The 19th R. Brdička Lecture

Professor Gabor A. Somorjai

(Department of Chemistry and Lawrence Berkeley National Laboratory, University of California, Berkeley)

"MOLECULAR FOUNDATIONS OF HETEROGENEOUS METAL CATALYSIS"

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J. Heyrovsky Institute of Physical Chemistry,v.v.i.
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Department of Chemistry and Lawrence Berkeley National Laboratory,
University of California, Berkeley

Heterogeneous metal catalysts are nanoparticles that carry out reactions at high reactant gas pressures or in the liquid phase. Instruments developed in Berkeley for molecular studies under these conditions are sum frequency generation vibrational spectroscopy, high pressure scanning tunneling microscopy and ambient pressure X-ray photoelectron spectroscopy. Model surfaces were used to study heterogeneous catalytic reactions that permitted to control and monitor the atomic surface structure, composition and reaction intermediates and simultaneously measure reaction rates and selectivities. This way precises quantitative correlations could be obtained between catalytic reaction kinetics and the molecular factors that control reaction dynamics. Single crystal surfaces were used at first as model catalysts followed by the use of metal and bimetallic nanoparticles that were synthesized with precise size and shape using colloid techniques. Catalytic studies that produce a single molecule (ethylene hydrogenation, CO oxidation) were redirected to focus on reaction selectivity in multipath chemical processes. Reactions were found to induce restructuring of the metal surfaces and mobility of adsorbed molecules. Reaction selectivity and rates can be altered by changing the nanoparticle size in the 0.8 – 10 nm range and shape (surface structure). Transition metal catalysts that are nanosize achieve facile restructuring and rapid change in surface composition under reaction conditions as their low atom coordination permits rapid bond rearrangements. Exothermic surface reactions can cause the flow of hot electrons at oxide metal interfaces and the clustering of metal atoms at the interface, which dramatically increases the metal oxide interface area. Improvements of techniques for molecular studies of surfaces that provide better time resolution and spatial resolution will enhance our ability to study the dynamics of surfaces, which are key to both activity and selectivity during catalysis. The control of metal nanoparticle size and shape provides opportunities to achieve superior reaction selectivity. Combined studies of nanoparticle catalyst synthesis, characterization and reaction studies will accelerate developments of this important field of chemical sciences and chemical energy conversion.

Gabor A. Somorjai (1935)

is a Professor of Chemistry at the University of California, Berkeley, and a Principal Investigator in the Materials Sciences Division of the Lawrence Berkeley National Laboratory.

Gabor A. Somorjai was born in Budapest, Hungary. He was a fourth year student of Chemical Engineering at the Technical University in Budapest in l956 at the outbreak of the Hungarian Revolution. He left Hungary and emigrated to the United States, where he received his Ph.D. degree in Chemistry from the University of California, Berkeley in l960. He became a U.S. citizen in l962. After graduation, he joined the IBM research staff in Yorktown Heights, New York, where he remained until l964. At that time, he was appointed Assistant Professor of Chemistry at the University of California, Berkeley. In l967, he was named Associate Professor, and in l972 promoted to Professor. Concurrent with his faculty appointment, he is also a Faculty Senior Scientist in the Materials Sciences Division, and Group Leader of the Surface Science and Catalysis Program at the Center for Advanced Materials, at the E.O. Lawrence Berkeley National Laboratory. Professor Somorjai has educated more than 115 Ph.D. students and 200 postdoctoral fellows. He is the author of more than 1000 scientific papers in the fields of surface chemistry, heterogeneous catalysis, and solid state chemistry. He has written three textbooks.

He has received numerous awards and honors including the 2009 Miller Senior Fellow, the 2008 Priestley Medal from the American Chemical Society, the 2007 Langmuir Prize from the American Physical Society,the 2002 National Medal of Science, the 2000 Linus Pauling Medal for Outstanding Accomplishment in Chemistry, the 1998 Wolf Prize in Chemistry, the 1997 Von Hippel Award, Materials Research Society, the 1994 Adamson Award in Surface Chemistry, American Chemical Society, the 1989 Peter Debye Award in Physical Chemistry, American Chemical Society.

Professor Somorjai's research interests are in the field of surface science. His group is studying the structure, bonding, and reactivity at solid surfaces on the molecular scale. This knowledge is then utilized to understand macroscopic surface phenomena; adsorption, heterogeneous catalysis, and biocompatibility on the molecular level. To this end, he also develops instruments for nanoscale characterization of surfaces. These include sum frequency generation surface vibrational spectroscopy (SFG) and high pressure scanning tunneling microscopy (high pressure STM) and high pressure X-ray photoelectron spectroscopy (ambient pressure XPS).

Research is carried out in the following areas:

- Studies of catalytic reactions on single crystals, nano-particles, or other well-characterized surfaces. The rate and product distribution of catalyzed reactions are correlated to surface composition, valency, and atomic structure. As part of these studies, hydrocarbon reactions on platinum and rhodium single crystal surfaces are investigated. Monodispersed metal nanoparticles in the 1-10 nm range are synthesized in solution and deposited on oxide films as two-dimensional arrays using the Langmuir-Blodgett technique and used as model catalysts. A combination of SFG and high pressure STM is used in these studies.
- Encapsulation of metal nanoparticles in mezoporous oxide channels is used to produce high surface area catalysts that exhibit high reaction selectivity.
- Polymer surfaces, both hydrophobic and hydrophilic are utilized to study the adsorption, structures and transformations of amino acid and polypeptide monolayers. The adsorption of peptides with increasing molecular weight and different amino acid compositions is investigated. A combination of SFG and quartz microbalance (QCM) is used in most of these studies.

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.

BRDIČKA LECTURES

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 **GRAETZEL***
    (Ecole Polytechnique Federale de Lausanne, Switzerland
    "Mesoscopic Electrodes for Generation and Storage of Electric Power from Sunlight"