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

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Report on the visit of prof. Prof. Johannes Kästner

[WP3]

Level of dissemination: PUBLIC

Warsaw, November 2019

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. Johannes Kästner 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. Kästner was invited to IPC to deliver seminar lecture on his studies.

Johannes Kästner is professor of Computational Chemistry at the Institute for Theoretical Chemistry, University of Stuttgart. He received his PhD in theoretical physics from the Technical University of Clausthal. He was a postdoctoral research associate at the Max Planck Institute for Coal Research and a researcher at Daresbury Lab in the UK. 2008, he joined the University of Stuttgart, initially as a Junior-professor. 2014, he received tenure and is now professor of computational chemistry. 2012, he received the Hans G. A. Hellmann award in theoretical chemistry. Since 2015 **prof. Kästner is a recipient of an ERC Consolidator Grant** for his work about chemical reactions in quantum mechanical tunnelling.

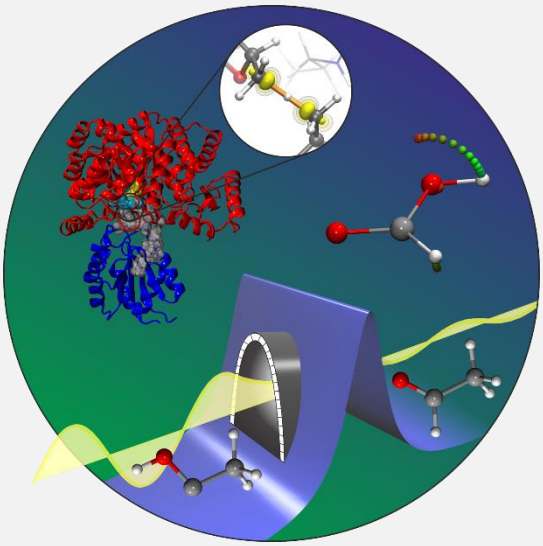
Professor Kästner's research focuses on computer simulations to investigate chemical and biochemical reactions. These include enzymes, biological receptors, but also astrochemistry, materials properties and catalysis. To make such investigations more efficiently and more accurately in the future, his group has been developing some new methods for chemical simulations. These include methods to calculate atom tunnelling rates, free-energy differences as well as optimization of chemical structures, possibly involving thousands of atoms. Their latest field is the use of machine learning techniques in computational chemistry.

THE COURSE OF THE VISIT

The visit of prof. Johannes Kästner took place on the 6th – 7th, November, 2019 [see annex 1 for the agenda].

On the 7th of November prof. Kästner delivered seminar entitled *"Tunnelling Processes in Chemistry Simulated with Instanton Theory"*. 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.

Abstract of the seminar



The tunnelling of atoms accelerates many chemical reactions from catalysis via biochemistry to astrochemistry. Most reactions involving hydrogen atoms will be influenced by tunnelling even at room temperature. Lower temperatures allow the tunnelling of heavier atoms. Among the different techniques to evaluate tunnelling rate constants, instanton theory is a promising compromise between accuracy and computational efficiency. The theory will be briefly reviewed along with applications such as the decay of carbenes, proton transport along Grotthus chains or water-formation reactions in the interstellar medium.

J. Meisner, J. Kästner, **Angew. Chem. Int. Ed**. 55, 5400 (2016)
S.R. McConnell, A. Löhle, J. Kästner **J. Chem. Phys**. 146, 074105 (2017)
J. Meisner, T. Lamberts J. Kästner **ACS Earth Space Chem**. 1, 399 (2017)

The seminar of prof. Johannes Kästner, assembly hall, the 18th November, 2019.

After the seminar and also during the first day of his visit prof. Johannes Kästner visited selected laboratories. The aim of these visits was to familiarize with IPC, establish contacts with synergic groups supporting the ERA Chair holder and discuss possibility of the future cooperation. The purpose of these visits was also to assess the research conducted in individual groups and to identify possible problems.

Meetings with the following research groups were organized:

- **Prof. Jacek Waluk** – head of Department of Photochemistry and Spectroscopy
- **Dr hab. Gonzalo Angulo** – head Group of Dynamics of photoinduced bimolecular reactions
- **Dr hab. Adam Kubas** – Modern Heterogenous Catalysis Group
- **Dr Marcin Gronowski** – Group of Laboratory astrochemistry

Prof. Kästner found the research at the IPC very interesting. Number of IPC groups have been working on problems that involve quantum tunnelling. The instanton theory developed by Prof. Kästner allows to describe quantum tunnelling in chemical systems in efficient way. The discussions between prof. Kästner and above mentioned researcher focused on the way how the theory can be used to explain number of phenomena observed in complex systems studied at IPC such as hydrogen transfer in porphyrins or tunnelling effects in catalysis. Prof. Kästner provided IPC researchers with the access to his code DL-FIND including assistance with installation. He pointed out that newly developed python code ChemShell will provide us great environment to integrate various quantum chemical software with his programme.

During the meetings IPC researchers introduced Prof. Kästner into the Polish scientific system including the way how dr hab. and prof. degrees are granted. He found this important in the context of reviewing grant proposals of Polish researchers.

The meetings were concluded with the intention to write common COST action proposal in the nearest future to support knowledge exchange between prof. Kästner group and groups based at IPC.

ANNEX 1.

Agenda of the visit of prof. Johannes Kästner

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CREATE lecture

The Institute of Physical Chemistry of the Polish Academy of Sciences

Wednesday, November 6th, 2019

12.30	pick-up from the airport
13.00	Lunch
15.00	**lab visits** (part I) **prof. Jacek Waluk** head of Department of Photochemistry and Spectroscopy
19.30	dinner

Thursday, November 7th, 2019

8.45	pick-up from the hotel
9.45	checking the presentation in the IPC lecture hall
10.00	**Prof. Dr. Johannes Kästner– seminar lecture** ***„Tunneling Processes in Chemistry Simulated with Instanton Theory"***
11.00	**lab visits** (part II) **Dr hab. Gonzalo Angulo** head Group of Dynamics of photoinduced bimolecular reactions
12.00	Lunch
13.00	**lab visits** (part III) **Dr hab. Adam Kubas** – Modern Heterogenous Catalysis Group **Dr Marcin Gronowski** – Group of Laboratory astrochemistry
15.00	Departure

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