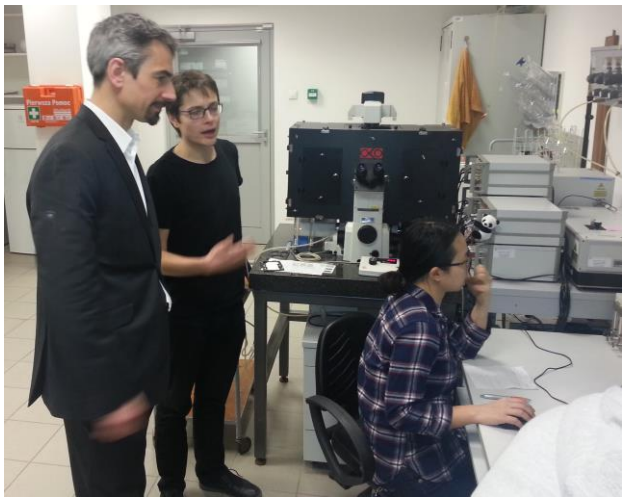
The Art of Leading a Research Group

Leading a research group requires some of the skills we thought we would never need when we decided to become a scientist. After years of post-doctoral work where scientific reasoning, realism and painstaking attention to detail counts everything, we are suddenly confronted with writing ambitious grant proposals that promise to solve the many problems of this world. After a 10-minute conversation with the interviewee we should be able to tell if he/she makes a successful PhD student or Postdoc or if most of the answers given were just hot air. We are supposed to motivate our group members, comfort them if experiments give zero results after years of preparations and encourage them to become the leaders of the future. The "human component" that comes into play when leading a group should not be underestimated - it is (almost) as important as the science itself. I will give a (necessarily) personal view on some of the issues a scientific group leader faces, including best practices in leading a group, optimal group size, hints about hiring and interviewing, publishing and writing of grant applications.

During the first and the second day of his visit, professor Blumberger visited selected laboratories. The aim of this visits was to familiarize with IPC, establish contacts with "synergic groups" from CREATE project supporting the ERA Chair holder and discuss possibility of future cooperation. Meetings with the following research groups were organized:

Modern Heterogeneous Catalysis Group

Prof. Blumberger visited the laboratory of the Modern Heterogeneous Catalysis Group and had a possibility to talk to **dr hab. Anna Śrębowata**, Prof. IPC PAS, and **dr Adam Kubas,** Adjunt. He learned about hydrogenation reactions and theoretical calculations that are carried out in the group. In particular – sophisticated, built in-house hydrodechlorination set-up for water purification attracted his attention. He also discussed new outcomes regarding theoretical calculations on iron-sulfur systems for biological electron transport and expressed his interest to perform some of additional calculations in his group.

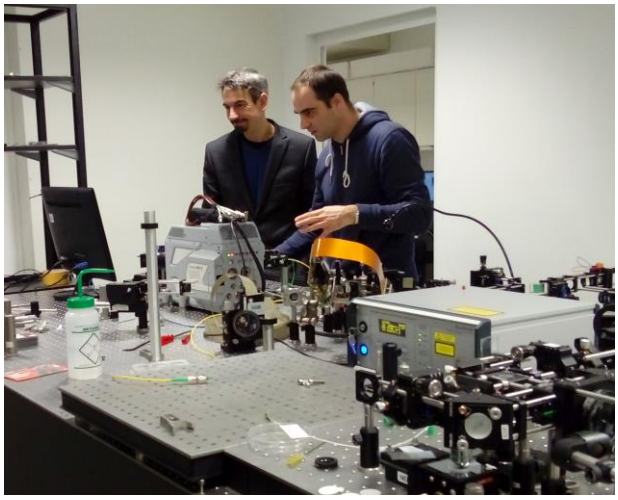


Research group of Soft Condensed Matter

Prof. Blumberger visited laboratories of the Soft Condended Matter Group, where he was guided by **dr Krzysztof Sozański** and **Krzysztof Szczepański**. The visit was focused on the fluorescence microscopy facility and cell culture labs. A natural starting point for the discussion was how a quantitative, physics-driven approach can be applied to solve biological problems. It was also a great occasion to share some valuable insights on the synergy effect obtained through parallel use of theoretical and experimental methods in particular biophysical research projects.

Organometallic and Materials Chemistry Group

In Prof. Janusz Lewiński's laboratory, Jochen Blumberger was exposed to diverse scientific fields explored by this group, including reactions that involve dialkilzinc species, synthesis of nano-ZnO and advanced mechanochemical transformations. The discussion with Prof. Lewiński was very fruitful as it may constitute a background for new collaboration in order to understand unusual charge-transport properties of nano-ZnO obtained in the group.



Physical Optics and Biophotonics Group, Department of Physical Chemistry of Biological Systems

Professor Jochen Blumberger met with the POB group members including the head of the group - prof. Maciej Wojtkowski, ERA Chair holder. The guest was introduced to POB's high throughput swept source full field oct system. During the meeting the discussion on distinguishing features and limitations of the setup as well as potential took place. POB's members pointed out possibility of registering dynamic reactions on demand in 3D. This kind of observations might be accomplished with POB's device, since it can be externally triggered and acquire 3D data within 5 ms.

After visiting selected laboratories, on the second day of the visit, the summary of the visit and discussion on recommendations for the Institute took place in a group of:

- ✓ **Prof. Jochen Blumberger** – the visiting guest,
- ✓ **Prof. Maciej Wojtkowski** – the ERA Chair holder, head of Department of Physical Chemistry of Biological Systems, IPC PAS ,
- ✓ **Prof. 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 between prof. Robert Hołyst, prof. Maciej Wojtkowski, Agnieszka Tadrzak and prof. Jochen Blumberger (from left).

The discussion lasted ca. 1 hour. The following topics were discussed:

- approach of University College London (UCL) to doing research on the boarder of different disciplines,
- different forms of cooperation between theorists and experimentalists,
- career development, different career paths, and promotion,
- approach to evaluation of researchers,
- other types of positions at UCL supplementing competencies of researchers.

Professor Blumberger positively assessed IPC capacities in terms of linking different fields of science in a single institute. Answering a question of professor Hołyst he described formulas of engaging theorists at University College London (UCL). At UCL theorists constitute separate groups capable of conducting own studies, but there are also experts in experimental groups giving explanations and building theoretical bases for obtained results. He also assumed that engaging external experts can a good idea but it depends on the expert's profile.

Professor Blumberger also stated that researchers at UCL have very clearly defined professional duties (e.g. research, incl. publications and grant applications, and admitting students for PhD studies). Career paths and requirements for different positions are clearly defined in a document entitled: "*UCL Academic Careers Framework*". Promotion of an individual (incl. wage increase) is a subject for an application and assessment. Only evaluation of individuals is conducted. The whole group is not the subject for assessment. Technicians are not admitted to individual research groups but they constitute of separate group serving the whole UCL community.

After the meeting some new recommendations aimed at IPC organizational and structural change, were formulated, incl. necessity to describe variety of career paths at IPC taking into account differentiated employees' profiles, flexibility as regards to research groups composition, in particular it refers to hiring technicians, theorists and experimentalists.

ANNEX 1.

Full agenda of the visit of Prof. Jochen Blumberger

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CREATE lectures

The Institute of Physical Chemistry of the Polish Academy of Sciences

Agenda

February 22, 2018

12:00 – 1:00 pm	**Lunch**
1:00 – 1:40 pm	**Lab visit**
	Anna Śrębowata, PhD; Adam Kubas, PhD
	Modern Heterogenous Catalysis Group *Department of Catalysis on Metals*
2:00 – 3:30 pm	**Seminar - Prof. Dr. Jochen Blumberger**
	„Inorganic Interfaces, Organic Materials and Energy Converting Enzymes: The Power of Computational Chemistry"
	"The Art of Leading a Research Group"
4:00 – 5:00 pm	**Lab visits**
4:00-4:30	Krzysztof Sozański, PhD
	Soft Condensed Matter Group *Department of Soft Condensed Matter*
4:30-5:00	prof. Janusz Lewiński
	Organometallic and Materials Chemistry *Department of Physicochemistry of Supramolecular Complexes*
8:00 – 11:00 pm	**Dinner**

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February 23, 2018

8:45 – 9:45 am	**Lab visit and meetings with POB group members**
	Physical Optics and Biophotonics Group (POB), Department of Physical Chemistry of Biological Systems
8:45 – 8:55	Paweł Wnuk, PhD
8:55 – 9:05	Paulina Niedźwiedziuk
9:05 – 9:15	Mounika Rapolu
9:15 – 9:25	Patrycjusz Stremplewski, PhD
9:25 – 9:35	Piotr Ciąćka, PhD
9:35 – 9:45	Dawid Borycki, PhD
9:45 – 10:30 am	**Meeting with ERA Chair Project Coordinator and ERA Chair holder**
	Short discussion, summary of the visit and recommendations for IPC PAS

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ANNEX 2.

Poster promoting the seminar

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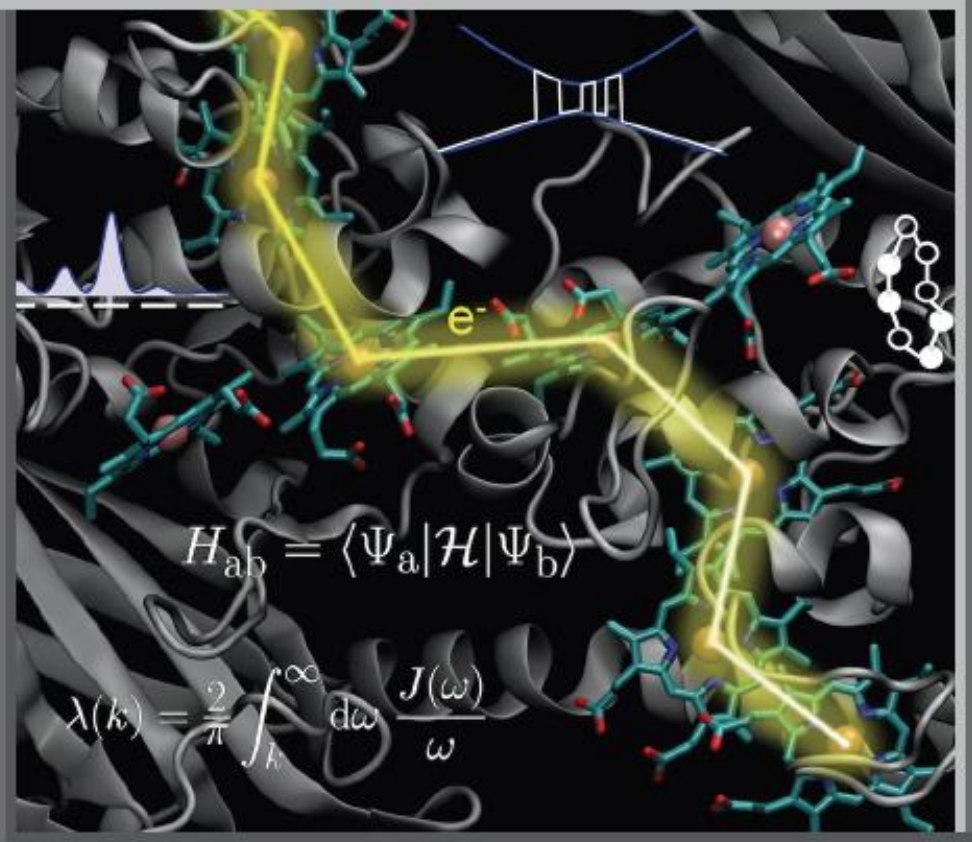
INSTITUTE OF PHYSICAL CHEMISTRY PAS - **SEMINAR LECTURE**

Prof. Dr. Jochen Blumberger

University College London,
Department of Physics and Astronomy, London, UK

Inorganic Interfaces, Organic Materials and Energy Converting Enzymes: The Power of Computational Chemistry

The Art of Leading a Research Group



22 February 2018 (Thursday), **14:00-15:30**
Assembly hall of the IPC PAS
Warsaw, 44/52. Kasprzaka

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