The 25th Rudolf Brdička Memorial Lecture

Professor Ulrike Diebold

Institute of Applied Physics,
TU Wien, Vienna, Austria

Surface Science of Metal Oxides

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

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Ulrike Diebold

Institute of Applied Physics, TU Wien, Vienna, Austria

e-mail: diebold@iap.tuwien.ac.at

With the advent of Scanning Tunneling Microscopy (STM) a dream has come true in surface chemistry: to directly watch how a single molecule adsorbs on a surface and undergoes a chemical transformation. Combined with first-principles theory, such measurements allow identifying specific surface sites, as well as reaction processes and mechanisms that are at the heart of heterogeneous, photo- and electrocatalysis.
In the talk I will give an overview of the insights gained from such combined STM/DFT investigations. I will mainly focus on TiO_2, the prototypical system for surface science experiments on metal oxides; technologically important, yet fundamentally challenging materials. The semiconducting properties of TiO_2 (and the fact that it is cheap, stable, readily available, and can be produced in a variety of nanostructures) make it popular in well-established fields, such as photocatalysis, and emerging technologies, such as memristive switching.
To be meaningful, surface science studies are best conducted on single-crystals in ultrahigh vacuum, although recent STM studies in aqueous solutions point towards the potential of using this technique in other environments as well. The surface geometrical and electronic structures of various facets and polymorphs of TiO_2 are now well understood. An important aspect are surface defects, in particular O vacancies that form easily in reducible metal oxides. Such defects can be judiciously created by electron bombardment, and with STM one can inspect individual defects and even manipulate them. I will discuss adsorption, diffusion and photo-induced processes for various molecules. The results will be compared with other systems systems, e.g. iron oxides, where vacancies in the cation sublattice influence surface properties in a profound way.

References

U. Diebold, “The Surface Science of Titanium Dioxide”, Surface Science Reports, 48 (2003) 53 – 229

Y. He, A. Tilocca, O. Dulub, A. Selloni, and U. Diebold, “Local ordering and electronic signatures of submonolayer water on anatase TiO_2(101)” Nature Materials 8 (2009) 585 - 589

M. Setvin, U. Aschauer, Ph. Scheiber, M. Schmid, A. Selloni, U. Diebold “Reaction of O_2 with Subsurface Oxygen Vacancies on TiO_2 Anatase (101)” Science, 341 (2013) 988

R. Bliem, E. McDermott, P. Ferstl, M. Setvin, O. Gamba, M. A. Schneider, M. Schmid, U. Diebold, P. Blaha, L. Hammer, G. S. Parkinson “Subsurface Cation Vacancy Stabilization of the Magnetite (001) Surface” Science, 346 (2014) 1215

BRDIČKA LECTURES 1991-2014

1.	***(1991)***	*Edgar* ***HEILBRONNER*** *(Eidgenossische Technische Hochschule, Zürich)* "**The old Hűckel 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 Collége 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 Natkional 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"**

Rudolf BRDIČKA
(1906-1970)

Professor of physical chemistry at Charles University, founding member of the Czechoslovak Academy of Sciences, founder and 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.