



The 27th Rudolf Brdička Memorial Lecture

Professor Frank NEESE

*Max-Planck Institute for Chemical Energy Conversion,
Mülheim, Germany*

**Analysis of complex catalytic
mechanisms by High-level
spectroscopy and quantum
chemistry: The case of water
oxidation in PSII**

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**J. Heyrovský Institute of Physical Chemistry, v.v.i.
Academy of Sciences of the Czech Republic
Prague 8, Dolejškova 3**

Analysis of complex catalytic mechanisms by High-level spectroscopy and quantum chemistry: The case of water oxidation in PSII



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The combination of high-level spectroscopy (EPR, MCD, various X-ray techniques, resonance-Raman, Mößbauer etc) and high-level quantum chemistry offer unique opportunities for disentangling complex reaction mechanisms. Using spectroscopic observables as a means to gauge theoretical calculations is a powerful means to implement the important concept of falsification. As a theoretician, one no longer has to rely on small energy differences. As an experimentalist one profits from the ability to correctly interpret complex spectra. The concepts are illustrated by an in-depth study one of the most important chemical reactions: the oxidation of water by the oxygen evolving complex of photosystem II.

Born at 13.12.1967 in Wiesbaden. From 1987 - 1993 studies of biology (Diploma 1993); 1997 Promotion at University of Konstanz. 1997 - 1999 Postdoctoral Fellow at the Stanford University (California, USA); 1999 - 2001 Habilitation (Bioinorganic und theoretical chemistry) at the University of Konstanz; 2001 - 2006 group leader at the Max Planck Institute for radiation chemistry (since 2003 Max Planck Institute for Bioinorganic Chemistry); 2006 - 2011 Full Professor and Chair of Theoretical Chemistry at the University of Bonn. In addition from 2008 - 2011 Fellow of the Max Planck Society and since 2011 Director und Scientific Member at the Max Planck Institute for for Chemical Energy Conversion. Since 2013 Honorary Professor at the Rheinische Friedrich-Wilhelms-Universität of Bonn.

Frank Neese has been honored with a number of awards, including the Karl-Arnold Prize (2005), Klung-Wilhelmy-Weberbank Award (2008), the Early Career Award (2009), and the Leibniz-Award (2010). In 2013, he was received into the Leopoldina German National Academy of Sciences.

BRDIČKA LECTURES 1991-2016

1. (1991) Edgar **HEILBRONNER** (*Eidgenössische Technische Hochschule, Zürich*)
"The old Hückel formalism"
2. (1992) Kamil **KLIER** (*Lehigh University, Bethlehem, Pennsylvania*)
"Physical chemistry in two dimensions"
3. (1993) Joshua **JORTNER** (*Tel Aviv University, Tel Aviv*)
"Clusters – a bridge between molecular and condensed matter chemical physics"
4. (1994) David J. **SCHIFFRIN** (*The University of Liverpool*)
"Electrochemistry in two-dimensional systems"
5. (1995) Josef **MICHL** (*University of Colorado, Boulder, Colorado*)
"Molecular kit for new materials"
6. (1996) Gerhard **ERTL** (*Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin*)
"Self-organization in surface reactions"
7. (1997) Roger **PARSONS** (*University of Southampton*)
"Electrochemistry in the last 50 years: from Tafel plotting to scanning tunnelling"
8. (1998) G. Barney **ELLISON** (*JILA and University of Colorado, Boulder, Colorado*)
"The chemical physics of organic reactive intermediates in combustion and atmospheric processes"
9. (1999) Henry F. **SCHAEFER III** (*University of Georgia, Athens, Georgia*)
"The third age of quantum chemistry"
10. (2000) Alexis T. **BELL** (*University of California and Lawrence Berkeley Laboratory, Berkeley, California*)
"Progress towards the molecular design of catalysts – lessons learned from experiments and theory"
11. (2001) Mario J. **MOLINA** (*Massachusetts Institute of Technology, Cambridge, Massachusetts*) "The Antarctic ozone hole"
12. (2002) Jean-Marie **LEHN** (*Université Louis Pasteur, Strasbourg a Collège de France, Paris*) "Selforganization of supramolecular nanodevices"
13. (2003) Helmut **SCHWARZ** (*Technische Universität Berlin*)
"Elementary processes in catalysis: looking at and learning from "naked" transition ion"
14. (2004) Rudolph A. **MARCUS** (*California Institute of Technology, Pasadena*)
"Strange isotope effects in stratospheric ozone and in the earliest minerals in the solar system"
15. (2005) Avelino **CORMA** (*Instituto de Tecnología Química, Valencia*)
" Supramolecular Entities Based on Molecular Sieves for Catalysis and Synthesis of New Materials"
16. (2006) Paul **CRUTZEN** (*Max Planck Institute for Chemistry, Mainz*):
"Atmospheric Chemistry and Climate in the 'Anthropocene'"
17. (2007) Harry B. **GRAY** (*California Institute of Technology, Pasadena*)
"The Currents of Life: Electron Flow through Metalloproteins"
18. (2008) Michael **GRÄTZEL** (*Ecole Polytechnique Fédérale de Lausanne*)
"Mesoscopic Electrodes for Generation and Storage of Electric Power from Sunlight"
19. (2009) Gabor. A. **SAMORJAI** (*Department of Chemistry and Lawrence Berkeley National laboratory, University of California, Berkeley*)
"Molecular Foundations of Heterogeneous Catalysis"
20. (2010) Pavel **HOBZA** (*Institute of Organic Chemistry and Biochemistry of the AS CR*)
"Noncovalent Interactions and their Role in Chemistry and Biochemistry"
21. (2011) Klaus **MÜLLEN** (*Max-Planck Institute, Mainz, Germany*)
"Carbon Materials and Graphenes"
22. (2012) Enrico **GRATTON** (*University of California, Irvine*)
"Nanoimaging technique with high time and spatial resolution: Mechanisms of translocation through the nuclear pore complex"
23. (2013) J. Peter **TOENNIES** (*Göttingen, Germany*)
"Superfluid Helium Nanodroplets: Very Cold and Extremely Gentle"
24. (2014) Christian **AMATORE** (*CNRS Paris, France*)
" Seeing, Monitoring, Measuring and Understanding Vesicular Exocytosis of Neurotransmitters with Ultramicroelectrodes"
25. (2015) Ulrike **DIEBOLD** (*TU Wien, Austria*)
"Surface Science of Metal Oxides"
26. (2016) Ferdi **SCHÜTH** (*Max-Planck-Institut, Mülheim, Germany*)
"Controlled nanostructures for applications in catalysis and beyond"



Rudolf BRDIČKA
(1906-1970)

Professor of physical chemistry at Charles University, founding member of the Czechoslovak Academy of Sciences, founder and the first director of the Institute of Physical Chemistry of the Czechoslovak Academy of Sciences.

An outstanding electrochemist renowned in particular by his pioneering work on kinetic polarographic current and on applications of polarography in medicine. A brilliant university teacher, author of an internationally recognized textbook of physical chemistry. He has crucial merits for development of modern physical chemistry in this country.

To commemorate his work and personality, the Institute of Physical Chemistry of the Academy of Sciences of the Czech Republic has organized since 1991 annually a festive R. Brdička Lecture. Invited speakers have been eminent scientists active in some field relating to the research currently pursued in the Institute.