



*The **CRE**ation 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. Markus Reiher

[WP3]

Level of dissemination: PUBLIC

Warsaw, February 2021



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

TABLE OF CONTENT

INTRODUCTION 3
THE COURSE OF THE VISIT 3

INTRODUCTION

On December 10th, 2020, an open lecture under the series of cyclical lectures on emerging interdisciplinary research was delivered by prof. Markus Reiher. Due to the pandemic situation, the lecture was delivered online via the zoom platform. All researchers and PhD students employed at IPC were invited to participate in this seminar.

Markus Reiher is a full professor at the Department of Chemistry and Applied Biosciences in ETH Zürich. He received his diploma in chemistry from the University of Bielefeld in 1995, where he then conducted his PhD studies in theoretical chemistry in the research group of Professor Juergen Hinze. After his PhD in 1998, his habilitation followed in theoretical chemistry at the University of Erlangen with Professor Dr Bernd Artur Hess in 2002. After that, he worked in the Department of Theoretical Chemistry at the University of Bonn. In December 2004, he was offered a full professor in theoretical chemistry at the University of Groningen and a professor for physical chemistry (designation: theory) at the University of Jena. He accepted the latter in 2005.

Professor Reiher' research is devoted to general theoretical chemistry. The main focus is on the development of theory and algorithms for the calculation of electronic structures based on the first principles of quantum mechanics.

THE COURSE OF THE VISIT

The online visit of prof. Markus Reiher took place on December 10th 2020. Prof. Reiher delivered a seminar entitled **"Have you ever pulled on a molecule? - Chemical Reactivity by Interactive Quantum Mechanics"**. The seminar was delivered via the Zoom platform, and all researchers and PhD students employed at IPC were invited to participate in this seminar.

Abstract of the seminar

Our capability to describe molecular structures based on the first principles of quantum mechanics has reached a breathtakingly high degree of sophistication, maturity, and feasibility. At the same time, theoretical chemistry as a research field has diversified dramatically over the years. Significant progress has been made in all its diverse subfields. Its capabilities, as well as the open challenges, are very well understood. Moreover, many unexpected new concepts - in electronic structure theory, vibrational spectroscopy, data-driven chemistry, quantum information and quantum computing, etc. – developed in the past twenty years highlight the enormous current impetus and momentum of the field.

In my talk, I will reflect on some of these developments and then focus on our new concept of real-time quantum chemistry that allows one to get immersed into molecular reactivity through interactive quantum mechanics.

ICChF
Institute of Physical Chemistry PAS: Create Lecture series

Prof. Markus Reiher
ETH Zürich

1998 PhD Uni. Bielefeld
2003 Habilitation Uni. Erlangen-Nuremberg
2003 – 2005 Priv.-Doz. Uni. Bonn
since 2006 at ETH Zürich

Multiple **research stays**: Tel Aviv (2000), Budapest (2001), Tromsø (2003/2004), Lund (2006), and Singapore (2009)

Multiple **awards**

- 2010 the OYGA award, Jerusalem
- Golden Owl of the students of ETH Zürich
- 2018 the Löwdin Lecture of the University of Uppsala
- Credit Suisse Best Teaching award

Participants: Maciej Wojtkow..., Patrycja Niton, Adam Kubas, mreih, Michał, Adams, joanna, M Kochman, Jacek Waluk, Bartosz Zawadzki

HAVE YOU EVER PULLED ON A MOLECULE?

CHEMICAL REACTIVITY BY INTERACTIVE QUANTUM MECHANICS

Markus Reiher
ETH Zürich
Laboratorium für Physikalische Chemie
www.reiher.ethz.ch
markus.reiher@phys.chem.ethz.ch

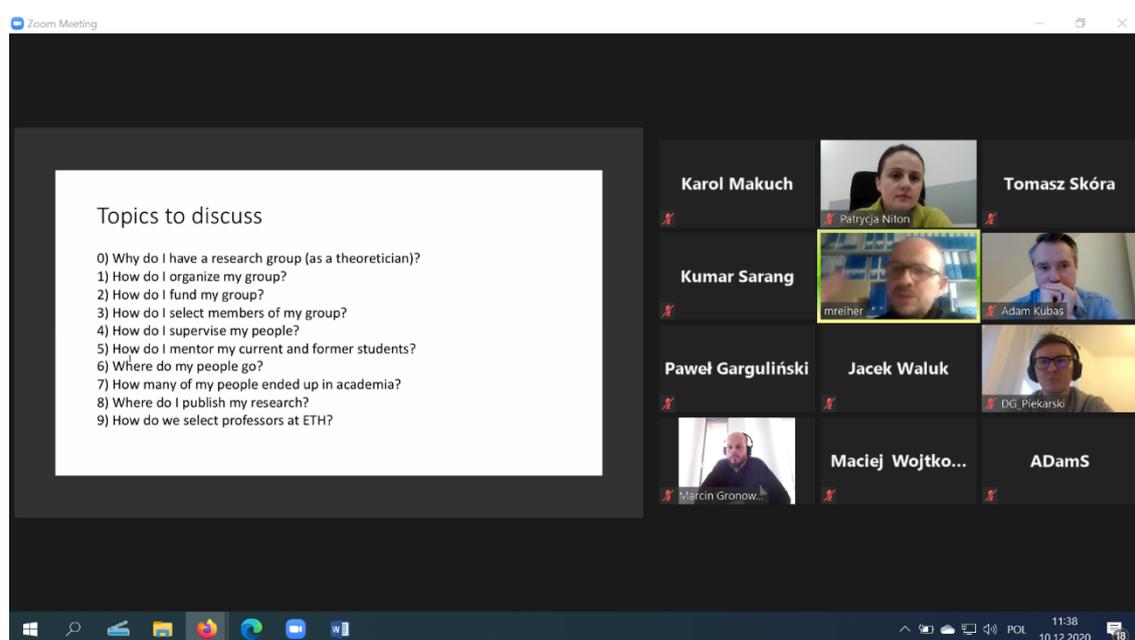
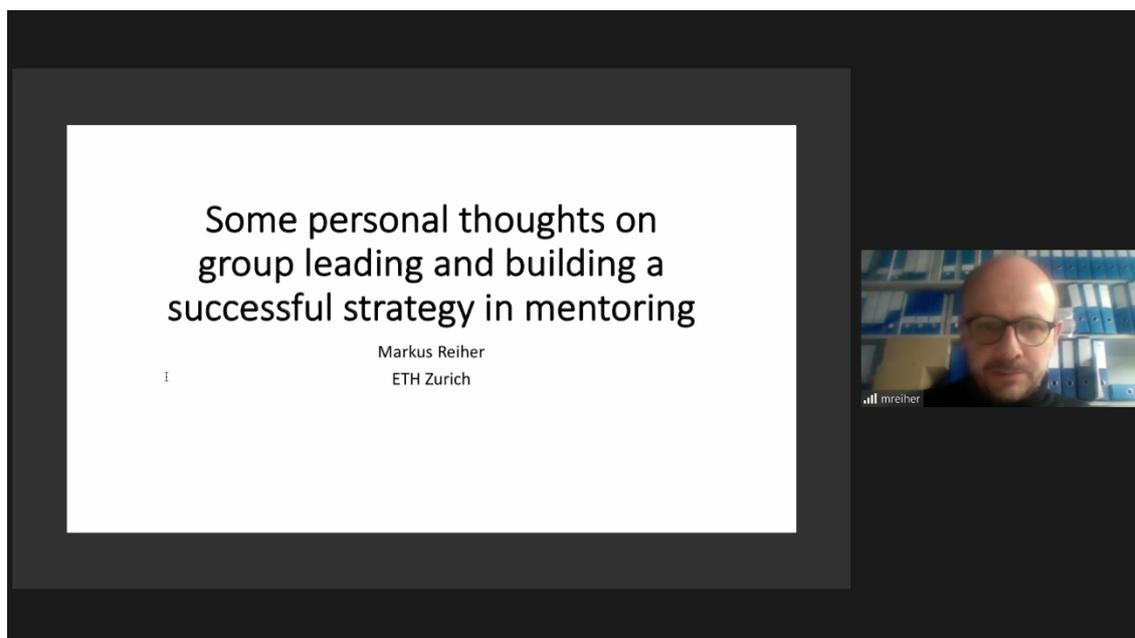
Participant: mreih

Participants: Tomasz Skóra, Patrycja Niton, Adam Kubas, Kumar Sarang, Maciej Wojtkow..., mreih

Zoom controls: Unmute, Stop Video, Security, Participants (109), Polls, Chat, Share Screen, Record, Breakout Rooms, Reactions, More, End

The first part of the seminar of prof. Markus Reiher, Zoom platform, the December 10th, 2020.

After the first part of the seminar, active discussion on scientific aspects took place. Then, professor Reiher moved to the second part of the seminar. He presented his personal thoughts on group leading and gave valuable tips on how to build a successful strategy in mentoring.



The second part of the seminar of prof. Markus Reiher, Zoom platform, the December 10th, 2020.

After the seminar, prof. Reiher met with prof. Maciej Wojtkowski and several researchers from the IPC. These meetings aimed to familiarise with IPC, establish contacts with the groups supporting the ERA Chair holder and discuss the possibility of future cooperation. The zoom meetings with the following researchers were organised:

- **Prof. dr hab. Maciej Wojtkowski** – the ERA Chair holder, head of the Physical Optics and Biophotonics Group;
- **dr Dariusz Piekarski** – member of the Cooperative Catalysis Group;
- **dr Michał Kochman** – member of the Cooperative Catalysis Group;

➤ **dr Marcin Gronowski** – member of the Laboratory Astrochemistry Group.

During the meeting with Prof. Wojtkowski, the management of research groups was discussed. Prof. Reiher pointed out the need to meet frequently with his group members and to maintain a very high level of self-discipline in matters of regular discussions about current projects.

He pointed out that communication within the group is crucial for effective team progress. He also emphasised the great role of doctoral students and proper mentoring. He described his research group's functioning scheme and shared his experiences from the team's daily organisation. In addition, the discussion turned to issues related to the dissemination of knowledge and systemic solutions at the University, which enable the efficient building of recognition. Prof. Reiher stated that the group members' involvement is also crucial in the PR process and gave examples of doctoral students' initiatives that helped him advertise his group activity.

European grants were another topic of discussion between Prof. Wojtkowski and Prof. Reiher. Prof. Reichert concluded that relying on ERC or Horizon funding cannot be the basis of the group's activities, and he appreciated the continuous funding from the University. The latter allows to undertake research on any topic without defining the predictable effects of the grant. He pointed out that such highly competitive grant processes reduced efficiency and low effectiveness of operations in the short term.