



# The 20<sup>th</sup> R. Brdička Lecture

**Professor Pavel Hobza**

*Institute of Organic Chemistry and Biochemistry,  
Academy of Sciences of Czech Republic*

**“Noncovalent Interactions and their Role  
in Chemistry and Biochemistry”**

**June 23, 2010 at 14:00 am**

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

## NONCOVALENT INTERACTIONS AND THEIR ROLE IN CHEMISTRY AND BIOCHEMISTRY



***Pavel Hobza***

*Institute of Organic Chemistry and Biochemistry,  
Academy of Sciences of Czech Republic*

Noncovalent interactions play a key role in biodisciplines and they determined the structure of biosystems. The function of biomacromolecules is largely determined by their structures, e.g. the double helix of DNA is responsible for the storage and transfer of genetic information. The experimental study of noncovalent interactions is still challenging problem and the interpretation is not always unambiguous. On the other hand theoretical methods of quantum chemistry combined with methods of molecular dynamics provide a unique and consistent picture of noncovalent interactions under different conditions, e.g. in different environments or at different temperature. In this lecture, different types of noncovalent interactions, their character and their role in nature will be presented. In addition, the reliability of different methods to describe these interactions will be discussed, starting from the most accurate nonempirical approaches with chemical accuracy up to semiempirical and empirical methods which allow to study systems with several thousand of atoms. Finally, selected projects from our laboratory will be briefly presented with a special emphases on in silico drug design.

## BRDIČKA LECTURES

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 GRAETZEL (Ecole Polytechnique Federale de Lausanne, Switzerland)*  
"Mesoscopic Electrodes for Generation and Storage of Electric Power from Sunlight"
19. (2009) *Gabor A. SOMORJAI (University of California, Berkeley)*  
"Molecular Foundations of Heterogeneous Metal Catalysis"



**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.