

Scientific Report

New trends in molecular assembling and electronics: experiment and theory.

1) Summary

The workshop '*New trends in molecular assembling and electronics: experiment and theory*' took place at *Czech Technical University, Prague, Czech Republic* between 4.-6.July 2011. The aim of this meeting was to bring together leading scientists in the field of surface science, chemistry and molecular electronics from both experimental and theoretical fields to discuss recent progress and challenges in the field. The workshop included of 14 invited talks (40 minutes) and 6 regular talks (20 minutes). In total, we had 32 participants from 13 countries (France, Spain, Netherlands, Italy, Switzerland, Finland, Germany, Ireland, Austria, Poland, UK, Canada and Czech Republic). The event was organized as a satellite workshop of the 13th International Conference on the Formation of Semiconductor Interfaces organized by the Institute of Physics of the AS CR in Prague, Czech Republic in July 2011. More information is available on a webpage ntmae.fzu.cz.

Among main topics addressed by the workshop were: (i) adsorption of a single molecule on surfaces ; (ii) self-assembling molecular processes, intermolecular interactions ; (iii) advanced characterization, high-resolution and modification of molecules at atomic scale ; (iv) the electron transport through individual molecules and molecular layers ; (v) molecular switching and motors and (vi) advanced molecular chemistry towards new functionalized molecules.

List of Invited Speakers:

Wesley Browne, Univerisity of Groningen, The Netherlands

Christopher Gerber, University of Basel, Switzerland

J. A. Martin Gago, ICMM-CSIC Madrid, Spain

Peter Liljeroth, Aalto University School of Science, Finland

Ernst Meyer, University of Basel, Switzerland

Nikolaj Moll, IBM, Zurich, Switzerland

Jose Ortega, Universidad Autónoma de Madrid, Spain

Jascha Repp, Universitaet Regensburg, Germany

Mario Ruben, INT Karlsruhe, Germany

Ivan Rungger, Trinity College Dublin, Ireland

Ivo Starý, Institute of Organic Chemistry and Biochemistry ASCR, Czech Republic

Marek Szymonski, Jagiellonian University, Poland

Stefan Tautz, Forschungszentrum Jülich GmbH, Germany

Dietrich R.T. Zahn, Chemnitz University of Technology, Germany

2) Description of scientific meeting

An exploration of new material properties and assembling of artificial structures at nanoscale is a key factor to maintain the current technological progress. One of the promising strategies to obtain nanostructures of desired material properties is a formation of self-assembled molecular layers on surfaces. Recently, substantial progress has been made in various fields of the creation of molecular nanostructures. Despite of the large effort devoted studying the molecular systems at the nanoscale, functional molecular devices suitable for electronic industry are still far from the reality. Mainstream activities in the field of molecular nanostructures are focused on layers on metal substrates.

The aim of the workshop was to bring together leading scientists from the experimental and theoretical sides to exchange ideas needed for new horizons in the field and to discuss next steps in the close future of molecular electronic and molecular assembling.

The opening lecture was given by Prof. Ch. Gerber, the co-inventor of Atomic Force Microscope. He provided a brief overview of history of AFM, its achievements and impact to different scientific areas including Solid State Physics, Chemistry and Biology.

The second block, including invited lectures given by E. Meyer, M. Szymonski and J.A. Martin-Gago, was devoted to experimental studies related to deposition of organic molecules on surfaces by means of Scanning Probe Microscopy (SPM). Particular attention was paid to formation of self-assembled nanostructures from individual molecules. Also new possibilities to induce new chemical reactions on surfaces were pointed out. Finally, the importance of proper interpretation of experimental data obtained by SPM was critically discussed.

The afternoon block of three invited talks (S. Tautz, J. Ortega and N. Moll) was related to both experimental and theoretical studies of adsorption of single molecules on surfaces. Possibility of high resolution imaging of individual molecules by means of Atomic Force Microscopy (AFM) using a functionalized probe has been discussed by N. Moll. Also possibility to form molecular junction consisting of only a single molecule by means of SPM has been reported by S. Tautz. The formation of molecular junction between STM probe and molecule/surface interfaces has been revealed by simultaneous measurement of the tunneling current and the chemical force. This combination opens a completely new way to study single-molecule junctions. J. Ortega discussed in details the importance of proper theoretical treatment of organic/metal interfaces going beyond standard techniques based on one-electron picture (such as Density Functional Theory).

The late afternoon section has been devoted to advanced experimental characterization of molecular layers on surfaces. Two different experimental techniques (AFM and Near Edge X-ray Absorption Fine Structure (NEXAFS)) has been adopted to understand orientation of individual molecules on surfaces. During the talks, the mechanical properties of molecular layers has been also discussed. A. Shluger presented a theoretical work discussing a mechanism of reconstruction of ionic surfaces induced by organic molecules.

The second day began with a block of lectures related to chemistry on surfaces. M. Ruben discussed problems and challenges in building functional spinotronic devices based on supramolecular structures. He paid special attention to connecting individual building blocks to functionalized units and the introduction of spin degree of freedom by the presence of magnetic atoms. W. Browne discussed different strategies how to prepare molecular motors by means of electro- and photoswitching. In particular, he focused on effects of surface immobilization of molecules on the conformational chemistry of an electro- and photoswitchable molecules. Finally I. Stary explored the possibilities to use nonplanar π -electron systems for synthesis and self-assembly of complex nanostructures on solid surfaces.

In the second session on Tuesday, J. Repp discussed experimental understanding of the electron transport through single molecules deposited on thin insulating films. In particular, he focused on the charging effect of weakly coupled molecules and possibility to induce molecular switching by injection of electrons into molecules. P. Liljeroth presented exciting experimental work about quantum confined electronic states in atomically well-defined graphene nanostructures. In particular, he revealed the existence and the importance of so called edge electronic states present in graphene flakes. Finally, I. Rungger presented a new way to theoretically calculate forces induced by current flowing through nanostructures (such as metallic wires). He also discussed a solvent effect on nanoscale junctions and a way how this effect can be effectively introduced in theoretical calculations.

The last block of the workshop has been devoted to regular talks addressing formation of complex molecular layers and their material properties. Also a new theoretical technique allowing simulation of time-dependent evolution of electronic states and their transitions has been reported by E. Abad. This technique opens new ways to study switching mechanism in molecular systems induced by electronic excitations.

3) Assessment and impact of the workshop

The aim of the workshop was bring together leading scientists from the experimental and theoretical sides to exchange ideas needed for new horizons in the field and to discuss next steps in the close future of molecular electronic and molecular assembling. We think the workshop met this goal.

The scientific discussion between participants during the workshop established better synergy between synthetic chemistry, surface and material science. We believe that especially the gap between chemistry and physics has been reduced. There was an intensive debate how to prepare and deposit supramolecular structures on surfaces still keeping new functionalities. In particular, special attention has been paid to 2D topological character of surfaces and interaction between entities having certain impact on formation processes.

The detail knowledge of atomic and electronic structures of a molecule/surface interface is crucial for the further development of molecular electronics. In general the reliable information can be achieved by combining both experimental and theoretical techniques. Therefore, the importance of combined experimental and theoretical analysis required for better understanding of material properties of nanostructures has been stressed many times.

Intensive debate was opened about complex characterization of molecular structures on surfaces. In the ideal case, local probe techniques (such as AFM or STM) should be complemented with macroscopic spectroscopic methods, such as photoemission, NEXAFS or ESCA, giving the information on electronic band and atomic structures in k-space over a large sample area. It is evident that only the combination of these approaches with theoretical ones offers the desired complex analysis of molecular nanostructures on a semiconductor surface.

Inherent limitations of DFT (strong electron correlations, van der Waals interactions) have been discussed in a way accessible to the experimental audience. On addition, discussion between presented theoreticians suggested several ways going beyond standard DFT method.

The workshop joined to the 13-th International Conference on the Formation of Semiconductor Interfaces. We believe that the synergy between the workshop and the conference brought benefits to both events. The transfer of knowledge about modification of semiconductor surfaces stimulated new ideas about preparation of molecular nanostructures. On the other hand, the advanced transport measurements and complex characterization with ultimate resolution discussed during the workshop attracted the interest of many regular participant of the ICFSI conference.

4) Annexes: Programme of the meeting and list of speakers and participants

Workshop Programme

Mon 4/7

9:00-10:00 Ch. Gerber **SPM Technologies past, present, future**

10:00-10:40 Coffee break

10:40-11:20 E. Meyer **Force microscopy from contact to non-contact**

11:20-12:00 M. Szymonski **Atomic-Scale Technologies for Assembling and Characterization of Molecular Nanostructures at Semiconductor Surfaces**

12:00-12:40 J.A. Martin-Gago **Organic Adsorbates on the TiO₂(110) surface**

12:40-14:00 Lunch time

14:00-14:40 S. Tautz **Metal-Molecule Contacts: From Adsorption to Charge Transport**

14:40-15:20 J. Ortega **Energy level alignment at the molecule-metal interface**

15:20-16:00 N. Moll **Functionalized tips leading to atomic-resolution force microscopy**

16:00-16:40 Coffee break

16:40-17:20 D.R.T. Zahn **Ultra-thin organic films on semiconductor substrates: How can we control molecular orientation?**

17:20-17:40 A. Shluger **The mechanism of reconstruction of ionic surfaces induced by organic molecules**

17:40-18:00 Q. Shen **Characterization of azimuthal orientations on second-layer islands of para-hexaphenyl thin films with well-defined polygonal shapes**

Tue 5/7

10:00-10:40 Coffee break

10:40-11:20 M. Ruben **Supramolecular Spintronic Devices**

11:20-12:00 W. Browne **Effect of surface immobilization on the conformational chemistry of an electro- and photoswitchable overcrowded alkene**

12:00-12:40 I. Stary **Nonplanar π -electron systems: their synthesis and self-assembly on solid surfaces**

12:40-14:00 Lunch time

14:00-14:40 J. Repp **Scanning tunneling spectroscopy of molecules on thin insulating films**

14:40-15:20 P. Liljeroth **Quantum confined electronic states in atomically well-defined graphene nanostructures**

15:20-16:00 I. Rungger **Current induced forces and solvent effects in nanoscale junctions**

16:00-16:40 Coffee break

16:40-17:00 M. Canepa **Selenide induced Hg segregation and "poisoning" of alkanediselenide self-assembled monolayers on Au**

17:00-17:20 E. Abad **Tully's surface hopping method in practice: FIREBALL calculations of photoactive organic materials**

17:20-17:40 M. Abel **Single polymeric phthalocyanine sheet obtained on metals or thin insulating surfaces**

17:40-18:00 S. Ababou-Girad **Covalent attachment of metallic cluster cores (ReSe, MoBr) on silicon (111) surfaces via alkyl chains: surface characterization and electronic properties**

19:00-23:00 Workshop diner

List of participants

Speakers	
Name	City, Country
Dr. Soraya Ababou-Girard	Rennes, (FR)
Dr. Enrique Abad	Madrid, (ES)
Dr. Mathieu Abel	Marseille, (FR)
Professor Wesley R. Browne	Groningen, (NL)
Dr. Maurizio Canepa	Genova, (IT)
Professor Christoph Gerber	Basel, (CH)
Professor Peter Liljeroth	Espoo, (FI)
Dr. José Angel Martín Gago	Madrid, (ES)
Professor Ernst Meyer	Basel, (CH)
Dr. Nikolaj Moll	Rüschlikon, (CH)
Professor José Ortega Mateo	Madrid, (ES)
Professor Jascha Repp	Regensburg, (DE)
Professor Mario Ruben	Eggenstein-Leopoldshafen, (DE)
Dr. Ivan Rungger	Dublin 2, (IE)
Dr. Quan Shen	Leoben, (AT)
Professor Alexander Shluger	London, (UK)
Dr. Ivo Starý	Prague, (CZ)
Professor Marek Szymonski	Krakow, (PL)
Professor Stefan Tautz	Julich, (DE)
Professor Dietrich R. T. Zahn	Chemnitz, (DE)

[Add a Participant](#)

Participants	
Name	City, Country
Dr. Martin Švec	Praha, (CZ)
Dr. Vladimír Cháb	Praha, (CZ)
Dr. Yannick Dappe	Strasbourg, (FR)
Professor Fernando Flores	Madrid, (ES)
Dr. Prokop Hapala	Praha, (CZ)
Dr. Zsolt Majzik	Praha, (CZ)
Professor Alastair B. McLean	Kingston, (CA)
Dr. Pingo Mutombo	Praha, (CZ)
Dr. Peter Puschnig	Leoben, (AT)
Dr. Martin Setvín	Praha, (CZ)
Dr. Martin Vondráček	Praha, (CZ)
Dr. Vladimír Zobač	Praha, (CZ)