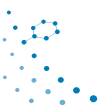


Abstracts



PROGRAM OVERVIEW

INVITED LECTURES

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Invited Lectures

*Abstracts listed in alphabetical order
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the lecturer's name*

Design and Manipulation of Functional Molecular Nanosystems at Interfaces

Johannes V. Barth

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The control and organization of molecular species at interfaces is key to advance molecular science, nanochemistry and the development of novel low-dim materials. The insights gained affect various fields of application, including catalysis, sensing, light-harvesting, nanomagnetism, organic electronics and single-molecular thermodynamics. We explore molecular modules, steer their behaviour and afford novel functions using well-defined homogenous surfaces, textured and sp^2 -nanotemplates as construction platforms. The devised bottom-up fabrication protocols implement biological and *de novo* synthesized building blocks, while exploiting error-corrective noncovalent bonding and metal-directed assembly, as well as covalent chemistry. Scanning probe real-space observations visualize structural features with atomic precision, revealing molecular recognition, assembly and bonding schemes mediating the expression of distinct nanoarchitectures. Multitechnique studies of flexible species such as metalloporphyrins exemplify the delicate interplay between conformational adaptation, electronic signature and axial ligation of adducts or magnetic features. Our approach provides a rationale for the interfacial control of single molecular units and the design of nanostructured materials with complex features, intricate dynamics and tunable functional properties. Complementary modeling efforts perfect the experimental insights and unravel underlying driving forces or complex phenomena. Furthermore selected examples of ongoing research efforts are presented.

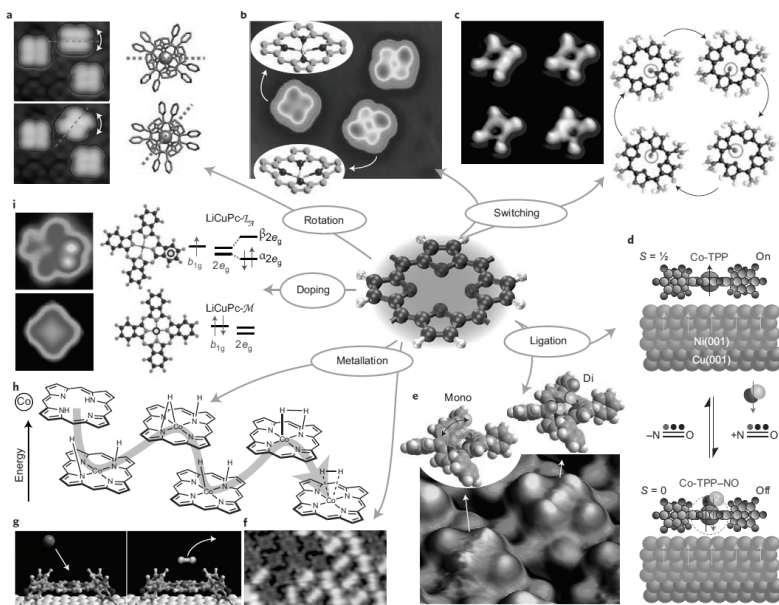


Figure: Functional properties and control of tetrapyrrole units confined at interfaces (DOI: 10.1038/nchem.2159).

Abstracts: Invited Lectures

Molecular Self-Assembly and Templating at the Liquid–Solid Interface

Manfred Buck

EastCHEM School of Chemistry, University of St Andrews, St Andrews, UK

Supramolecular networks (SMNs) where non-covalent interactions between flat lying molecules with extended π -systems play the decisive role, and self-assembled monolayers (SAMs) where chemisorption is the driving force to yield densely packed upright standing molecules, provide complementary approaches to the nanoscale. Defining dimensions with atomic precision, SMNs provide a relatively straightforward bottom-up access to ultraprecise templating on the sub-5-nm scale whereas SAMs enable a flexible functionalisation of surfaces and constitute elements of the top-down approach to nanostructures.

Even though the liquid/solid interface is more complex and less amenable to a detailed characterisation compared to a surface in a UHV environment, it offers a number of attractive features for molecular assemblies. Besides a simple setup, the thermodynamics and kinetics of interfacial processes can easily be varied over a wide range taking the solution based approach. The opportunities are further augmented at electrified interfaces as the precision at which rates and equilibria of reactions can be controlled and charges can be measured, makes the electrochemical approach most interesting for nanotechnology.

The talk will address opportunities of and challenges for hierarchical assembly controlled by hydrogen bonded networks, SAM/SMNs hybrid structures and electrodeposition templated by SAMs and SMNs.

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Abstracts: Invited Lectures

Atomic-Scale Studies of Metal Oxide Surfaces

Ulrike Diebold

Institute of Applied Physics, TU Wien, Vienna, Austria

Surface science studies of metal oxides have experienced a rapid growth. The reasons for this increasing interest are quite clear: after all, most metals are oxidized under ambient conditions, so in many instances it is the oxidized surface that deserves our attention. In addition, bulk metal oxides exhibit an extremely wide variability in their physical and chemical properties. These are exploited in established and emerging technologies such as catalysis, gas sensing, and energy conversion schemes, where surfaces and interfaces play a central role in device functioning. Hence a more complete understanding of metal oxide surfaces is desirable from both a fundamental and applied points of view.

By using Scanning Tunneling Microscopy measurements, in combination with Density Functional Theory calculations and area-averaging spectroscopic techniques, great strides have been made in understanding the atomic-scale properties of the surfaces of several oxide materials. In the talk I will give examples drawn from recent studies of bulk single crystals including TiO_2 , Fe_3O_4 , and selected perovskites.

PROGRAM OVERVIEW

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Spin Excitations in Single Molecules on Metals and Superconductors

Benjamin W. Heinrich, Olof Peters, Lukas Braun, Christian Lotze, Xianwen Chen, Jose I. Pascual, Katharina J. Franke

Fachbereich Physik, Freie Universität Berlin, Berlin, Germany

The magnetic properties of atoms and molecules on a surface are significantly affected by details in the atomic-scale surrounding. Manipulation of this surrounding provides the possibility to tune the electronic and magnetic functionality of surfaces on the nanometer scale. Here, we use scanning tunneling spectroscopy to resolve the magnetic properties of individual paramagnetic metal–organic complexes on normal metal and superconducting surfaces.

We show that the lifetime of excited spin states in the paramagnetic Fe–Octaethylporphyrin-Chloride (FeOEP-Cl) is orders of magnitude longer when the molecule is adsorbed on a superconductor as compared to a normal metal substrate. We ascribe this increase in spin relaxation time to the superconducting energy gap at the Fermi level, which prohibits efficient pathways of energy quenching into the substrate [1]. The small spin relaxation rates allow for pumping into higher spin states by large current densities.

The magnetic anisotropy of the individual molecules can be varied by the proximity of the STM tip. Approaching the tip to FeOEP-Cl leads to an increase in the axial anisotropy. We ascribe this behaviour to a modification of the crystal field resulting in a shift of the *d*-level energies. On a Au(111) surface, additionally, a Kondo resonance appears once the tip is in contact to the molecule, indicating a stronger coupling of the Fe core to the substrate electrons.

Removing the central Cl ligand changes the oxidation and spin state, respectively. The spin excitation spectra reveal a notable axial and transverse anisotropy, which are also affected by the presence of the STM tip.

[1] B.W. Heinrich et al., Nature Physics 9 (2013) 765.

Abstracts: Invited Lectures

PROGRAM OVERVIEW

Molecular Dynamics Simulations: The Theoretical Partner to Cluster and Dynamic SIMS Experiments

*25 years of collaboration between Jagiellonian University and Penn State.
The special honorary lecture related to Ted Madey Award of the AVS.*

Barbara J. Garrison, Nicholas Winograd

Department of Chemistry, Penn State University, University Park, PA, USA

The efforts of our research groups and our collaboration with scientists from Jagiellonian University have centered upon experimental studies of energetic (5–40 keV) bombardment of solids and computational modeling of the events. Applications of particle bombardment include surface cleaning, surface smoothing, implantation of dopants in semiconductors, focused ion beam milling for integrated circuit repair and TEM sample preparation, reactive ion etching, erosion of the moons of Saturn, and the analytical technique of secondary ion mass spectrometry (SIMS). The intriguing recent advance in the SIMS arena is the use of cluster beams that have expanded the applications to molecular depth profiling and 3D-imaging. The initial results show that 3D-images with hundreds of nm lateral by 10 nm depth resolution can be obtained, a level of resolution with molecular specificity unobtainable in other techniques. The talk will be aimed at a general audience with examples of experimental results or molecular depth profiling and the computational approaches for explaining the experimental data.

[1] R.J. Paruch, Z. Postawa, B.J. Garrison, *Anal. Chem.* 85 (2013) 11628.

[2] K. Shen et al., *Anal. Chem.* 85 (2003) 10565.

[3] N. Winograd, *Anal. Chem.* 87 (2015) 328.

INVITED LECTURES

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Abstracts: Invited Lectures

Interaction of Molecules with Single Atoms on Hydrogenated Semiconductors

S. Godlewski,¹ M. Englund,² M. Kolmer,¹ H. Kawai,³ R. Zuzak,¹ A. Garcia-Lekue,⁴ B. Such,¹ J. Lis,¹ A.M. Echavarren,⁵ C. Joachim,⁶ D. Sanchez-Portal,^{2,4} M. Saeys,⁷ M. Szymonski¹

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²*Centro de Fisica de Materiales CSIC-UPV/EHU, Donostia-San Sebastian, Spain*

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The interaction of organic molecules with single atoms attracts recently growing attention inspired by both the potential applications in the construction of nanoscale machines, rotors or electronic circuitries, light harvesting, heterogeneous catalysis as well as by the interest in the fundamental knowledge of elementary processes occurring between the molecules and atoms. Among several new concepts in electronic technology the idea of single organic molecules utilized as active parts of nanoscale electronic devices has gained growing attention and several prototypical single molecule electronic circuits have been demonstrated. To this day the most widely used substrates are metals. However, in order to reduce the unwanted electronic coupling of molecules with underlying substrate proper isolation of such molecular entities is required. It is expected that the problem could be resolved by application of passivated surfaces [1,2], and recent studies have shown that even a single layer of hydrogen on a semiconducting surface, i.e. Si(001):H or Ge(001):H, could efficiently decouple the molecules from the substrate [3,4]. Detailed characterization of molecular devices requires usage of sophisticated tools, which enable studies in the sub-nanometer range. This could be achieved by application of a scanning tunneling microscope, which not only provides amazing and unprecedented precision of measurements but makes also the fabrication of atomic and molecular devices feasible and controlled.

In the presentation we will characterize behavior of prototypical 3-input trinaphthylene molecules (Y molecules) on the hydrogenated Ge(001):H substrate with the application of low temperature scanning tunneling microscopy/spectroscopy (STM/STS) supported by the advanced theoretical modeling. We will demonstrate that with the application of the STM tip sophisticated surface nanostructures may be fabricated and the chemical bonds between the molecules and unsaturated surface defects could be reversibly formed and broken. We will further discuss the prospects for tip induced manipulation of single atoms and molecules and present the dynamical effects induced by tunneling electrons.

This research was supported by the Polish Ministry for Science and Higher Education (contract no. 0322/IP3/2013/72) and the 7th Framework Programme of the European Union Collaborative Project PAMS (contract no. 610446).

[1] M. Kolmer et al., Phys. Rev. B 86 (2012) 125307.

[2] M. Kolmer et al., Microelectronic Engineering 109 (2013) 262.

[3] S. Godlewski et al., ACS Nano 7 (2013) 10105.

[4] A. Bellec et al., Nano Lett. 9 (2009) 144.

Abstracts: Invited Lectures

Atomic-Scale Investigations with Kelvin Probe Force Microscopy

Leo Gross, Bruno Schuler, Fabian Mohn, Nikolaj Moll, Niko Pavlicek, Wolfram Steurer, Gerhard Meyer

IBM Research – Zurich, Rueschlikon, Switzerland

We investigated individual atoms [1,2], molecules [3,4], and defects [5] on thin NaCl layers on Cu using Kelvin probe force microscopy (KPFM). We employed tips functionalized by CO, Cu, Au, Cl and Xe made by atomic manipulation.

We demonstrate atomic resolution KPFM images with these tips on Cl vacancies and observed qualitatively tip-independent contrast of the local contact potential difference (LCPD) [5].

On molecules we found different height regimes of the LCPD contrast, that qualitatively reflect the electrostatic field above the sample. However, the direct deduction of partial charges within the molecule remains challenging due to the dominating contributions of higher order electrostatic multipoles at small tip heights [4].

On several layer thick NaCl films on different Cu surfaces we investigated the charge stability of Au adatoms and demonstrate charge state control and detection using KPFM [2].

[1] L. Gross et al., Science 324 (2009) 1428.

[2] W. Steurer et al., Phys. Rev. Lett. 114 (2015) 036801.

[3] F. Mohn et al., Nature Nanotech. 7 (2012) 227.

[4] B. Schuler et al., Nano Lett. 14 (2014) 3342.

[5] L. Gross et al., Phys. Rev. B 90 (2014) 155455.

PROGRAM OVERVIEW

INVITED LECTURES

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Create and Manipulate Quantum States on Surface Using Molecules

Nian Lin

Department of Physics, The Hong Kong University of Science and Technology, Hong Kong, PRC

We demonstrate that molecular and supramolecular structures assembled on metal surface provide an effective means to control and manipulate two-dimensional electron gas (2DEG). The first example is to use a cryogenic scanning tunneling microscope to arrange coronene molecules one by one into a triangular lattice on a Cu(111) surface [1]. As revealed by tunneling spectroscopy, the band structure and density of states of the 2DEG exhibit hallmark signatures of massless Dirac fermions. We then manipulated the quasi-particle spectra with aperiodically-arranged molecules, including zigzag and arm-chair edge nanoribbons, single vacancies, Stone–Wales defects and grain boundary dislocation lines. We detected enhanced density of states at or close to the Dirac point. In particular, we resolved edge states in the zigzag nanoribbons. The second example is to use supramolecular self-assembly on a Cu(111) surface to modulate 2DEG band structures [2]. The characteristics of the bands are tuned through changing the periodicity of the supramolecular networks and the molecule-to-surface interaction. In the last, we present a proposal for engineering topological superconductors using this technique, which aims at probing Majorana fermions [3].

[1] S. Wang et al., Phys. Rev. B 88 (2013) 245430.

[2] S. Wang et al., Phys. Rev. Lett. 113 (2014) 196803.

[3] Y. Lu et al., arXiv:1502.02548 (2015).

Solid–Liquid Interfaces Investigated by EC-STM and CV

B. Madry,¹ K. Wandelt,^{1,2} M. Nowicki¹

¹Institute of Experimental Physics, University of Wrocław, Wrocław, Poland

²Institute of Physical and Theoretical Chemistry, University of Bonn, Bonn, Germany

The co-adsorption of submono-, mono- and multi-layers of Cu with sulfate anions on a Au(111) electrode surface was investigated in electrochemical environment (0.1 mM CuSO₄ + 0.1 M H₂SO₄) by cyclic voltammetry (CV) and in-situ scanning tunneling microscopy (STM) [1,2]. Correlated with the STM investigations, the CV measurements indicate co-adsorption/co-desorption processes of Cu of submono-, mono- and multi-layer coverages with sulfuric acid species on Au(111). The formation of a quasi-hexagonal Moiré superstructure on terraces of copper multilayers was observed in situ by STM. In detail, the observed Moiré structure is similar but not identical to the one observed on the (111) surface of bulk copper [3,4]. Kinks of terrace edges correspond to single units of the Moiré mesh. The mean periodicity lengths of the Moiré structure in different directions as well as angles between these directions indicate distortions within the Cu surface, which exhibits characteristic domains. High resolution STM images show the formation of a ($\sqrt{3} \times \sqrt{7}$)-like sulfate structure on all multilayer copper terraces. The interfacial Cu–Au alloy formation is suggested at negative potentials and copper coverages higher than 1ML.

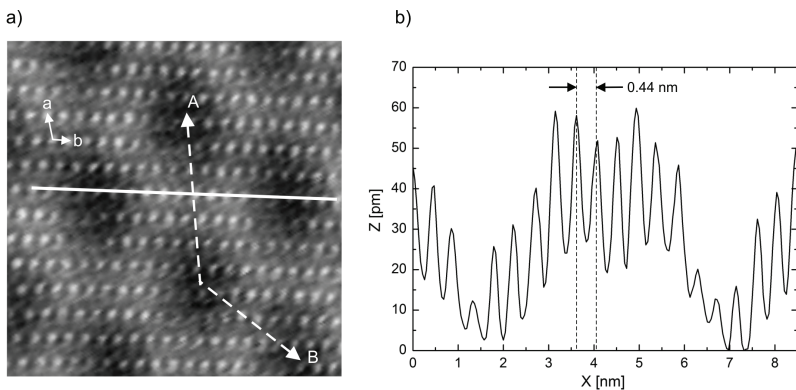


Figure: (a) High resolution STM image (9.24×9.24 nm²) of the ($\sqrt{3} \times \sqrt{7}$)-like sulfate structure (bright spots) superimposed on the Moiré superstructure (dark–bright modulation) on the Cu terrace after overpotential growth of Cu film on Au(111) in 0.1 mM CuSO₄ + 0.1 M H₂SO₄ solution. (b) Height profile along direction *b* of the sulfate anion lattice.

[1] B. Madry, K. Wandelt, M. Nowicki, *Surf. Sci.* 637–638 (2015) 77.

[2] B. Madry, K. Wandelt, M. Nowicki, to be published.

[3] M. Wilms et al., *Surf. Sci.* 416 (1998) 121.

[4] P. Broekmann et al., in: *Topics in Applied Physics*, vol. 85, *Solid–Liquid Interfaces: Macroscopic Phenomena – Microscopic Understanding*, K. Wandelt, S. Thurgate (Eds.), Springer, 2003, p. 141.

Reversible Phase Transitions and Dynamical Fluctuations on Semiconductor Surfaces

José Ortega, Daniel G. Trabada, Fernando Flores

Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, Madrid, Spain

Reversible phase transitions on semiconductor surfaces have been a subject of much interest in surface physics in the last years. In these temperature-induced transitions the dynamical fluctuations of the surface atoms give rise to a reversible change in the translational symmetry as a function of T ; this structural transition is often accompanied by an electronic insulator–metal (IM) transition. The atomic mechanisms responsible for these transitions have been under intense debate. Peierls instabilities and charge density wave formation, order–disorder processes, soft phonons, electron correlations, dynamical fluctuations, etc., have all been proposed, these mechanisms not being mutually exclusive.

In the first part of the talk a general overview of this topic will be presented, paying special attention to the paradigmatic cases Sn/Ge(111)– $(\sqrt{3}\times\sqrt{3})\leftrightarrow(3\times3)$ [1,2] and In/Si(111)– $(4\times1)\leftrightarrow(8\times2)$ [3,4]. In the second part of the talk experimental and theoretical evidence will be presented for a new reversible phase transition that takes place in Sn/Si(111):B [5]. This phase transition is explained by the 24-fold degeneracy of the ground state and a novel mechanism where a Sn tetramer moves along the surface visiting the different ground states.

[1] J. Carpinelli et al., Phys. Rev. Lett. 79 (1997) 2859.

[2] D. Farías et al., Phys. Rev. Lett. 91 (2003) 016103.

[3] H.H. Yeom et al., Phys. Rev. Lett. 82 (1999) 4898.

[4] C. González et al., Phys. Rev. Lett. 96 (2006) 136101.

[5] W. Srour et al., Phys. Rev. Lett. 114 (2015) 196101.

Abstracts: Invited Lectures

The Many-Body Path towards Quantitative Modeling of Complex Adsorption Systems

Alexandre Tkatchenko

Theory Department, Fritz Haber Institute of the Max Planck Society, Berlin, Germany

Reliable (accurate and efficient) modeling of the structure, stability, and electronic properties of complex adsorption systems remains a daunting task for modern electronic structure calculations. In the context of approximate density-functional theory, two thorny issues prevent us from reaching the goal of quantitative predictions: the (in)famous self-interaction error and the lack of reliable methods for an accurate description of van der Waals (vdW) interactions for hybrid inorganic/organic systems (HIOS). Both issues arise from the complexity posed by many-electron quantum mechanics, thereby demanding effective and novel solutions. Focusing on the role of vdW interactions, our recent developments of approximate many-body methods will be discussed along with a few surprises we found when applying these methods to HIOS: (1) The vdW energy can contribute more to the binding of covalently bonded systems than it does for physisorbed molecules; (2) the physically bound precursor state for aromatics on Pt(111) can be more stable than the corresponding chemisorbed state; (3) many-body vdW interactions lead to a binding energy for a fullerene molecule adsorbed on multi-layered graphene that decreases as a function of the number of underlying graphene layers. Finally, we discuss the challenges that lie ahead on the path towards fully quantitative many-body modeling of complex adsorption systems.

PROGRAM OVERVIEW

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Chemical Linkers, Quantum Interference and Other Effects in Single Molecule Circuits: Insight from First Principles

Héctor Vázquez

Institute of Physics, Academy of Sciences of the Czech Republic, Prague, Czech Republic

Single molecule circuits are ideal systems for studying a range of quantum phenomena, and theory and simulations are key in understanding fundamental processes taking place at these nanojunctions. In this talk I will give an overview of how first-principles calculations can be used to understand the flow of current through molecular circuits, focusing on two main topics where I have worked in the past: metal–molecule chemical linkers and quantum interference.

Molecular linker groups are necessary for the formation of stable and reproducible contacts in single molecule transport yet they strongly affect the conducting properties [1]. I will discuss the role played by the linker groups and I will highlight direct Au–C metal–molecule bonds, which result in very high calculated and measured conductance [2].

I will also address quantum interference effects in single molecule transport. Here, the structure, connectivity and spectral properties of the molecule result in exciting examples of constructive [3] and destructive [4] interference.

[1] F. Schwarz, E. Loertscher, *J. Phys.: Condens. Matter* 26 (2014) 474201.

[2] Z.-L. Cheng et al., *Nature Nanotechnol.* 6 (2011) 353.

[3] H. Vázquez et al., *Nature Nanotechnol.* 7 (2012) 663.

[4] C.M. Guedon et al., *Nature Nanotechnol.* 7 (2012) 305.

Abstracts: Invited Lectures

Molecular Electronics: Single Molecule Devices

Harold J.W. Zandvliet*Physics of Interfaces and Nanomaterials, MESA⁺ Institute for Nanotechnology, University of Twente, Enschede, The Netherlands*

In order to design and realize single-molecule devices it is essential to have a good understanding of the properties of an individual molecule. For electronic applications, the most important property of a molecule is its conductance. In this talk I will show how a single octanethiol molecule can be connected to macroscopic leads and how the transport properties of the molecule can be measured [1]. Based on this knowledge we have two single-molecule devices: a molecular switch [2] and a molecular transistor [3]. The switch can be opened and closed at will by carefully adjusting the separation between the electrical contacts and the voltage drop across the contacts. This single-molecular switch operates in a broad temperature range from cryogenic temperatures all the way up to room temperature. Via mechanical gating, i.e. compressing or stretching of the octanethiol molecule by varying the contact's interspace, we are able to systematically adjust the conductance of the electrode–octanethiol–electrode junction. This two-terminal single-molecule transistor is very robust, but the amplification factor is rather limited. In this second part of my talk I will show the feasibility of controlling an atomic scale mechanical device by an external electrical signal. The nanomachine that I will discuss is comprised of only four atoms and exhibits a very rich dynamic behaviour [4].

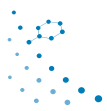
[1] R. Heimbuch et al., Phys. Rev. B 86 (2012) 075456.

[2] A. Kumar et al., J. Phys.: Condens. Matter 24 (2012) 082201.

[3] K. Sotthewes et al., J. Chem. Phys. 139 (2013) 214709.

[4] A. Saedi et al., Nano Lett. 9 (2009) 1733.

Abstracts



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*Abstracts listed in alphabetical order
according to
the presenting author's name*

Abstracts: Oral Presentations

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Identification of an On-Surface Reaction Pathway by Means of Atomic Force Microscopy

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¹*Institute of Experimental and Applied Physics, University of Regensburg, Regensburg, Germany*

²*IBM Research – Zurich, Rüschlikon, Switzerland*

³*Institute of Nanotechnology (INT), Karlsruhe Institute of Technology (KIT), Eggenstein–Leopoldshafen, Germany*

⁴*Institut de Physique et Chimie des Matériaux de Strasbourg (IMCMS), CNRS–Université de Strasbourg, Strasbourg, France*

We study the pathway of a thermally-activated on-surface planarization reaction in detail by analysis of reactant, intermediates and reaction products from atomically resolved atomic force microscopy (AFM) images and spectroscopy with CO functionalized tips [1]. Due to the three dimensional (3D) structure of the reactant, a helical diphenanthrene derivative, the reaction pathway involves an out-of-surface rotation of one phenanthrene moiety.

The characterization of the on-surface reaction in three dimensions is enabled by acquisition and analysis of the AFM signal in a 3D dataset [2]. This way, the structure and geometry of non-planar molecules as well as their unexpected reaction pathway can be determined.

[1] L. Gross et al., *Science* 325 (2009) 1110.

[2] F. Mohn, L. Gross, G. Meyer, *Appl. Phys. Lett.* 99 (2011) 53106.

INVITED LECTURES

ORAL PRESENTATIONS

POSTER PRESENTATIONS

Translation and Rotation in the Surface Diffusion of Cobalt Phthalocyanine on Ag(100)

G. Antczak,¹ W. Kamiński,¹ A. Sabik,¹ Ch. Zaum,² K. Morgenstern³

¹Institute of Experimental Physics, University of Wrocław, Wrocław, Poland

²Leibniz University Hannover, Hannover, Germany

³Chair for Physical Chemistry I, Ruhr-Universität Bochum, Bochum, Germany

The phthalocyanine molecules are model molecules that are, among others, investigated with respect to optoelectronics [1], sensors [2], and quantum computing [3]. This is the reason why it is important to know the stability conditions of those molecules on surfaces. We have used time-lapsed scanning tunneling microscopy in the temperature range of 43 to 50 K and density functional theory to explore the surface diffusion of quasi-isolated cobalt phthalocyanine (CoPc) molecules on the Ag(100) surface. In the presentation, we will show the details of adsorption of this large organic molecule and determine the effective values of the prefactor and the activation energy for its diffusivity. Additionally, we will explore the basic events as translation and rotation, involved in the motion, and how these events are correlated with respect to the molecule–surface interactions. Our combined experimental and theoretical study thus shows that the surface diffusion of CoPc molecule on the Ag(100) surface has a more complex nature than observed for a single adatom mobility.

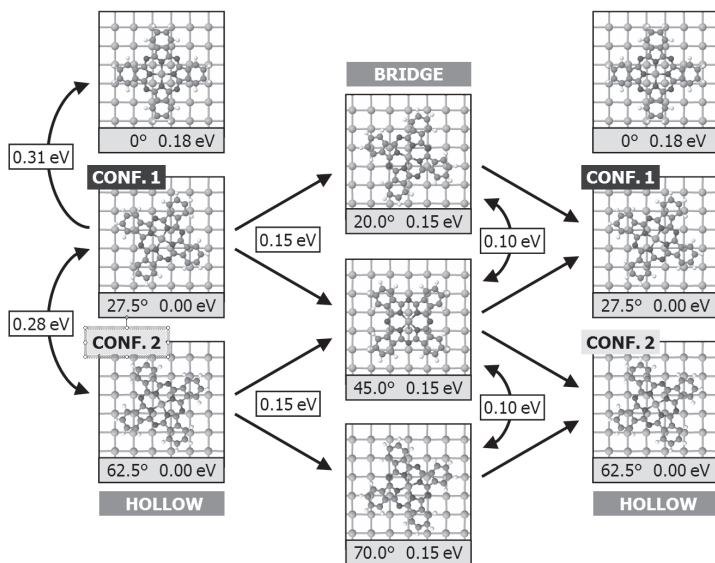


Figure: Diagram with the energy barriers for the combined translational and rotational paths of the CoPc molecule on the Ag(100) surface.

[1] M. Neghabi et al., Mater. Sci. Semicond. Process. 17 (2014) 13.

[2] A.M. Paoletti et al., Sensors 9 (2009) 5277.

[3] M. Warner et al., Nature 503 (2013) 504.

Abstracts: Oral Presentations

Molecular Structure Transformation at the Liquid–Solid Interface

Izabela Cebula,^{1,2} James C. Russell,¹ Jason M. Garfitt,¹ Matthew O. Blunt,¹ Lidong Ma,¹ Matteo Baldoni,² Elena Bichoutskaia,² Maria del Carmen Gimenez–Lopez,² Martin Schröder,² Neil R. Champness,² Peter H. Beton¹

¹*School of Physics and Astronomy, University of Nottingham, University Park, Nottingham, UK*

²*School of Chemistry, University of Nottingham, University Park, Nottingham, UK*

Terphenyl-3,3",5,5"-tetracarboxylic acid (TPTC) and quarterphenyl-3,3"',5,5''-tetracarboxylic acid (QPTC) structure formation at a liquid–solid interface on a graphite surface (HOPG) has been previously studied. TPTC in the presence of nonanoic acid forms rhombus tilings characterized by the existence of 5 different arrangements [1] whereas QPTC assembles forming exclusively one type of the structure [2].

Our interest is to study the role of the solvent played in organic adlayers formation at liquid–solid interface as an important and emerging factor in the control of the adsorbed structures [3].

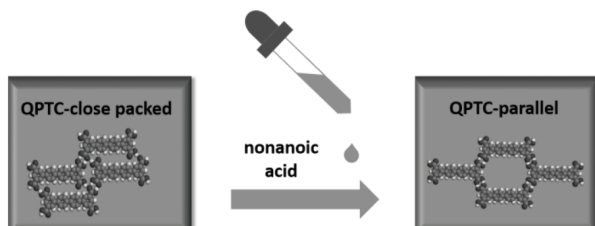


Figure: Schematic representation of the experimental concept.

We present here experimental and theoretical results of the investigation of the structural transformation observed upon solvent introduction. Using the method reported previously [4] we prepared solvent-free films. Highly ordered, close-packed adlayers made of carboxylic acids are formed on HOPG and are characterized using Scanning Tunneling Microscopy (STM). Initially formed structures transform into less dense networks upon exposure to the solvent. We discuss obtained results with the previously reported investigations of TPTC and QPTC systems at liquid–solid interface. Experimentally observed molecular arrangements fit well with models predicted by theory.

[1] M.O. Blunt et al., *Science* 322 (2008) 1077.

[2] M. Blunt et al., *Chem. Comm.* 20 (2008) 2304.

[3] U. Mazur, K.W. Hipps, *Chem. Comm.* 51 (2015) 4737.

[4] I. Cebula et al., *J. Phys. Chem. C* 117 (2013) 18381.

Investigating Intra-Molecular Contributions to the Inelastic Electron Tunneling Signal in Conjugated Molecular Junctions

Giuseppe Foti, Héctor Vázquez

Institute of Physics, Academy of Sciences of the Czech Republic, Prague, Czech Republic

Inelastic electron tunneling spectroscopy (IETS) provides fundamental information about the interaction of tunneling electrons and vibrations in molecular junctions [1] and has been extensively used to study the electronic, structural and vibrational properties of molecular adsorbates.

Previous works addressing the origin of the inelastic signal have identified propensity rules describing the probability of such inelastic processes [2] in terms of the symmetry of the conducting channels and of the vibrational modes.

Here we consider a benzene-based molecular junction and use first-principles simulations [3] to explore the intra-molecular contributions to the inelastic peaks associated with the vibrational modes. Our calculations show how the partial contributions of each atom and bond in the molecule combine in the total inelastic signal. This local picture allows us to obtain a map of the relative importance of the individual molecular components in the IETS peaks.

[1] K.W. Hipps, U. Mazur, J. Phys. Chem. 97 (1993) 7803.

[2] M. Paulsson et al., Phys. Rev. Lett. 100 (2008) 226604.

[3] T. Frederiksen et al., Phys. Rev. B 75 (2007) 205413.

Abstracts: Oral Presentations

Strain Effects on Properties of Water and Ethanol Adsorbed on Transition Metal Substrates

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The adsorption of water and ethanol on transition metal (TM) surfaces is very interesting in view of the hydrogen production. This work is aimed to obtain an understanding of surface strain effects [1] on the adsorption properties of water and ethanol. We investigated structural and energetic properties for these molecules on Cu(111), Pt(111), Au(111), $X_n/Pt_nX_{9-n}/X(111)$ and $Pt_n/X_9/X(111)$ ($X = \text{Cu, Au}; n = 5, 9$), performing a spin-polarized Density Functional Theory calculations within the generalized gradient approximation as proposed by Perdew, Burke and Ernzerhof (PBE). To improve the description of our systems we employed van der Waals corrections proposed by Tkatchenko and Scheffler [2]. As found before [3], alcohol molecules adsorb on TM systems through the oxygen atom on on-top sites nearly parallel to the surface. We can manipulate the TM surface reactivity by depositing layers of another metal, inducing some strain in the system. For PBE, we found that Pt mono- and sub-monolayers on Au(111) increase the adsorption energy of water and ethanol, if compared to Au(111), while for Cu(111) surfaces we found a decrease. This work can contribute to a better understanding of the strain effects, originated from different TM surfaces, on the adsorption properties of water and ethanol.

Work supported by CNPq (R.L.H. Freire Scholarship), CAPES and FAPESP.

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Scanning Quantum Dot Microscopy

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Imaging electric potential on the nanoscale in three dimensions has so far proved to be a great challenge for scanning probe microscopy. Although in recent years Kelvin probe force microscopy has shown its considerable promise for imaging electrostatic interactions [1], it has its drawbacks, most notably that it is measured as a contact potential between two extended surfaces which causes strong averaging effects. We introduce an imaging technique, which we name *Scanning Quantum Dot Microscopy* (SQDM), which quantitatively maps electric potentials in three dimensions with sub-nanometre lateral resolution [2]. By registering charging events of a single molecule quantum dot attached to an NC-AFM/STM tip we have measured the quadrupole field of a single molecule adsorbed on a clean metal surface, and demonstrated the remarkable sensitivity of the method to the dipole field of a single adatom up to 7 nm away.

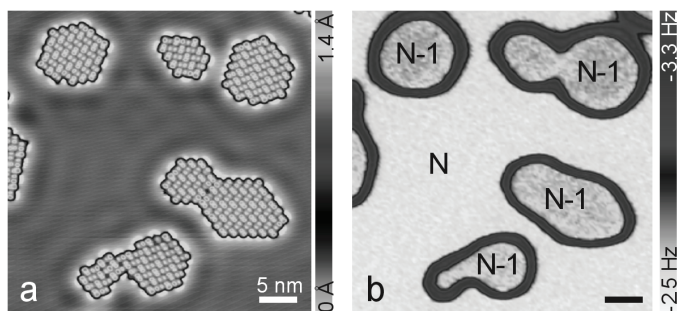


Figure: (a) STM image of PTCDA islands with Ag tip; $V = -0.35$ V, $I = -0.1$ nA. (b) Constant height dipole field image with SQDM tip; thick solid dark lines represent equipotentials where charging events occur, with N and $N-1$ representing the electron population of the QD.

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Abstracts: Oral Presentations

PROGRAM OVERVIEW

Understanding High Resolution STM, AFM and IETS Imaging with Minimalistic Models

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In previous articles we have shown that relaxation of flexible probe particle (PP) attached on the tip is the dominant mechanism leading to sharp sub-molecular contrast observed in AFM, STM [1] and IETS [2] images. The same mechanism is also responsible for appearance of intermolecular features in the position of hydrogen bonds [3,4].

Here we would like to focus on mapping of electrostatic field around molecules from distortion in high resolution AFM/STM images. We will also discuss latest developments of our model for description of STM and IETS images which we achieved by considering nodal structure of electronic states of molecule on the surface.

[1] P. Hapala et al., Phys. Rev. B 90 (2014) 085421.

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INVITED LECTURES

ORAL PRESENTATIONS

POSTER PRESENTATIONS

Abstracts: Oral Presentations

The Growth and Structure of the Ag/Pt(111) Surface-Confined Alloy Investigated with SPA-LEED and LEEM

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We have investigated the growth and structure of the Ag/Pt(111) surface-confined alloy and initial growth of thin silver films on Pt(111) using low energy electron microscopy (LEEM) in microscopy and diffraction mode, and spot profile analysis low energy electron diffraction (SPA-LEED).

We confirmed the formation of a surface confined alloy in the first layer. The in-situ experiments show the intermixing of the material at sub-monolayer coverage, which leads to the development of ordered Pt-rich and Ag-rich phases. During growth we find complex alloying and de-alloying behavior. We confirm the initial alloying followed from about 0.5 monolayers onwards by de-alloying, resulting in a transient relaxation of the Ag film at a coverage of 0.85 ML. Approaching completion of the first layer re-entrant alloying and formation of pseudomorphic layer is observed.

Unconventional growth of the second layer with a remarkable transient heterogeneity was observed. Initially, a mixed layer propagates from the ascending step into the terrace. Later a disordered low density bilayer film emerges, which is seen as the expansion of cauliflower shaped branches from the growth front moving out from the steps. The subsequent densification of this film is accompanied by the emergence of a dislocation network which accommodates surface misfit and unveils itself through the appearance of satellite spots near the integer order peaks in the SPA-LEED diffraction patterns. The growth of thicker films, above 2 ML of Ag, results in periodically undulated Ag layers whose specific symmetry and periodicity is initially set by the buried dislocation network.

[1] H. Brune et al., Phys. Rev. B 49 (1994) 2997.

[2] K. Ait-Mansour et al., Phys. Rev. B 86 (2012) 085404.

[3] M. Jankowski et al., Phys. Rev. B 89 (2014) 235402.

[4] M. Jankowski et al., J. Chem. Phys. 140 (2014) 234705.

PROGRAM OVERVIEW

INVITED LECTURES

ORAL PRESENTATIONS

POSTER PRESENTATIONS

A Study of the Two Dimensional Electron Gas at the InAs(001) Surfaces

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Angle-resolved photoelectron spectroscopy (ARPES) is used to study a few differently reconstructed, sulphur passivated InAs(001) surfaces. On the surfaces we find downward band bending and an electron accumulation layer, i.e. a two dimensional electron gas confined in a subsurface well. Within the layer electron energies associated with the coordinate normal to the surface are discrete and this is indicated by a number of quantized subbands visible in the ARPES spectra.

Depending on the preparation/passivation procedure a few different surface reconstructions and band bending values, are obtained. Here we discuss three examples with the band bending values: 0.23 eV, 0.30 eV, 0.58 eV, shown in the figure below. As seen two or three subbands are found populated by electrons.

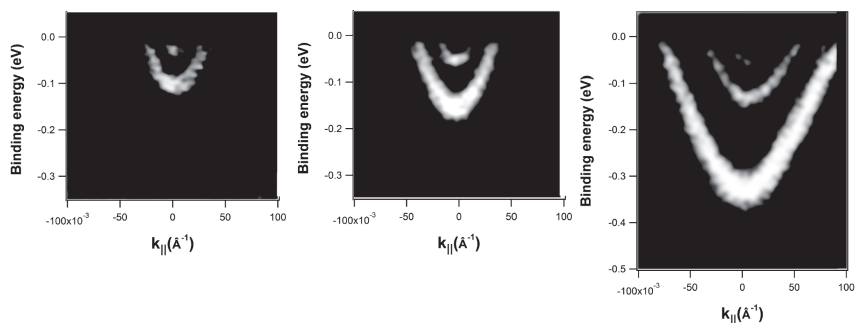


Figure: Quantized subbands within the conduction band of the sulphur passivated InAs surfaces, for band bending values: 0.23 eV, 0.30 eV, and 0.58 eV (left to right).

The results are modeled using the charge screening model. First, for given band bending, the crystal electrostatic potential close to the surface is found by a solution of the self-consistent Poisson equation and second the Schrödinger equation with the obtained potential is solved. Attention is paid to choose realistic boundary conditions at the surface. The theoretical subbands separations are in remarkable agreement with the experimentally measured ones. The electron effective mass is found to be dependent on the band bending magnitude which is tracked down to varying conduction electron concentration near the surface.

We acknowledge financial support by Polish NCN (2011/03/B/ST3/02070). The research was carried out with the equipment purchased thanks to European Regional Development Fund/Polish Innovation Economy Operational Program (POIG.02.01.00-12-023/08).

Quasi 1D Lead Ribbons on the Si(1 10) Surface

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Silicon (1 10) surface has rectangular symmetry and may be considered as a template for the formation of one dimensional structures. However, a (16×2) reconstruction characteristic for the pristine surface [1] as well as (7×2) Pb-induced reconstruction extend along the <11-2> directions [2]. This results in a complex structure of two domains rotated by 70.5° with respect to each other.

In this report we present the results of the formation of one domain system induced by the Pb atoms. The crystallographic and electronic structures of the Si(1 10)-Pb surface are investigated with the reflection high energy electron diffraction and angle resolved photoelectron spectroscopy techniques. Deposition of 1.3 monolayers Pb with subsequent annealing at 260 °C results in the formation of quasi one dimensional ribbons. The Pb ribbons are parallel to the [1-10] direction and reveal the $3a_{\text{Si}} = 16.3 \text{ \AA}$ periodicity along the [001] direction. The electronic structure shows highly anisotropic metallic bands with parabolic dispersion in the [1-10] direction.

The morphology of the surface together with its band structure resemble those obtained for other strongly anisotropic system of Si(553)-Pb [3,4].

This work was partially supported by the National Science Centre under Grant 2013/11/B/ST3/04003.

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[3] M. Kopciuszyński et al., Appl. Surf. Sci. 305 (2014) 139.

[4] M. Kopciuszyński et al., Phys. Rev. B 88 (2013) 155431.

Abstracts: Oral Presentations

Sensing the Charge State of Au at the CeO₂(111) SurfaceK. Kośmider,^{1,2} O. Stetsovych,³ M.V. Ganduglia–Pirovano,⁴ O. Custance,³ R. Pérez¹¹Universidad Autónoma de Madrid, Madrid, Spain²Academy of Sciences of the Czech Republic, Prague, Czech Republic³National Institute for Materials Science, Tsukuba, Japan⁴Consejo Superior de Investigaciones Científicas, Madrid, Spain

Ceria supported gold has attracted significant attention [1] as a potential catalyst for the industrially important water–gas shift reaction. However, despite a large volume of research, there is only little experimental work at the atomic scale, and fundamental understanding of the Au–Ceria interaction is still missing. For example there is no clear picture of a charge transfer in this system. According to density functional theory (DFT) calculations charge transfer depends on an adsorption site, and may even change sign in the presence of oxygen vacancies [2]. But DFT provides conflicting results for the Au/CeO₂(111) depending on exchange-correlation functional. Thus, to understand charge transfer in this system closer cooperation between theory and experiment is needed. Recent scanning tunneling microscopy study [3] (under high vacancies concentration) shows the Ce³⁺ → Au transfer accompanied with an appearance of characteristic Au atom pairs. Unfortunately — despite a proof [4] of capabilities to distinguish between charge polarization of Au atom — no atomic force microscopy (AFM) results considering Au on CeO₂ is available so far.

Here we present a systematic DFT+*U* study of the Au/CeO₂(111) system. Analysis of charge transfer at different adsorption site and surface stoichiometry is shown as an introduction to the force spectroscopy AFM simulation of oppositely charged Au atoms. We consider different tips, including O- and OH-terminated tips [5], and analyze their influence on AFM contrast. Our results could be used as a guideline for prospect AFM measurements.

[1] J.A. Rodriguez et al., *Science* 318 (2007) 1757.[2] C. Zhang et al., *Phys. Chem. Chem. Phys.* 13 (2010) 22.[3] Y. Pan et al., *Phys. Rev. Lett.* 111 (2013) 206101.[4] L. Gross et al., *Science* 324 (2009) 1428.[5] A. Yurtsever et al., *Phys. Rev. B* 85 (2012) 125416.

Au and Si Spin Chains on a Vicinal Si(553) Surface

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Band splitting, spin polarization and topological states generated by spin–orbit interactions (SOI) at surfaces have attracted much attention due to their relevance to spintronics applications [1]. The gold decorated vicinal Si surfaces are prime examples where SOI plays an important role [2–5]. In the case of Si(553)-Au surface SOI is responsible for splitting of a doublet of one-dimensional (1D) metallic Au–Si bands [4–6].

In the present work we discuss the results of our spin-polarized angle-resolved photoelectron spectroscopy (SARPES) and first-principles density functional theory (DFT) investigations of electronic properties of the Si(553)-Au surface. The SARPES data clearly show the existence of the spin-split 1D electronics states, interestingly, with a substantial out of plane component. The DFT calculations reproduce well the experimental data.

This work has been supported by the National Science Centre under Grant No. 2013/11/B/ST3/04003.

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- [2] D. Sanchez–Portal et al., Phys. Rev. Lett. 93 (2004) 146803.
- [3] T. Okuda et al., Phys. Rev. B 82 (2010) 161410.
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- [6] M. Krawiec, Phys. Rev. B 81 (2010) 115436.

Abstracts: Oral Presentations

PROGRAM OVERVIEW

CO₂ Hydrogenation on Rhodium Surfaces: A Study by Field Emission Techniques

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This work addresses the adsorption of CO₂ and the interaction of H₂/CO₂ gas mixtures over single nano-sized rhodium crystallites. This system has been studied using Field Ion (FIM) and Field Emission Microscopies (FEM). FEM and FIM methods are able to image the surface of a metal conditioned as a thin tip with nanoscale and even atomic lateral resolution, respectively. Dynamic evolutions of the surface composition can be followed in real time.

The structure of rhodium nanocrystals has been characterised by FIM, whereas CO₂ adsorption and dissociation have been followed by FEM. Depending of the local work function of the surface, brightness analysis is used to monitor the reaction while it proceeds.

When pure CO₂ gas is introduced in the chamber, the brightness decreases with the dissociative adsorption of CO₂ gas to O(ads) and CO(ads) species. Upon increase of the hydrogen pressure, reaction phenomena were observed from 650 to 700 K. The increasing brightness indicates the occurrence of a reaction between adsorbed hydrogen and adsorbed oxygen.

Crossing our results with literature data allows to propose a coherent chemical scenario. The Reverse Water Gas Shift reaction (CO₂(g) + H₂(g) → CO(g) + H₂O(g)) is most probably in operation in our case [1]. These assumptions are in line with direct local chemical analysis performed by atom probe techniques consisting in the coupling of a FIM device with a Time of Flight mass spectrometer operated during the ongoing processes using field pulses.

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INVITED LECTURES

ORAL PRESENTATIONS

POSTER PRESENTATIONS

Steering the Self-Assembly of Bridged Triphenylamines on KBr(001)

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Molecules on insulating surfaces usually suffer from a weak unspecific molecule–surface interaction, which often leads to the growth of unordered structures. Through a careful design of the molecules functional groups, we were able to tune the self-assembly of bridged triphenylamines from porous and compact two-dimensional networks to nearly upright standing π – π stacked one-dimensional molecular aggregates on KBr(001).

Here, we present a low temperature non-contact atomic force microscopy (nc-AFM) study in ultra-high vacuum on the adsorption and self-assembly of hydrogen-bonding and halogen functionalized triphenylamines on KBr(001). We discuss the role of the intermolecular and molecule–surface interactions based on molecularly resolved nc-AFM images and DFT calculations. We show that triphenylamines bridged with bulky dimethylmethylene side groups adopt flat-lying adsorption geometries, while more compact carbonyl side groups favor intermolecular π – π interaction leading to nearly upright adsorption geometries of the molecules. To clarify the molecule–surface interaction we compare the self-assemblies on KBr(001) to the ones observed on Au(111).

Abstracts: Oral Presentations

PROGRAM OVERVIEW

Enantiospecific Spin Polarization of Electrons Photoemitted through Layers of Homochiral Organic Molecules

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INVITED LECTURES

The relationship between chirality and magnetism has long puzzled researchers. Here we report on spin-polarized photoemission experiments in which monolayer-thick films of chiral 1,2-diphenyl-1,2-ethanediol (DPED) have been studied [1]. This molecule has two chiral centers and presents two chiral enantiomers which are designated according to their conformation and optical activity as (R,R)-(+)-DPED and (S,S)-(-)-DPED. The molecular layers were adsorbed in ultra-high vacuum on ferromagnetic Co films grown on Cu(100) whose in-plane spin polarization served as an *in situ* reference. The photoelectrons emitted through adsorbed layers of both chiral enantiomers display a clear spin polarization at room temperature, independent of their binding energy. The spins point along different directions in space: in-plane for (R,R)-(+)-DPED and out-of-plane for (S,S)-(-)-DPED, which makes the DPED molecule a prototype system to study enantioselective spin filtering. Furthermore, since the electrons were excited with linear light, this is the first demonstration of enantiosensitive response to irradiation not requiring circularly polarized (i.e. chiral) radiation. More recent experiments carried out on a similar molecule, 1,2-diphenylethylenediamine, will also be discussed.

These findings may create opportunities for applications not only in organic-based molecular spintronics but also in other fields such as asymmetric chemical synthesis, as well as provide some insight into the origins of the chiral asymmetries found in Nature.

[1] M.Á. Niño et al., Adv. Mater. 26 (2014) 7474.

ORAL PRESENTATIONS

POSTER PRESENTATIONS

Abstracts: Oral Presentations

Planarized Cyano-Functionalized Triarylaminines on Coinage Metal Surfaces: Intermolecular vs. Molecule/Substrate Interactions

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The interplay of molecule–substrate and intermolecular interactions is of utmost importance in molecular self-assembly on metal surfaces as well as for the electronic properties of these self-assembled structures. While the intermolecular interactions can be controlled by the use of specific functional groups, the molecule–substrate interactions are steered by the corrugation of the adsorption potential, the reactivity of the substrate, its crystal structure and possible surface reconstructions.

We conducted a detailed study of the adsorption of a planar triarylamine derivative functionalized with cyano groups on different (111)-oriented coinage metal surfaces. By using scanning tunneling microscopy and density functional theory studies we found that the substrate plays a crucial role in the self-assembly process. While on Au(111) two different well-ordered phases with micrometer-sized domains stabilized by dipolar coupling, hydrogen bonding and metal coordination were found [1], on Cu(111) only small patches of close-packed molecules were observed next to a disordered phase. In contrast, only one close-packed phase stabilized exclusively by hydrogen bonding was found on Ag(111). This study shows that although the coinage metals Ag and Au are considered relatively inert they can strongly influence the molecular self-assembly due to their different electronic and structural corrugation.

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PROGRAM OVERVIEW

INVITED LECTURES

ORAL PRESENTATIONS

POSTER PRESENTATIONS

Abstracts: Oral Presentations

STM Studies on C₆₀ Molecules Growth on Vicinal Si(553) Surface Passivated with Pb

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Engineering self-assembly of molecular nanostructures, especially one-dimensional (1D) molecular chains on silicon surfaces [1], has been a fascinating subject in the emerging field of nanoelectronics, since it may integrate the vast range of well-controlled flexible structures and functionalities of organic molecules into the main-stream semiconductor electronics seamlessly. However, molecules form strong covalent bonds with the chemically active bare Si surfaces, which inhibit their diffusion on the surfaces, resulting in disordered arrangement [2]. Partially, this problem can be solved by passivation of the Si surface with hydrogen, however, limited success have been achieved [3]. An alternative way to passivate silicon surface is deposition of metal atoms onto Si.

Here, we report first experimental results, showing growth of C₆₀ molecules on vicinal silicon surface passivated with Pb. Bare Si(553) surface covered with 1.3 ML of Pb and annealed transforms into long-range ordered surface with uniform steps and terraces distribution over macroscopic area [4]. Lead forms five-atom wide nanoribbons, weakly coupled to the substrate on each Si(111) terrace, separated by 1.48 nm in [112] direction. C₆₀ molecules deposited on this template at room temperature usually form islands. Locally, at the domains edges molecules form regular, anisotropic, complex chain-like structures.

This work was supported by Polish Science Foundation under HOMING PLUS grant no. 10/2013-08/.

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[4] M. Kopciuszynski et al., *Phys. Rev. B* 88 (2013) 155431.

Two-Dimensional Dielectric on a Semiconductor

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Using the angle resolved photoelectron spectroscopy (ARPES) we investigate the formation of a junction between the isolator and semiconductor on a model KBr/*c*(8×2)-InSb system. KBr (rocksalt structure, lattice constant 6.60 Å, band gap ~7.6 eV) and InSb (zinc blend structure, lattice constant 6.48 Å, band gap ~0.17 eV) are epitaxially matched and nearly layer-by-layer growth mode for KBr on InSb(001) is obtained. We show how the KBr film and the substrate electronic bands evolve during growth of the film.

Our studies show that formation of the KBr film does not destroy electronic band structure of InSb surface—the InSb surface bands are found attenuated but not much changed under the film. The upward band bending is observed. The first KBr monolayer (ML) wets the *c*(8×2)-InSb(001) surface and next layers grow in imperfect (due to a presence of the Schwoebel barriers) layer-by-layer regime [1,2]. It is found that a bilayer of KBr already has the same electronic structure as much thicker films. The maximum of well formed 2 ML KBr film valence band (VBM) is found aligned 5 eV below the VBM of InSb. With this we are able to explain recent scanning tunneling microscopy results for KBr/InSb system, demonstrating that the tunneling from occupied states 2 eV below the Fermi level gives an image of the interfacial Sb sublattice.

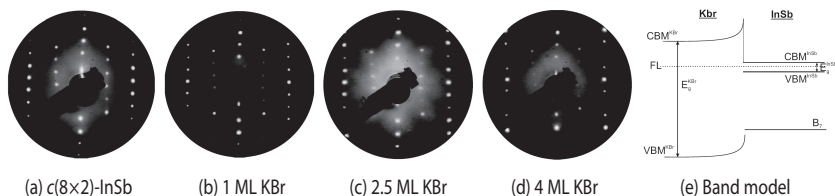


Figure 1: Comparison of the LEED patterns (a–d) for the InSb(001)-*c*(8×2) surface which is covered by KBr. Part (e) presents the band diagram of isolator–semiconductor interface.

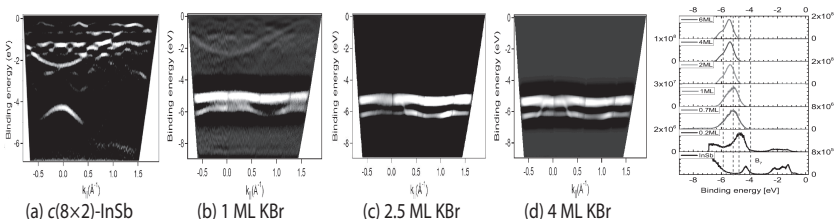


Figure 2: Electronic band structure along the Γ – J' direction for selected coverage of KBr on InSb(001).

We acknowledge financial support by Polish NCN (2011/03/B/ST3/02070). The research was carried out with the equipment purchased thanks to European Regional Development Fund/Polish Innovation Economy Operational Program (POIG.02.01.00-12-023/08).

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Abstracts: Oral Presentations

Theoretical Study of Oxygen Adsorption on Iron (110) Surface

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Oxygen adsorption on iron surfaces is intensively studied due to importance of this process in oxide formation. Previous experimental and theoretical studies have demonstrated that oxygen adsorbs dissociatively on iron surfaces [1]. Both experiment and theory suggested that on the Fe(110) surface oxygen is adsorbed in twofold coordinated long bridge sites. Our accurate DFT calculations show that adsorption of oxygen is energetically preferred in pseudo-threefold coordinated hollows [2]. However, at low oxygen coverage, a long bridge and pseudo-threefold hollow sites are nearly degenerated in energy. This is in contrast to the experiment and to earlier theoretical studies which reported the threefold coordinated hollow sites to be unstable [1,3]. We show that the preference for an oxygen adsorption in the threefold hollow sites, which results from our calculations, can be reconciled with experimental observations. We also discuss how this site switch affects the interpretation of different on-surface oxygen structures observed experimentally [4]. The effect of accounting for strong correlations between Fe 3d electrons on the properties of the O/Fe(110) system, by including Hubbard correction, will be discussed.

Work supported by the National Science Centre (NCN), Poland (Grant No. 2012/07/B/ST3/03009).

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Theoretical Investigation of Au Nanostructures on Hematite (0001) Surface

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In recent years supported gold nanoparticles have attracted significant interest for their unusual catalytic properties in a broad range of reactions. Highly dispersed gold particles supported on iron oxides are very active catalyst for the oxidation of CO at ambient temperatures. In this work the adsorption of Au atoms [1] and small Au_n nanoclusters ($n = 2, 3, 4$) on α -Fe₂O₃ (hematite) (0001) surfaces is investigated using density functional theory (DFT) with Hubbard corrections for strongly correlated Fe 3d electrons (DFT+U). The structural, energetic, and electronic properties are examined for the stable vertical and tilted orientations of Au_n nanostructures adsorbed on both Fe- and O-rich terminated hematite surfaces. The tilted orientations are energetically more favored on both terminations. The different character of both terminations of hematite is reflected in different character of changes of the adsorption binding energy with the size of the Au_n cluster. On the Fe-terminated surface the binding energy increases with the number of Au atoms in a cluster, whereas on the O-rich termination it decreases with increased cluster size. Changes in the electronic structure of the Au_n nanostructures and the oxide support and consequences for their interactions with CO are discussed.

Work supported by the National Science Center (NCN), Poland (Grant No. 2012/07/B/ST3/03009).

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Abstracts: Oral Presentations

The Photocatalytic Growth of Silver Nanoparticles on Titanium Dioxide Coatings

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The size and number of silver nanoparticles (AgNPs) grown on the titanium dioxide (TiO₂) surface using photo-assisted method are influenced by many factors [1]. Usually, AgNPs are used to enhance the photocatalytic and antibacterial properties of TiO₂-based materials [2,3]. However, the mechanisms of photocatalytic growth of AgNPs are still in the center of interest of many research groups. Since the final properties of AgNPs strongly depend on their size, it is of great importance to gain the knowledge related to the phenomenon of their growth.

In this study, we investigate the kinetics of AgNPs growth by monitoring of their primary nucleation stages using microscopy techniques. It was found that changes in size and number of AgNPs are especially dynamic during first 10–30 s of UV illumination. These changes have their origin in the release/diffusion of Ag⁺ ions and their migration to TiO₂ surface. For longer illumination periods (up to 180–300 s) this effect can be also observed as preferential enlargement of some particles combined with simultaneous decrease of size and subsequent disappearance of small, non-stable silver clusters. On the basis of these observations we propose the Ostwald ripening model as possible mechanism of AgNPs growth on TiO₂ [4].

The preparation of AgNPs on TiO₂ having homogenous size distribution as well as control of particle surface density are very important due to their vast applications not only in photocatalysis but especially in enhancement of fluorescence and Raman scattering signals in surface investigations.

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Silicene on Ultrathin Pb Films

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Silicene, two-dimensional layer of Si atoms ordered in the honeycomb lattice, both in terms of atomic and electronic structure is a silicon equivalent of graphene. Silicene has been successfully produced only on a few different substrates so far, but the main effort is put into the study of silicene on the surface of silver. The electronic structure of such a system, particularly with regard to existence of Dirac cone, is still under an intense discussion [1–3].

In the presentation we propose the use of thin layers of lead as a substrate for silicene. Since binding energy in this case is up to three times lower than for bulk silver, the linear dispersion around the K points of Brillouin zone is maintained [4]. The research include results for different numbers of lead layers, which allows us to analyze how the properties of the system like binding energy, distance between silicene and the topmost layer of Pb atoms and position of Dirac cone oscillate with thickness of the substrate.

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Study of the Substrate Influence on the Properties of Physisorbed Self-Assembled Molecular Layers: Azabenzene 1,3,5-Triazine on Graphite and Graphene on Metals

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The properties of SAMs on inorganic substrates depend on a delicate balance between intermolecular and overlayer–substrate interactions. We present a combined experimental and theoretical study of azabenzene 1,3,5-triazine layers grown on both graphite and G/Pt(111). STM experiments show different large Moiré structures for the two substrates [1]. In our ab initio DFT calculations (using VASP) we use different functionals (PBE, hybrids) and vdW implementations [2] to fully characterize the intermolecular (H-bonds + vdW) and molecule–substrate (vdW attraction + Pauli repulsion) interactions. Our results confirm that the molecule–substrate interactions fix a relative orientation between substrate and SAM while H-bonds preserve the lattice symmetry of the isolated monolayer. The graphene layer modifies the H-bonds with respect to an isolated layer but no significant differences are found between the substrates. Smaller adsorption distances would imply larger adsorption energies which would be determinant in order to achieve results much closer to the experimental values. This exhaustive characterization shows the theoretical limitations to describe these weakly interacting systems even with state-of-the-art approaches.

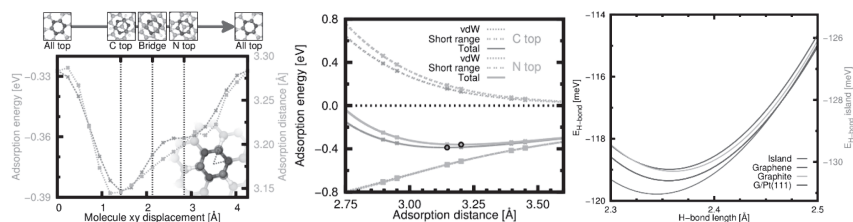


Figure: Left and center plots show the energy dependence with the xy position (over the Moiré) and z position (adsorption distance) of the triazine, respectively, for a graphene substrate. The right plot shows no change between substrates in the H-bond distance.

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Adsorption of Organic Molecules on Thin Cobalt Oxide Films

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While the properties of organic molecules on metal surfaces have been intensively studied in recent years, much less is known about their properties on oxide surfaces. Using cobalt oxide CoO(111) thin films grown on Ir(100) as a well characterized transition metal oxide substrate [1] we studied the adsorption and self-assembly of some common organic molecules using Scanning Tunneling Microscopy. Aiming at understanding the basic interaction mechanisms between the molecules and the surface we focused on monolayer or sub-monolayer organic films. We varied the oxide film thickness from monolayer to multilayer thickness thus covering the range from metal-oxide hybrid phases to true oxide surfaces.

The molecules studied are pentacene (Pn), Co-phthalocyanine (CoPc) and biphenyl-dicarboxylic acid (BDA). All molecules adsorb flat-lying on the oxide surface. While Pn is a representative of a π -system interacting with the substrate, CoPc provides an anchoring point in form of the coordinated metal ion, and BDA combines the π -system with the additional potential of creating hydrogen bonds with molecular neighbours. For all systems we observe that on the single bilayer CoO(111) film [2] the molecule–substrate interaction is relatively strong resulting in a site-specific adsorption geometry that is influenced by the corrugation of the oxide surface. As a consequence the first molecular layer is less dense than what could be achieved considering the molecular geometry only. On thicker oxide films the molecule–substrate interaction is weakened leading to a dense assembly of molecules in islands.

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Abstracts: Oral Presentations

PROGRAM OVERVIEW

Interference TiO_x/Ti/TiO_x/Glass Systems Produced in the Industrial Scale Using GIMS Method

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In the last decades titanium oxides are intensively studied because of their exceptional properties. These oxides are used in some high-tech applications including electrochromic devices and dye-sensitized solar cells. Moreover, TiO₂ (also in the doped form) can be used as protective and antireflective coatings. Furthermore, titanium oxides and (oxy)nitrides can be applied as a decorative material for architecture, the automotive industry, electronics and jewellery [1,2].

The opaque and semitransparent TiO_x/Ti/TiO_x/glass systems were deposited using gas injection magnetron sputtering (GIMS) method [3,4] in the Bohamet S.A. company. The industrial magnetron was successfully adopted to produce an opaque TiO_x/Ti/glass glazing [1]. The thickness of dielectric film directly determines the interference colour of coating. In turn, the thickness of Ti film affects the transparency of TiO_x/Ti/TiO_x/glass system.

Optical and microstructural properties of thin metallic films strongly depend on growing conditions. In this study, the influence of the deposition time on optical and microstructural properties of Ti layers was examined and characterization of TiO_x/Ti/TiO_x/glass systems was performed.

The produced samples were investigated by means of spectroscopic ellipsometry (SE), atomic force microscopy (AFM) and confocal optical microscopy (COM). Additionally, the reflectance (R) and transmittance (T) measurements were performed.

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INVITED LECTURES

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Visualizing Local Reaction Kinetics: Hydrogen Oxidation on Rhodium

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Recently, the *local kinetics by imaging* approach was developed, which is based on the correlation between the local catalytic activity of particular surface regions and the local photoemission yield [1]. Both quantities depend on the surface coverage of adsorbates which serve as reactants in a catalytic reaction: the catalytic activity does it directly and the photoemission yield depends on the coverage via work function. This correlation is scalable down to the nm-scale and allows to obtain the laterally-resolved kinetic information with the resolution of the corresponding photoemission sensitive device, e.g. PEEM (photoemission electron microscope). The approach has been realised using the digital analysis of the PEEM video-sequences recorded during the ongoing surface reaction and was applied first for the CO oxidation on individual μm -sized Pt and Pd grains of polycrystalline foils and on the supported Pd powder [1–4].

In present contribution we apply this approach for the first time to study the local kinetics of the H_2 oxidation on individual Rh(hkl) domains of a polycrystalline Rh foil and on the zirconia-supported Ph powder.

This work was supported by the Austrian Science Fund (FWF) [SFB F45 FOXSI].

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Self-Organization of S Adatoms on Au(111): $\sqrt{3}R30^\circ$ Rows at Low Coverage

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Using scanning tunneling microscopy (STM), we observe an adlayer structure that is dominated by short rows of S atoms, on unreconstructed regions of a Au(111) surface in ultrahigh vacuum. This structure forms upon adsorption of low S coverage (less than 0.1 monolayer) on a fully reconstructed clean surface at 300 K, then cooling to 5 K for observation. The rows adopt one of three orientations that are rotated by 30° from the close-packed directions of the Au(111) substrate, and adjacent S atoms are separated by $\sqrt{3}$ times the surface lattice constant a . Monte Carlo simulations performed on DFT-derived lattice-gas models, with pairwise interactions extending to $5a$, plus simple trio interactions, successfully reproduce the linear rows of S atoms at reasonable temperatures. The observation of individual S atoms is compared to other observations of sulfur-derived structures on Cu(111) and Ag(111) surfaces under essentially-identical conditions.

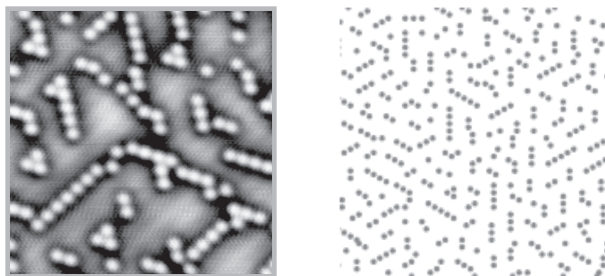


Figure: Left: Scanning tunneling micrograph of individual S atoms self-assembled into short $\sqrt{3}a$ linear rows; $10 \times 10 \text{ nm}^2$. Right: Snapshot of an ab-initio Monte Carlo configuration; $39 \times 39 \text{ nm}^2$.

On the Formation of Two-Dimensional Alloys of Sn and Pb Coadsorbed on Ru(0001)

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Atoms of immiscible Pb and Sn metals have been recently shown to form locally a two-dimensional ordered alloy on Ru(0001) [1]. The identified alloy phase, observed upon subsequent deposition of 0.15 ± 0.05 ML of Pb and 0.40 ± 0.05 ML of Sn, exhibited a slightly incommensurate structure of a $(\sqrt{7} \times \sqrt{7})$ symmetry and a close-packed hexagonal-like arrangement of Sn and Pb adatoms with an average composition corresponding to PbSn_3 .

Motivated by this experimental work, we employ DFT simulations to establish the conditions for the occurrence of Sn–Pb ordered alloys on Ru(0001). To this end, we calculate the surface phase diagram of Sn and Pb coadsorbed on the Ru(0001) substrate and determine ranges of doses of deposited Sn and Pb when the formation of a binary alloy is energetically more favorable than the growth of segregated pure phases of Sn and Pb. We identify the preferred Sn–Pb alloy structures in terms of their stoichiometry, lateral symmetry, as well as the optimal adatom configuration within the surface unit cell. Main electronic characteristics of the postulated alloy phases are discussed, including the analysis of partial density-of-states spectra and spatial distributions of electronic charge. The corresponding STM images are also simulated. Our DFT predictions are contrasted with the experimental results reported in [1].

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Abstracts: Oral Presentations

Clean and Adsorbed 4H-SiC{0001} Surfaces: A DFT Study

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The wide band-gap semiconductor silicon carbide has attracted a great interest during the past decades because of number of properties which make it very attractive for many applications in electronic devices. For electronic applications purposes hexagonal 4H-SiC is the preferred polytype. One of the main problems in the development of the SiC-based electronics is still poor quality of the SiC crystals. There have been theoretical studies of both clean and adsorbed ideal 4H-SiC{0001} surfaces. Therefore, it is necessary to understand the interaction of basic building bricks like Si, C, Si₂C and SiC₂ with the surface. Since hexagonal SiC crystals grow along <0001> direction, the interaction of Si, C and Si₂C interaction with Si- and C-terminated {0001} surfaces is examined within DFT framework. The most favourable adsorption sites are identified for two adsorbate coverages. We found that Si₂C molecule lies almost flatly on both surfaces with Si atom connected to the underlying topmost substrate atom. Qualitative ab initio molecular dynamic simulations show that molecules bind to both examined surfaces without dissociation. It is confirmed by quantitative DFT studies showing that there is no barrier for the molecule adsorption. Moreover, a possible mechanism of Si₂C on-surface dissociation is examined. Then, the coadsorption of another Si₂C molecule is studied.

Real surfaces are stepped ones and chemical processes important for crystal growth can occur at steps or in their vicinity. Therefore, we also present DFT calculations of clean steps along <10-10> and <11-20> directions on Si- and C-terminated 4H-SiC{0001} surfaces. We applied two different models for steps with various heights. For each model tests were performed aiming at finding a minimal step width by increasing the step width from 4 to 14 atomic layers. We searched for the sufficient step width to describe correctly flat terraces between steps. Our research shows that even for the widest steps examined the corrugation on terraces is still observed. It exists in both models and is especially pronounced on Si-terminated surfaces. It is an indication of strong long-range stress induced by steps.

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Para-Hexaphenyl as a Molecular Sensor of TiO₂(110) Surface Quality: Influence of Ion Beam Irradiation and Air Passivation of Substrate Surface

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²Montanuniversitaet Leoben, Leoben, Austria

We report on molecular ultra-thin films grown on titanium dioxide single crystal surfaces, either atomically flat or ion beam modified. The surface morphology of the developed para-hexaphenyl (6P) structures was studied: *in situ* by means of non-contact AFM and *ex situ* by tapping-mode AFM and SEM.

The atomically flat TiO₂(110)(1×1) surfaces were prepared in UHV by cycles of Ar⁺ sputtering and subsequent annealing. For the ion-beam induced surface modification, the samples were irradiated by 2 keV Ar⁺ ions under either normal or oblique incidence resulting in isotropic or anisotropic (*rippled*) surface structures, respectively.

It will be shown that the chain-like para-hexaphenyl molecules can be used as a molecular sensor of substrate surface quality. For the atomically flat substrate, the formation of tens of micrometers long 6P nanoneedles composed of lying molecules is observed. Subsequent air exposure initiates a dewetting process resulting in the formation of small features between the nanoneedles — crystallites. When the procedure is reversed (air exposure proceeding the deposition) it results in the formation of dendritic islands, composed of upright standing molecules.

Also ion beam irradiation of titanium dioxide surface influences molecule–substrate interaction and causes para-hexaphenyl molecules to form upright-standing islands. We will show that by tailoring the surface structure properties like anisotropy, height and lateral size, the islands sizes, shapes and degree of attachment can be controlled.

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Spin-Polarized Photoemission from Ultrathin Ag Films on Si(111)

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The spin-polarized surface states have been observed experimentally for the first time on Au(111) [1]. Since then the Rashba effect has been studied for many various surfaces and ultrathin layers of high Z number metals [2]. The effect is caused by the breaking inversion symmetry at the crystal surface and is due to the spin-orbit interaction. The influence of the spin-orbit interaction can also be observed for the bulk continuum states at the surface region [3]. A strong polarization of photoelectrons from such states has been reported for Bi(111) [4]. Among many studied systems, however, there are no reports of this effect for materials with the low Z number.

In this contribution the results of spin-polarized photoemission from Ag ultrathin layers grown on the Si(111) surface are presented. The d states of Ag reveal spin polarization with the polarization vector parallel to the sample surface. The spin-split states are visible for the Ag films as thin as 1 monolayer. It is also shown that the Si(111) surface with $(\sqrt{3} \times \sqrt{3})$ Ag reconstruction reveals clear spin-polarized states. The results are discussed within the framework of the bulk continuum states and influence of the photoemission process on the polarization of photoelectrons.

This work was partially supported by the National Science Centre under Grant 2013/11/B/ST3/04003.

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Abstracts

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Using Two-Dimensional Correlation Spectroscopy and Principal Component Analysis to Enhance Spectral Information Available from XPS Spectra for Ti–O–N System

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When XPS (X-ray photoelectron spectroscopy) is used to study changes on a sample surface, the information about prominent peaks for elemental identification and concentration calculations is typically obtained. Two-dimensional correlation spectroscopy (2D-COS) and principal component analysis (PCA) can help extract the maximum amount of information from the collected spectral data. The objective of this work is to study the surface reaction of the titanium–oxide–nitride system during annealing by using these two methods. To obtain a better initial understanding about the XPS data structure we employed the PCA method. The main advantage of using PCA is that there is no need to construct peak models for strongly overlapped features. The result shows that the first two principal components provide useful information about the changes in the peaks and the peak positions in terms of binding energy. More deeply, these changes can be monitored by 2D-COS analysis. 2D-COS technique allows us to enhance spectral resolution and make band assignments. The main use is to determine the sequence of emergence of the spectral peaks. The spectral peaks are spread across the x and y axes and the result is a contour map where the peak intensities indicate the degree of correlation. From the analysis of the 2D XPS correlation spectra, we suggest a mechanism of the formation and changes in the chemical states for the analysed Ti–O–N system.

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Abstracts: Poster Presentations

Bridging Scales in the Surface Oxidation of Zr: XPS, PEEM, FIM, FEM and DFT Studies**I. Bespalov, M. Datler, S. Buhr, J. Zeininger, P. Blaha, G. Rupprechter, Y. Suchorski***Institute of Materials Chemistry, Vienna University of Technology, Vienna, Austria*

One of the main uses of Zr and Zr-alloys is in nuclear technology, as e.g. cladding of fuel rods in nuclear reactors [1]. Since the surface oxidation of Zr is an important process in such applications, it is extensively studied presently. Mostly, the composition, the structure and the oxidation state are studied and much less the kinetics and the mechanism of the oxide formation [2,3].

The Zr “hcp-to-bcc” phase transition occurring at temperatures usual in nuclear reactors remains mainly disregarded in the Zr oxidation studies. In the present contribution we apply XPS, PEEM, FIM, and FEM for the studies of zirconium oxide formation via oxidation of the polycrystalline Zr surface, also of those subjected to the “hcp-to-bcc” transition. DFT calculations are in accord with the experimental findings including the formation of Zr-suboxides.

The “hcp-to-bcc” phase transition in Zr is visualized by PEEM for the first time and the structure and surface morphology changes caused by this phase transition are observed. The role of Zr suboxides in the oxidic support of catalytically active metal particles is discussed.

This work was supported by the Austrian Science Fund (FWF) [SFB F45 FOXSI].

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Oxygen-Assisted Morphological Changes of Pt Nanosized Crystals: A Study by Field Ion Microscopy

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The studies of thermal faceting of crystals of platinum group metals induced by oxygen adsorption were triggered among others by their rich catalytic properties and widespread in numerous catalytic applications. In this context Field Ion Microscopy (FIM) is an advanced experimental tool for studying the crystal morphology. The specimen—a metal tip of radius of curvature around 15–25 nm—can be regarded as a good model of a particle of a real catalyst, by its size and its shape. Faceting experiments carried out on curved surfaces can show morphological and structural changes of many different planes simultaneously, giving an insight into the evolution of shape of the microcrystals of the catalyst.

In this contribution the influence of oxygen adsorption on the shape of the Pt nanosized crystal will be presented. The clean Pt tip annealed at around 700 K exposed only low index {001} and {111} planes. For low oxygen exposures the crystal shape did not change considerably. When the crystal was exposed to more than 100 L at around 300 K the development of {113}, {111}, {100} planes was observed after annealing of the tip at 700 K. The planes of such reconstructed crystal were separated by relatively broad zones of corrugated, rounded 'edges', which is in contrast to sharp interplanar edges observed during faceting of Pd [1] and Ir [2] crystals adsorbed with low amounts of oxygen.

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Structure of the Sulphur-Passivated InSb (001) Surface

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Using low energy electron diffraction and angle-resolved photoelectron spectroscopy we study the (001) InSb surface passivated with an adsorption of sulphur dimers, coming from an electrochemical source.

On the clean (001) InSb surface prepared by ion beam annealing $c(8 \times 2)/(4 \times 2)$ reconstruction is formed. The surface is then subjected to the passivation process at elevated temperature (230 °C) with the sulphur dose equal to 20 L. It is then annealed repeatedly to increasingly higher temperatures up to 470 °C.

Immediately after passivation the surface is found to be weakly ordered and exhibits no distinct diffraction peaks. Annealing at 435 °C leads to the formation of $c(4 \times 8)$ reconstruction. Crystallographic order on the surface is improved by annealing to the temperatures up to 455 °C. Above this temperature one-dimensional disorder appears on the surface, as indicated by streaking of diffraction reflexes in LEED pattern. It is worth noting that we have observed similar effect on the sulphur-passivated InAs (001) surface.

Annealing to the temperature of 470 °C leads to the formation of $c(4 \times 12)$ surface reconstruction. Further studies are needed to explain the structure of S-passivated InSb (001).

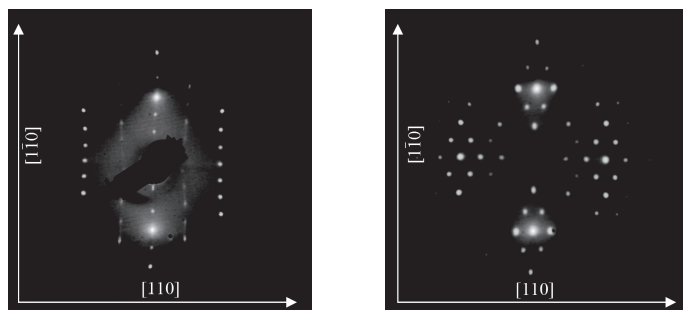


Figure: LEED pattern of InSb (001) surface before (left) and after (right) S-passivation and annealing at 455 °C, incident electron energy $E = 65$ eV.

We acknowledge financial support by Polish NCN (2011/03/B/ST3/02070). The research was carried out with the equipment purchased thanks to European Regional Development Fund/Polish Innovation Economy Operational Program (POIG.02.01.00-12-023/08).

Abstracts: Poster Presentations

Mapping the Reaction Front Nucleation and Propagation in H₂ Oxidation on Rh

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The surface of a catalytically active polycrystalline foil, which consists of crystallographically different μm -sized domains, provides a suitable system for a direct comparison of catalytic behaviour of differing crystallographic orientations. A prerequisite for such a comparison is the ability to evaluate the reaction behaviour of individual domains in parallel measurements, i.e. spatially-resolved analysis of the reaction kinetics on a μm -scale is required. The *kinetics by imaging* approach, based on the *in situ* PEEM imaging of surface reactions, provides such a possibility, as it was recently demonstrated for the CO oxidation on individual Pt(hkl) and Pd(hkl) domains [1–3]. Apart from the local kinetic data, such approach provides simultaneous information about the nucleation and propagation of the reaction fronts on different domains at identical conditions and can also help to reveal e.g. the role of defects in the behaviour of the reaction fronts [4].

We apply herewith the above approach for the first time to the monitoring of the reaction front nucleation and propagation on individual Rh(hkl) domains of a polycrystalline Rh foil and on the ZrO₂ supported Rh powder in the H₂ oxidation. The role of defects and grain boundaries in the present observations is discussed.

This work was supported by the Austrian Science Fund (FWF) [SFB F45 FOXSI].

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Formation of Metal/CuPc Films on the HOPG and InSb Substrates Studied by Electron Spectroscopies

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The results of thin layers of metals: In, Sn and Ti on a thick layer of Cu-Phthalocyanine (CuPc) are presented. CuPc layers were formed by vacuum evaporation on the surface of graphite (HOPG) and on the surfaces of single crystals: InSb(111), unreconstructed InSb(001) and reconstructed InSb(001)-c(8×2). The formation of multilayers was monitored using a quartz microbalance and then examined using Auger electron spectroscopy (AES) and X-ray photoelectron spectroscopy (XPS). The atomic composition of the films was determined by measuring the profiles using XPS spectroscopy. Then films were annealed and the diffusion of atomic components from the substrate and top metallic layer into the CuPc film was observed.

Additionally, we present preliminary results from these layers using characteristic electron energy losses and very low energy electron diffraction (VLEED) in the target current measurement regime (TCS). Peaks in sample current derivative $S(E) = dI/dE$ correspond to the edges of unoccupied states and the d^2I/dE^2 spectrum corresponds to the density of unoccupied states.

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Abstracts: Poster Presentations

Studies of Nanostructures on the Cleavage Surface of InSe Layered Crystal Intercalated by Nickel

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The nanoscale self-assembling systems obtained by intercalation of 3d elements (e.g. Ni) into a matrix of InSe semiconductor layered crystal are interesting in terms of creating materials with paramagnetic properties for use in spintronic devices. The bulk metal nanostructures in the interlayer gaps become surface ones after cleavage, and thus could be studied by low electron energy diffraction (LEED) and scanning tunneling microscopy/spectroscopy (STM/STS) methods.

Nickel intercalated InSe crystals have been grown by the Bridgman method from the pre-synthesized components. Synthesis was carried out by a special procedure to prevent the formation of nickel selenides. Further thermo treatment of grown crystals in evacuated quartz ampoules, carried out for 60 h at 870 K, led to Ni intercalation. LEED data were analyzed using the SPECS SAFIRE Diffraction Image Acquisition and Processing System. The STM/STS data were acquired using the Omicron NanoTechnology STM/AFM System.

The clear LEED spots of InSe hexagonal structure are observed for InSe (Ni). The calculated values of the two-dimensional lattice constants $a = b = 4.0 \text{ \AA}$, located in the (0001) InSe (Ni) cleavage surface plane correspond to the ones for bulk InSe crystal. Therefore, it was confirmed that Ni was introduced in the interlayer gap. The additional spots corresponding to metallic Ni phase are determined at high primary electron beam energies (~190–200 eV).

STM suggests the unreconstructed structure of (0001) surface covered by intercalate, which is similar for pure InSe. However, some clusters are observed on the surface in the form of local blurring of hexagonal structure. 2D-FFT filtering of these clusters revealed the structure with 3.5 Å period characteristic for metallic nickel. The analysis of density of states by STS confirms the “metallic nature” of local areas on InSe (Ni) surface.

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Mechanical and Microstructural Properties of Ti Layers Deposited on Glass Using GIMS and PMS Techniques

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It is commonly known that forming a coating by different magnetron sputtering method may result in different microstructural properties of coatings [1]. We would like to compare mechanical and microstructural properties such as instrumental hardness, Young's modulus, adhesion as well as roughness, crystalline structure and average size of nanocrystallites for titanium layers deposited on float glass by the recently developed gas injected magnetron sputtering method (GIMS) [2,3] and the commonly known pulsed magnetron sputtering method (PMS) [1]. Titanium layers were applied at three different argon pressures. Additionally, a part of Ti coatings were deposited on the TiO₂-coated float glass. Mechanical properties of such obtained coatings were measured by microindentation tester and scratch tester (CSM Instruments). In turn, the microstructural properties of the fabricated Ti coatings were investigated by atomic force microscope (Bruker), confocal optical microscope (Olympus) and X-ray diffractometer (PANalytical). The obtained results show that the features of Ti coatings are strongly affected by the argon pressure and in some cases also by the depositing method.

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Abstracts: Poster Presentations

Role of Orbital Structure in High-Resolution STM of Molecules

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Most features visible in high-resolution AFM images of molecules can be explained by simple mechanical model considering relaxation of an atomistic particle attached to the tip [1,2]. On top of this, we introduced a simple model for calculating STM current considering only inter-atomic hoppings between relaxed atomistic particle and molecule [1]. The simple model is able to reproduce the main characteristics of high-resolution STM maps in close distance regime where the relaxation effects prevail. But since it completely neglects the electronic structure of the scanned sample, it fails at far distances where the electronic structure is dominating in the STM current.

In this work, we implemented an efficient method for simulation of the high resolution STM images considering the molecular electronic structure and the atomistic particle relaxation as well. The method is able to reproduce observed contrast in both the close distance and the far distance regimes, including the gradual transition between them. It gives solid theoretical background for better understanding of high-resolution STM experiments.

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Surface Diffusion on Tungsten and Molybdenum Single Crystals

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The growth and surface diffusion of indium, tin and titanium thin films deposited on tungsten and molybdenum single crystals were studied. Present work is a continuation of our previous reports [1,2].

Thin films were deposited using standard effusion cell and electron-beam evaporation (EBV) sources. Growth of thin layers was analysed by means of Scanning Tunneling Microscopy (STM) and Low Energy Electron Diffraction (LEED). Surface diffusion was observed using X-ray Photoelectron Spectroscopy (XPS) with analyser operating in spatial mode. Surface diffusion was investigated along different crystallographic directions of the substrate. An attempt was made to determine surface diffusion coefficients.

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An Investigation of Oxidised Polycrystalline Fe–Cr Alloys Studied by Mössbauer and X-ray Photoelectron Spectroscopies

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In the last few years, there has been much interest in mechanical, thermodynamic and magnetic properties of Fe–Cr alloys [1–3] which are candidate materials for advanced fission reactors (Generation IV), accelerator-driven systems using spallation neutron sources or fusion reactors [4]. These types of steels are able to perform reliably for long time under high irradiation levels and at high temperatures. Moreover, high-chromium steels are known for their excellent corrosion resistant properties — in this case formation of a stable chromium oxide film on the surface, which prevents further oxidation of an alloy deeper into the bulk.

In this work the oxidised polycrystalline iron-based Fe–Cr alloys were investigated using X-ray photoelectron spectroscopy (XPS), transmission Mössbauer spectroscopy (TMS) and conversion electron Mössbauer spectroscopy (CEMS). This unique combination of experimental techniques allows us to take data simultaneously from the surface (XPS), from the 300 nm pre-surface region (CEMS) and from the bulk (TMS) of studied materials. This investigation gives the answer about the oxidation and segregation processes in Fe–Cr alloys. Before measurements, the samples were exposed to air at 600 °C for several hours. This type of treatment allows us to obtain valuable information about the formation of oxide layer on the surface and oxygen diffusion into the bulk. Moreover, exposure to air more closely resembles the conditions in which that type of construction material is utilised.

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INVITED LECTURES

ORAL PRESENTATIONS

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Oxidation and Surface Segregation of Silicon in Fe–Si Alloys Studied by Mössbauer and X-ray Photoelectron Spectroscopy

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The room temperature ^{57}Fe Mössbauer and XPS spectra were measured for polycrystalline pure iron and iron-based Fe–Si alloys. The spectra were collected using three techniques: the transmission Mössbauer spectroscopy (TMS), the conversion electron Mössbauer spectroscopy (CEMS) and the X-ray photoelectron spectroscopy (XPS). This unique combination of experimental techniques allows us to take data simultaneously from the surface of studied alloys by the X-ray photoelectron spectroscopy (XPS), from the 300 nm pre-surface region by the conversion electron Mössbauer spectroscopy (CEMS) and from the bulk by the transmission Mössbauer spectroscopy (TMS). The observed differences in Si concentration on the surface, in the pre-surface region and bulk should give the answer about segregation process in Fe–Si alloys.

The second part of our study concerns the oxidation process of the pure Fe as well as Fe–Si alloys. The experimental techniques used in this study are very sensitive to the presence of iron oxides (TMS, CEMS, XPS) and silicon oxides (XPS). Before measurements, the samples were annealed in the vacuum and then exposed to air in two different ways: (1) at room temperature for 30 days, and (2) at 600 °C for 2 h. This type of treatment allows us to obtain valuable information about the formation of oxide layer on the surface and oxygen diffusion into bulk. Worth noting is the fact that the majority of previous experimental studies on surface segregation and oxidation processes of Fe–Si alloys were performed on single crystals or under controlled oxygen exposure [1–4]. Taking into account that iron alloys are one of the most important engineering materials [5], it seems appropriate to investigate polycrystalline samples which were obtained in a process widely used by modern industry, such as melting. Moreover, exposure to air more closely resembles the conditions in which this type of construction material is utilized.

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Abstracts: Poster Presentations

Emergence of a Stress Induced Dislocation Network During Initial Growth of Ag-Films on Pt(111)

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We have investigated the emergence, growth and relaxation of a stress induced dislocation network during the initial growth of silver films on Pt(111) at 800 K using low energy electron microscopy (LEEM) in microscopy and diffraction mode, and spot profile analysis low energy electron diffraction (SPA-LEED). We confirmed the formation of a surface confined alloy in the first layer which near completion of the first layer results in a pseudomorphic layer. Further deposition results in re-entrant (partial) alloying. Unconventional growth of the second layer with a remarkable transient heterogeneity was observed. Initially, a mixed layer propagates from the ascending step into the terrace. Later a disordered low density bilayer film emerges, which is seen as the expansion of cauliflower shaped branches from the growth front moving out from the steps. The subsequent densification of this film is accompanied by the emergence of a dislocation network which accommodates surface misfit and unveils itself through the appearance of satellites spots near the integer order peaks in the SPA-LEED diffraction patterns.

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Abstracts: Poster Presentations

Supramolecular Organization of Thiophene Disubstituted Diketopyrrolopyrrole Donor–Acceptor–Donor Semiconducting Derivatives: Effects of the Size and Position of Electron Donating Units and Alkyl Substituents

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Diketopyrrolopyrroles symmetrically disubstituted with bi- or terthiophene units, abbreviated as DPPnTs, are novel semiconductors with: small optical band gap, tunable photoluminescence of high quantum yield and high charge carrier mobility of electrons and holes, which allows their use in organic electronics. Electrical properties of thin layers of DPPnTs strongly depend not only on molecular structure but also on morphology of the layer being an effect of self-organization.

Scanning Tunneling Microscopy (STM) has been used to examine 2D supramolecular organization of 6 DPPnTs derivatives deposited on HOPG. We consider effect of the length and position of alkyl substituents and the size of electron-donating segments containing 2 or 3 thiophene rings. The results show a strong tendency of studied compounds to form well-ordered monolayers of regular lattice-like structure. However, it was proved that details of their organization depend strongly on molecular topology. Evident differences in monolayer structures of investigated derivatives revealed two characteristic features of crucial importance: (i) clear effect of the alkyl substituent position and length (electron-accepting core vs electron-donating side blocks) on the alkyl chains interdigitation pattern, and (ii) influence of the position of the alkyl substituents in the terminal thiophene ring, α (C5) or β (C3), on molecular conformation on the surface affecting their 2D supramolecular organization. Additionally, self-assembly in monolayers have been compared with the 3D organization deduced from the powder X-ray diffractograms, indicating polymorphism for some derivatives.

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Investigation of Pb/Ru(0001) by Means of AES and LEED

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Auger electron spectroscopy (AES) and low energy electron diffraction (LEED) were used to study the growth mechanism, thermal stability and long range order of Pb on the Ru(0001) surface. The adsorption at 330 K leads to the formation of the wetting layer. The character of the Auger signal decay during the continuous Pb adsorption after the wetting layer formation suggests the growth of Pb islands and a significant decrease of the sticking coefficient for higher coverages. Increasing the sample temperature reduces the Pb sticking coefficient down to zero at around 600 K for Pb adsorbing on a completed wetting layer, which prevents nucleation of multilayer Pb islands at higher substrate temperatures. Formation of well-ordered first Pb adlayer is observed up to 890 K. The Auger signal, recorded during the heating of the adsorbed Pb layer, reveals a sudden agglomeration of 3D islands on the first wetting layer at about 600 K. Then the desorption of the adsorbate at elevated temperatures first from the 3D islands and then from the wetting layer is observed. A detailed analysis of LEED patterns recorded during the continuous Pb adsorption indicates the sequential formation of the $c(4 \times 2)$, $(2, 1; -0.25, 1.5)$, $(\sqrt{7} \times \sqrt{7})R19.1^\circ$ and $(2.4, 0.7; -1, 2.45)$ structures. The mutually rotated adsorbate domains were identified within each structure. The registered LEED patterns show the continuous transformations $c(4 \times 2) \rightarrow (2, 1; -0.25, 1.5)$ and $(\sqrt{7} \times \sqrt{7})R19.1^\circ \rightarrow (2.4, 0.7; -1, 2.45)$ at increased Pb coverages. The discontinuous transformation was found for the $(2, 1; -0.25, 1.5) \rightarrow (\sqrt{7} \times \sqrt{7})R19.1^\circ$ structural change [1,2].

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Tuning the Conductance of Benzene-Based Molecular Junctions

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Single molecule junctions provide an excellent opportunity to study transport properties of nanoscale devices, and therefore are essential for the development of molecular electronics. Transport characteristics of a metal/organic-molecule/metal junction are determined by several parameters, such as structural and electronic properties of both the molecule and the electrodes, conformation of the molecule, and its interaction with metallic leads.

Calculations based on non-equilibrium Green's functions approach [1] are performed within the density functional theory using the FIREBALL code [2]. Electron transport is studied in detail by means of the analysis of transmission spectrum, density of states distribution, current–voltage characteristic and eigenchannel decomposition [3].

According to recent studies [4], the linker atoms, connecting the molecule with electrodes, play a crucial role in optimizing the transport properties as well as thermodynamical stability of a single molecule junction. In order to understand this issue, we consider N, O, S and Se atoms as potential linkers anchoring the benzene molecule to the Au(100) electrodes. The results show that the choice of linkers indeed strongly affects the conductance of the junctions under study: at low bias regime, the current through N-linked molecules is remarkably higher as compared to the case of S and Se linkers, whereas the thermodynamical stability is similar. This offers an additional means of modifying the current–voltage characteristic of a given molecular junction by an appropriate selection of linkers.

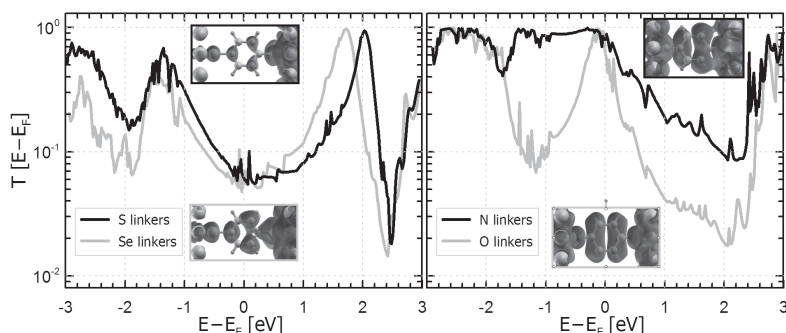


Figure: Electronic transmission spectra at zero-bias for benzene molecule connected to gold electrodes by (a) S and Se, and (b) N and O symmetric linkers. The eigenchannels of the biggest probability for all linkers at the Fermi energy are presented as insets in (a) and (b).

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Abstracts: Poster Presentations

XPS Analysis of Oxidized and Nitrided Titanium Thin Films Prepared in Flow Through High-Pressure Reactor

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The oxidized and nitrided titanium thin films prepared on different substrates in flow through high-pressure reactor were studied. The part of measurements was performed on titanium plate. Before any reactions the substrates were cleaned by ion sputtering. Another set of samples were prepared as set of thin titanium layers on crystalline silicon and SiO₂/silicon substrates. The thin layers of titanium were created by Electron Beam Evaporation (EBV) technique in ultra-high vacuum conditions. As the next step the samples were oxidized and nitrided by controlling the pressure of gas injection and temperature of samples.

The surface chemistry of material and chemical state of samples were analyzed by X-ray Photoelectron Spectroscopy (XPS). We also studied the chemical composition and state as a function of sputtering time by Ar ion depth profiling. The opto-electronic properties and thickness of layers were determined by Spectroscopic Ellipsometry (SE) measurements. We also analyzed the topography of samples by using Scanning Probe Microscopy (SPM).

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Si(110)–(16×2) as a Template for PTCDI-C8 Adsorption: Organic Films on Inorganic Semiconductors

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Understanding and control of physicochemical properties of organic–inorganic interfaces are key issues in the development of organic electronics. Main features of such interface depend on the structure of molecular layer grown on inorganic substrate. While the abilities to produce organic films of well-defined morphology on metal surfaces evolve, production of such films on semiconductor surfaces encounter obstructions. The basic problem in ordered organic layer preparation on semiconductor surfaces is the interaction of organic molecules with dangling bonds. The presence of dangling bonds favor adsorption at random position and prevent surface diffusion over significant distances. The formation of ordered layers can be supported by the use of substrates that exhibit template structure into which adsorbed molecules can be locked. For the molecules of appropriate dimensions the reconstructed Si(110)–(16×2) surface with its characteristic stripe-like structure seems to be promising as a template for ordered growth.

In order to check the template effect we have studied growth of PTCDI-C8 (N,N'-Dioctyl-3,4,9,10-perylenedicarboximide) films on Si(110)–(16×2) surface. The results of X-ray photoelectron spectroscopy (XPS), ultraviolet photoelectron spectroscopy (UPS) and scanning tunneling microscopy (STM) measurements combined with the density functional theory (DFT) calculations, allow us to characterize the morphological properties of PTCDI-C8 film at various stages of growth and the evolution of electronic properties of the interface caused by the film growth. High-resolution topographic STM images show that the template effect occurs only for low coverage (up to 0.4 molecular layer). Further increase of the amount of adsorbate destroys the adsorption layer ordering. Spectroscopic measurements show significant changes in electronic structure of the interface caused by adsorbate–surface and intermolecular interactions. The changes were observed for the core levels as well as for the valence band. XPS results indicate the importance of oxygen in the molecule–substrate bond formation—oxygen atoms of the molecule are bonded with silicon atoms of the surface.

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Electronic Transport in Graphene/h-BN Heterostructures

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Two-dimensional atomic sheets of graphene represent a new class of nanoscale materials with potential applications in electronics [1–3]. Recent advancements in fabricating graphene heterostructures by alternately layering graphene with crystalline hexagonal boron nitride (hBN) have led to an order of magnitude improvement in graphene device quality [1,4]. Since the lattice constant of hBN is about 1.8% longer than that of graphene, even perfect crystalline alignment of graphene on hBN exhibits a maximum moire wavelength of about 14 nm [5]. In this context we examine the changes in the electronic transport process due to electrostatic potential (Klein tunneling) [4,6,7].

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Abstracts: Poster Presentations

Electropolymerization of Pyrrole on Au(111) in Sulphuric Acid and Sodium Hexafluoroaluminate Solutions Revealed by Electrochemical Scanning Tunneling Microscopy

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The polymerization of pyrrole has been studied so far by one of us on polycrystalline gold with the use of cyclic voltammetry (CV), electrochemical impedance spectroscopy (EIS), scanning electron microscopy (SEM), and electrochemical quartz crystal microbalance (EQCM) [1]. Here, we present the results of investigations of polypyrrole on Au(111) with the use of CV and in-situ scanning tunneling microscopy (STM) in sulphuric acid and sodium hexafluoroaluminate supporting solutions. The cyclic voltammograms reveal the characteristic peak at positive potentials, which indicates the polymerization of pyrrole. Because of the irreversibility of this process no corresponding maximum is noted in the reverse potential scans. The multiple potential scans show a steady increase of the current at the same potential values and exhibit additional peaks associated with the redox reactions of formed polypyrrole.

Before polymerization, at negative potential $E = -490$ mV the STM images reveal the reconstructed Au(111) surface, as it is reported in the literature [2,3]. After several CV cycles in the potential range from -780 mV to 150 mV vs. platinum reference electrode, the STM images show the first stages of pyrrole polymerization. The polymer in the form of flat islands of about 1.5 Å height and 90 Å length is observed on terraces. The population of observed islands increases with CV cycles. The results are discussed in the context of two different supporting electrolytes used in electrodeposition of pyrrole.

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P3HT:PCBM Bulk–Heterojunction Thin Films Prepared by Novel Dual Feed Ultrasonic Spray Method for Application in Organic Solar Cells

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In polymer:fullerene bulk–heterojunction (BHJ) organic solar cells (OSC) the morphology of the active layer plays very vital role in the performance of solar cells. Formation of pure polymer and fullerene phases along with continuous interpenetrating networks of the phases are essential for optimum device performance. In conventional method, wherein both the polymer and the fullerene are dissolved in the same solvent, the required optimum morphology may not be achieved. We present here a new way of preparation of the polymer:fullerene BHJ which can lead to formation of pure phases. In this report, we present results of our initial experiments in this direction. The effect of process parameters on the thickness and surface roughness of the active layer has been discussed. The structural and optical properties have been studied using the optical microscope, UV-visible spectroscopy and photoluminescence (PL) spectroscopy. Significant PL quenching indicates efficient charge separation in the BHJ formed using this novel technique. Further, effect of other process parameters such as substrate temperature, nozzle to substrate distance, solution concentration and solution flow rate has also been studied. We have also compared the BHJ thin films prepared with this technique with the conventional single feed method indicating that smooth films can be formed with this new method as compared to the conventional method. The BHJ formed using this technique can be used as an active layer in OSC.

Abstracts: Poster Presentations

STM Study of the Si(1 1 1)/TI-(1 × 1) Surface as a Metal-like Passivated Si Substrate for Growth of Nanostructures

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Controlled growth of thin films on highly reactive silicon surfaces has been a challenge for decades. High density of surface dangling bonds, however, hinders the adsorbate diffusion and its self-organization. In our work, we use the TI-(1 × 1) layer as a passivating agent, which saturates all dangling bonds of the Si substrate [1]. We use room-temperature scanning tunneling microscopy to study structures formed on the Si(1 1 1)/TI-(1 × 1) surface after deposition of submonolayer amounts of three elemental adsorbates: Mn, In and Sn. Behavior of the adsorbates—however diverse—in all cases resembles interaction with metal substrates. Importantly, massive enhancement of adatom diffusivity is observed in all studied cases.

[1] P. Matvija et al., Appl. Surf. Sci. 331 (2014) 339.

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Large X-ray Circular Dichroism in Adsorbed Films of Homochiral Organic Molecules

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Enantio-pure ultrathin films of chiral 1,2-diphenyl-1,2-ethanediol deposited on Cu(100) at 100 K have been studied using circularly polarized X-ray absorption (XAS) at the carbon K edge. XAS excites element-specific core electrons to empty levels in the ground state thus probing the molecule's electronic configuration. The different features present in the absorption spectra have been identified and assigned to specific electronic transitions. The LUMO corresponds to the well-known π^* resonance of the C unsaturated bonds. Several other components also with π character follow in energy, which are assigned to the C–H bonds in the molecules, whereas broader features at higher energies correspond to σ -type C–C bonds.

Pairs of spectra with circularly polarized X-rays of opposite helicity were acquired and compared. Several clearly dichroic features have been observed and assigned to C–C and C–H π orbitals; the dichroic asymmetry shows opposite sign for the two enantiomers studied. Cross-check measurements using the non-chiral *meso*-DPED enantiomer confirm the direct relationship between the circular dichroism and the molecular handedness. Further photoemission microscopy (PEEM) experiments making use of the magnetic circular dichroism effect have also allowed us to image the magnetic state of the sample substrate—an epitaxial Fe film deposited on W(110)—and detect the enantiosensitive modifications induced by the adsorption of the chiral molecules. These findings lend additional support to the existence of some link between the molecular chirality and the electronic spin.

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Surface Relaxation of Pt(111) and Cu/Pt(111) Revealed by DEPES

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We present the results of atomic relaxation investigations of a clean Pt(111) surface as well as a pseudomorphic (1 × 1) Cu monolayer deposited on Pt(111). Formation of a pseudomorphic copper overlayer is attained during the course of continuous Cu adsorption at the substrate temperature equal to 450 K [1].

Our considerations include both the experimental and theoretical studies employing directional elastic peak electron spectroscopy (DEPES) [2], multiple scattering (MS) formalism [3], and density functional theory (DFT). A quantitative analysis of two-dimensional DEPES intensity distributions is presented and the contribution of subsequent Pt atomic layers to the measured signal is identified. The experimental DEPES distributions are compared with theoretical maps MS-simulated for a variable separation of the outermost atomic planes. For the clean Pt(111), the best fit is obtained assuming the outward relaxation of the surface layer by +0.7% with respect to the interplane distance in the bulk, confirming the slight expansion of the Pt(111) surface. A similar analysis performed for the Cu/Pt(111) adsorption system indicates the inward shift of the pseudomorphic Cu overlayer by -6.9% with respect to the substrate lattice continuation sites. Such determined surface relaxations of Pt(111) and Cu/Pt(111) agree well with the values predicted by the corresponding DFT computations.

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[2] S. Mróz, M. Nowicki, Surf. Sci. 297 (1993) 66.

[3] I. Morawski, M. Nowicki, Phys. Rev. B 75 (2007) 155412.

PROGRAM OVERVIEW

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Elastic Electron Scattering in Determination of Pb Adatom Positions on Ru(0001) Surface

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The forward focusing effect of incoming electrons is applied in study of Pb adatom positions in the sub-mono layer structure on the Ru(0001) surface. At low coverages up to 0.5 ML, the $c(4 \times 2)$ structure is created by Pb adatoms with their positions being significantly shifted from most symmetrical adsorption sites, i.e. hcp and fcc [1]. It provides additional maxima in elastically backscattered electron intensity when incoming electron beam strikes the investigated system along Pb–Ru directions. Due to high damping of the electron wave in the crystalline structure this effect is strongest for Ru atoms from first and second layer. Therefore DEPES (directional elastic peak electron spectroscopy) anisotropy maps [2] can provide direct and experimental information about Pb adatom positions within unit cell.

Investigations have been done for a middle electron energy range, i.e. from 700 eV up to 1600 eV in standard UHV electron spectroscopy equipment which is commonly used in low energy electron diffraction method.

[1] M. Jurczyszyn et al., Appl. Surf. Sci. 311 (2014) 426.

[2] I. Morawski, J. Brona, M. Nowicki, Appl. Surf. Sci. 258 (2012) 4848.

Abstracts: Poster Presentations

From Hydrogen Bonding to Metal Coordination and Back: Porphyrin Derivatives on Ag(111)

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Molecular self-assembly is one of the most promising routes to realize highly ordered molecular structures on surfaces. These structures are interesting from a fundamental point of view as well as for possible applications in organic electronic devices like organic field-effect transistors or organic solar cells. Usually weak non-covalent intermolecular interactions like hydrogen bonding, dipolar coupling, π - π stacking or metal coordination are employed for the fabrication of such structures.

In our studies we used a porphyrin derivative, which is functionalized at the trans meso positions with two pyridyl groups and two pentyl chains. We used scanning tunneling microscopy (STM) in order to investigate the structural arrangement of this molecule on Ag(111). For submonolayer to monolayer coverage, a close-packed rhombic network was observed, which is stabilized via hydrogen bonding between the pyridyl ligands and hydrogen atoms of neighboring pyrrole groups. Upon deposition of Co atoms, a porous hexagonal network formed by coordination of the pyridyl groups to the cobalt atoms. Upon thermal annealing at 450 K, the hexagonal network was transformed into a second close-packed rhombic structure. Additionally, we observed a change of the molecule-substrate interactions, which we assign to the metalation of the porphyrin core with cobalt atoms [1].

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Resolving of Subsurface Dangling Bond Triplets Created via Atomic Manipulation

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Atomic manipulation of the delta-doped B:Si(111)-($\sqrt{3} \times \sqrt{3}$)R30° surface was carried up using the Kolibri sensor based low temperature nc-AFM. To create a vacancy, a Si adatom was removed via a controlled vertical displacement of the probe. We succeeded to close the vacancy site by precisely placing a Si atom back, thus demonstrating that this process is completely reversible. During the manipulations, the rearrangement of the atoms at the tip apex occurs, leading to a sharpening of the tip. This enables us to look deeper inside the vacancy. It appeared that the removal of a Si adatom exposes subsurface Si dangling bond (DB) triplets, surrounding the B dopant in the first bilayer [1,2]. DFT calculations [3] reproduce nicely the experimental results and suggest that the tip is likely terminated by two Si atoms at the apex. Moreover, it is shown that the closing of the vacancy was possible only when atomic manipulation was performed with the tip placed off-center the vacancy site.

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[2] J. Berger et al., *Small* (2015), in press (DOI: 10.1002/small.201500092).

[3] J.P. Lewis et al., *Phys. Stat. Sol. B* 248 (2011) 1989.

Optical and Microstructural Characterization of Ti Layers Deposited Using PMS and GIMS Methods

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The magnetron sputtering is a technique where the vapour is obtained from a solid phase through the use of an arc discharge. Different materials can be synthesized by changing conditions in the vacuum chamber (e.g. a pressure of working/reactive gas, the temperature of substrate). Microstructural and optical properties of materials strongly depend on growing conditions. In this study the titanium layers were fabricated by using a standard magnetron process, PMS (Pulsed Magnetron Sputtering), and a method wherein the dynamically changing pressure of a working gas was applied, GIMS (Gas Injection Magnetron Sputtering) [1,2].

The influence of plasma generation method (PMS, GIMS), the time of deposition and the pressure of a working gas (Ar) on optical constants and microstructural properties of Ti films are considered. The prepared samples were investigated by means of spectroscopic ellipsometry (SE), atomic force microscopy (AFM), X-ray diffractometry (XRD) and confocal optical microscopy (COM). Additionally, a sheet resistance (4PP) of Ti layers was determined.

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[2] K. Zdunek et al., Surf. Coat. Tech. 228 (2013) 367.

Changes of Band Bending by UV-Induced Reaction on the S/InSb Surface

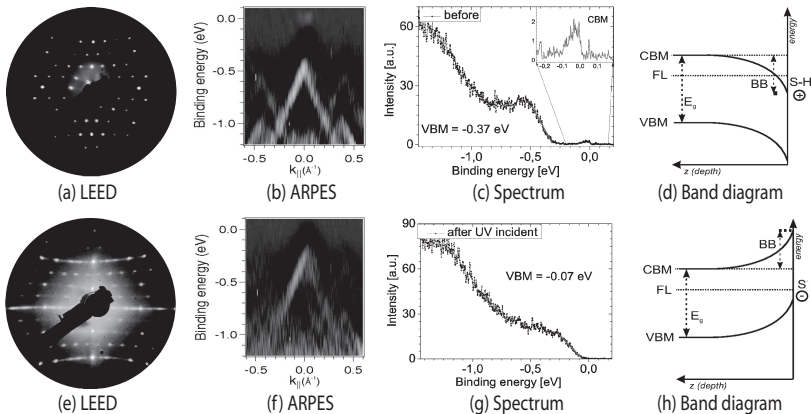
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Clean indium-terminated InSb(001)-c(8×2) surface exhibits upward band bending as a consequence of the InSb charge neutrality level lying at the valence band maximum [1]. However, it is expected that, similarly to other $A_{III}B_{IV}$ semiconductor surfaces [1,2], two-dimensional electron gas may be obtained by a sulphur passivation of the surface.

Using angle-resolved photoelectron spectroscopy (ARPES) we investigate electronic structure and band bending of the sulphur passivated indium antimonide (001) surface. It is found that the band bending is influenced by an exposure of the surface to the UV radiation. Also, as indicated by low energy electron diffraction (LEED), changes in surface reconstruction occur in parallel. We find that the changes are most likely caused by a photoreaction on the surface, i.e. by desorption of hydrogen, caused by UV radiation. The process is reversible: leaving the surface in UHV (where the predominant rest gas is the hydrogen) for a sufficiently long time restores the initial band bending and surface structure. It is also found that the electron accumulation layer is present on the hydrogenated S:InSb(001) surface.

In Figs. (a) and (e) there are presented LEED patterns of the sulphur passivated InSb(001) surface before and after exposition to the UV radiation (the dose $\sim 5 \times 10^{15}$ photons/cm²). As shown in Figs. (b–d) and (f–h) the dehydrogenation changes the sign of band bending. We think that S–H adsorbates act as electron donors and cause the downward band bending. In contrast the surface sulphur atoms act as electron acceptors and cause the upward band bending.



We acknowledge financial support by Polish NCN (2011/03/B/ST3/02070). The research was carried out with the equipment purchased thanks to European Regional Development Fund/Polish Innovation Economy Operational Program (POIG.02.01.00-12-023/08).

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[2] M. Betti et al., Phys. Rev. B 63 (2001) 155315.

Theoretical Study of CO Adsorption on Au₉ Clusters Supported on TiO₂(110)

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Small gold nanoparticles composed of few to several atoms dispersed on reducible metal oxide surfaces are very promising systems for CO oxidation reactions. The efficiency and durability of Au/metal-oxide catalysts depend strongly on the size and shape of Au nanoparticles. However, the functional shape and thus the properties of these nanoparticles are often significantly modified by coadsorbed molecules.

We present spin-polarized density functional theory (DFT) studies of CO adsorption on two types of the Au₉ clusters of different geometries, supported on the reduced TiO₂(110) surface. Clusters of both 3D and linear (row-like) structure [1] were investigated in order to compare their stability and properties in a presence of coadsorbed CO. On both Au₉ clusters several adsorption sites located on the cluster and its vicinity were examined. The binding of CO molecule depends on both adsorption site and the type of gold cluster. In general, the 3D cluster binds CO much stronger than linear one and for both clusters their shape is significantly changed. However, a row-like cluster is more flexible and better recovers its primary structure and functionality after CO is removed. Changes in the geometric and electronic structure of the Au₉ clusters and the oxide support induced by the adsorbed CO are discussed.

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Abstracts: Poster Presentations

Spin-Split Surface States at Tl/Si(111) and Pb/Si(111) and Chemical Probing with Cl and O Atoms

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The density functional theory ground state electronic structure of Tl/Si(111) shows large spin splitting of Tl induced surface states in the projected bulk band gap. By contrast, the ground state electronic structure of Pb/Si(111) does not show any spin-splitting of the Pb induced surface states. We show that in both systems the 2D electron gas (2DEG) that is formed within the adlayer is also decoupled from the substrate. As such the spin polarised 2DEG in Tl/Si(111) arises due to the broken in-plane inversion symmetry induced by the charge distribution within the adlayer. In Pb/Si(111) 2DEG is spin unpolarised as the corresponding in-plane symmetries within the adlayer are preserved. It is shown that for Tl/Si(111) the adsorption of O preserves the spin splitting and the Dirac point at K and M points of the surface Brillouin zone, respectively. The adsorption of Cl preserves the spin splitting at K and opens an energy gap at M .

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The Study of Self Assembled Monolayers Deposited on the Ti-6Al-4V Alloy

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Titanium and its alloys are one of the most commonly used materials in many industries. The extensive use of titanium is largely due to the high specific strength, and excellent corrosion resistance. In order to meet these expectations we present in this work a report about thin fluoroalkylsilanes and phosphonic acids films deposited on the Ti-6Al-4V alloy formed by the chemical adsorption on an active solid surface. These compounds as a self-assembled monolayer (SAM) consist of three building groups: a head group that reacts with a substrate, a backbone molecular chain group and a terminal group that interacts with the outer surface of the film [1,2].

SAM films were grown on Ti-6Al-4V surface by vapor phase deposition (VPD) and liquid method. In our work we measured SAM's with various structures. All films were characterized by means of a contact angle analyzer (surface free energy measurements, hydrophobicity) and X-ray photoelectron spectroscopy (XPS). The tribological behavior of SAM's films covalently adsorbed on alloy surfaces were characterized by atomic force microscopy (nanotribological properties) and the ball on disk tester (microtribological properties).

This work was supported by the National Science Centre, research grant No. 2014/13/B/ST8/03114.

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[2] M. Cichomski, Mater. Chem. Phys. 136 (2012) 498.

Abstracts: Poster Presentations

Adsorption of Pb and Formation of Chain-like Structures on Ge(001)

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Structural properties of the Ge(001) and Si(001) surfaces are very similar, however, the electronic properties of these systems are known to be considerably different. It was found, for example, that the electronic structure of Ge(001) depends on the number of atomic layers in asymmetric slabs used in calculations [1,2]. It was also demonstrated that the slab thickness affects the properties of the adsorbed Ge(001) substrate [3]. These results indicate the possibility of manipulating the physical, chemical and electronic properties of (001) oriented ultra-thin films of Ge by changing their thickness.

We have performed ab-initio, density functional theory, plane wave, pseudopotential calculations to examine the slab thickness effects on the adsorption of Pb on the Ge(001) substrate and the formation of the chain-like structures. It is shown that the slab thickness also affects the atomic and electronic structure of the group IV adsorbates on Ge(001). The obtained results are compared with the corresponding data for the Si(001) surface.

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Interaction of a Single Isopropyl Alcohol Molecule with the Si(001) Surface

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A computational, density functional theory study on the dissociative adsorption of a single isopropyl alcohol molecule on a Si(001) substrate has been performed. The total energy calculations have been carried out to determine the geometries and energetics of the adstructures grouped in ten distinct classes. In addition, the electronic local density of states projected on the adsorbed molecule for each of the considered configurations has been analysed. The obtained results are discussed in the context of the existing experimental (scanning tunneling microscopy) data.

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Work Function Changes of Cobalt Phthalocyanine on the Ag(100) Surface

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Investigations of complex systems like organic molecules on crystal surfaces require a very delicate, non-destructive probe. We study the changes in the work function induced by adsorption of cobalt phthalocyanine (CoPc) molecules on Ag(100) for coverages from submonolayer to multilayers. To this end, we modify the Anderson diode method and use very low intensity electron beam, which allows us to detect work function changes in the range of 0.01 eV without influencing CoPc molecules. Using LEED we characterize the molecular structure. Adsorption of a monolayer of CoPc lowers the work function. Additionally, the charge transfer occurs between the substrate and the molecular layer. The second CoPc layer partly eliminates the effect induced by the first layer. We obtain information about effective dipole moment, desorption temperatures and find out that multilayers desorb at noticeable lower temperature than the monolayer.

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A Computational Study of Coloured Interference Al₂O₃/Al and TiO₂/Ti/Al Systems

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Oxides on metal surfaces may serve different purposes. Firstly, they can protect the surface against corrosion. On the other hand, the dielectric layer can be used as a decorative coating. The typical example is a TiO₂/Ti system, which can be produced by a laser marking [1] and (also in industrial scale) by using electrolytic oxidation (anodizing) [2] as well as magnetron sputtering method [3]. Generally, titanium dioxide is a non-absorbing material in the visible spectral range and the colour is an effect of the interference of light in the thin dielectric layer.

Aluminium is a highly reflective metal. Aluminium oxide (Al₂O₃) formed on the Al plate does not produce (expressive) colours in contrast to the TiO₂/Ti system. Expressive colours of Al₂O₃-based coatings are prepared by adding an organic or inorganic (e.g. metal nanoparticles) dye to the highly porous aluminium oxide layer [4].

In this study we demonstrate an alternative method for the preparation of colour coatings on aluminium by the use the TiO₂/Ti double layer. The influence of dielectric layer (Al₂O₃, TiO₂) and metal film (Ti) thicknesses on reflective spectra of Al₂O₃/Al and TiO₂/Ti/Al systems as well as their L*a*b* parameters are examined. Performed computational study and obtained results clearly show the possibility of using the TiO₂/Ti double layer as the (expressive) colour coating (deposited) on aluminium.

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Influence of Electric Fields on Electronic and Magnetic Properties of a Copper–Dioxolene Complex Adsorbed on a Au(111) Surface

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The electronic and magnetic structure of a valence tautomeric complex [1] is considered. A copper–dioxolene molecule connected to Au(111) surface with an alkanethiol linker is investigated with the density functional theory. We systematically study the influence of electric field perpendicular to the surface on the properties of the adsorbed molecule.

The field steadily increases the charge and magnetic moment of the complex from $Q = +0.1|e|$ and $M = 1 \mu_B$ at $E = 0$ to $Q = +1.0|e|$ and $M = 2 \mu_B$ at $E = 0.5 \text{ V}/\text{\AA}$. Moreover, the molecule is reorientating along direction of the field due to its dipole moment. The ab-initio results were interpreted with a simple parametric model [2].

Our main conclusion is that the charge and spin state of the adsorbed complex could be well controlled by the electric field. This finding can be useful in development of memory storage or molecular switches [3].

This work has been supported by the National Science Center under the contracts DEC-2012/05/B/ST3/03208 and DEC-2012/07/B/ST3/03412. The computations were performed at the Poznań Supercomputing and Networking Center.

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INVITED LECTURES

ORAL PRESENTATIONS

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The Process of Dissociative Adsorption of Fluorine on Ge(001) Surface

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The process of dissociation of a fluorine molecule on the (001) surface of germanium has been analysed using density functional theory. Reaction paths during the dissociative adsorption are discussed. Dependence of the dissociation process on F_2 orientation with respect to the substrate, as well as the effect of the $p(1 \times 2)$ or $c(2 \times 4)$ surface reconstruction are shown.

The atomic and electronic structures, including spatial distributions of electron density of the adsorbate/substrate system, are discussed. Results for fluorine are compared with a similar process of dissociative adsorption of chlorine at the Ge(001)- $p(1 \times 2)$ surface [1].

[1] B. Stankiewicz, P. Mikołajczyk, Appl. Surf. Sci. 335 (2015) 198.

Abstracts: Poster Presentations

Electrical Resistance Asymmetry of Pb Atomic Chains on Si(553)Au

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Multiple Pb atomic chains on Si(553)Au are fabricated and studied with RHEED, four-point probe (4P) square geometry, STM and ARPES methods. For Pb on Si(553)Au a sequence of stable single, double and three atomic chain sets on each terrace was clearly resolved by all experimental methods used in the studies. The transition from insulating into metallic phase upon increasing number of Pb atomic chains on a single terrace was observed with ARPES.

In this report we demonstrate how the sequential growth of Pb atomic chains influences surface resistance of the Si(553)Au covered by sub-monatomic amounts of Pb, and how this phenomenon reveals in RHEED patterns. To measure resistance four tungsten current-potential tip probes were placed on Si(553) crystal slab and mounted in an UHV system equipped with LN₂ cryostat and RHEED diffractometer. Prior to Pb deposition, macroscopically ordered Si(553)Au surface was produced by deposition of 0.48 ML Au and annealing at 950 K. The resistance R was measured *in situ*, during Pb deposition by passing AC current of μ A range through two point contacts and measuring with lock-in voltage drop between another two point contacts.

The resistance measurements revealed different resistivities along different directions of the sample, clearly demonstrating its asymmetrical electrical properties, expected for surface covered with parallel aligned atomic chains. Moreover, the R vs Pb coverage curves showed a step-like shape, with steps centered around 0.12, 0.35 and 0.69 ML Pb (in units of one-half of a double Si(111) atomic layer), corresponding to completed, sequential growth of Pb atomic chains. The resistance data are completed by STM images of the Si(553)Au surface with single, double and triple Pb atomic chains.

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Complexity of Au(100): STM and DFT Study

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The massive reconstruction of Au(100) surface has been studied for decades (see for example [1–7]) and still the details of top-layer arrangements are not completely unraveled. Current understanding of the phenomenal arrangement is that the system lowers the surface energy by development of complicated, buckled quasi-hexagonal reconstructed, first layer on a square, weakly reconstructed, second layer. More puzzling is that in addition to the reconstruction, the top-layer can rotate up to $\pm 0.83^\circ$ with respect to the second layer. The rotation is responsible for various structural arrangements of the reconstruction. We have detected some very unexpected features of the surface and explored them by means of scanning tunneling microscope (STM) and density functional theory (DFT) calculations as implemented in the Vienna Ab-initio Simulation Package (VASP).

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Abstracts: Poster Presentations

PROGRAM OVERVIEW

Surface Segregation of Ge Wetting Layer in Thin Silver Films Deposited on SiO₂

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The influence of ultrathin germanium underlayer was studied on scattering and ohmic losses of surface plasmon–polariton (SPP) waves in Ag films deposited upon SiO₂ substrates at room temperature and 180 K. Samples morphology was examined by Atomic Force Microscopy (AFM), which confirmed the beneficial effect of wetting layer on the smoothness of the Ag surface and reduction of scattering losses. The gradual increase of the imaginary part of Ag permittivity in 500–800 nm spectral range was observed by spectroscopic ellipsometry (SE) measurements, thus suggesting Ge segregation towards the surface. The effect of Ge wetting layer on film resistivity was also measured by means of standard four-point probe method (M4PP). X-ray Photoelectron Spectroscopy (XPS) measurements combined with ion sputtering confirmed migration of germanium atoms toward the surface. The influence of additional thin Al₂O₃ and SiO₂ films as protecting layers on optical and compositional properties of Ag films was also studied.

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Imperfect Carbon Nanotube in a Field of a Point-Charge Probe: The Ab-initio Study

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Carbon nanotubes are one of the most promising materials for the future nanoelectronics. The presence and location of the structural defect in the carbon nanotube's wall modifies its electronic properties, therefore influences the functionality of a device [1].

We present numerical simulation of the transport properties of the defected carbon nanotube, where an external charge probe is applied. This probe acts as a local gate voltage. The considered simulation models the scanning probe microscopy measurement. The conduction maps obtained for the various structural defects are analyzed, the defect recognition scheme is proposed and its limitation is discussed. The numerical calculations are performed using SIESTA and GOLLUM package [2,3].

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PROGRAM OVERVIEW

INVITED LECTURES

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Geometrical Investigations on the Electronic Structure of Elemental Adsorption on Graphene

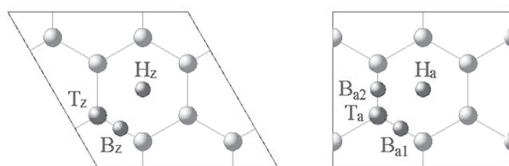
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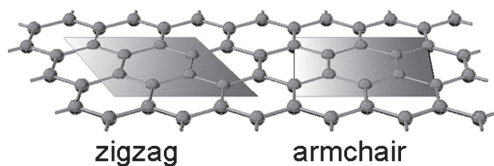
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Adding impurities or doping through adsorption is an effective way to modify the properties of graphene-based materials. The capability of making predictions pertinent to the trends of elemental adsorption on graphene is very instrumental towards a better understanding of the more complex adsorption cases. It also provides useful guidelines for fabricating 2-D graphene materials with novel properties. Properties of elemental adsorption on graphene have been calculated in terms of site (bridge, hollow, top), e.g. metal adatoms [1], H–Bi (except noble gases and lanthanides) adatoms [2]. However, it is found nonlinearity of the band gap on graphene with adsorbed O at atomic ratio of O/C of less than 30% [3]. This nonlinearity appears to be due to the positions of the adatoms relative to one another. This suggests that the electronic structure of elemental adsorption on graphene is affected not only by side of adsorption (single- or double-sided) and site of adsorption (bridge, hollow or top), but also by the relative orientation of the adsorbed sites (zigzag or armchair) (see figure below). In this contribution, we apply density functional theory (DFT) calculations to perform concerted investigation on the electronic structures of elemental adsorption on graphene in terms of absorption site and orientation, at various atomic ratios. This orientation effect adds an additional one degree of freedom in elemental adsorption on graphene. This calls for careful consideration of the orientation effect in element–graphene systems.



B=bridge, H=hollow, T=top



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Abstracts: Poster Presentations

Influence of the Surface Properties on Bactericidal Properties of Magnetron Sputtered Ti–Ag and Nb–Ag Thin Films

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The dynamic growth of interest in biomaterials representing various types of thin-film coatings has recently been focused on pure metals or their oxides due to their potential antimicrobial activity. In this study the comparative investigations on structural, surface and bactericidal properties of Ti–Ag and Nb–Ag thin films have been investigated. Ti–Ag and Nb–Ag coatings were deposited on silicon and fused silica substrates by magnetron co-sputtering method using innovative multi-target apparatus.

The physicochemical properties of prepared thin films were examined with the aid of X-ray diffraction, scanning electron microscopy, atomic force microscopy and X-ray photoelectron spectroscopy methods. Moreover, the wettability of the surface was determined. It was found that both, Ti–Ag and Nb–Ag thin films were amorphous. However, according to scanning electron microscopy and atomic force microscopy investigations the surface of Nb–Ag thin films was covered with visible grains, while Ti–Ag surface was homogenous.

The antimicrobial properties of the surface of thin films were also investigated. Studies of biological activity of deposited coatings in contact with *Escherichia coli*, *Staphylococcus aureus*, *Proteus species*, *Bacillus subtilis*, *Enterococcus hirae* and *Candida albicans* were performed. It was found that prepared coatings were bactericidal and fungicidal even in short-term contact. In the direct contact with organic medium Ti–Ag and Nb–Ag films were very stable as compared to pure silver film.

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Epitaxial Graphene on SiC Substrate: Raman Spectra, LEED and ARPES Studies

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Epitaxial graphene films are synthesized in ultrahigh vacuum on 4H-SiC(0001) surface, at the temperature around 1700 K, by desorption of silicon. Several techniques are applied for diagnostics of the obtained films. Raman spectroscopy is used in order to find the temperature of the graphitization onset. Low energy electron diffraction (LEED) and angle resolved photoemission spectroscopy (ARPES) are used to study the surface atomic and electronic structure.

It is found that the obtained graphene films have a well-defined orientation with respect to the substrate crystal structure. Both LEED and ARPES results are consistent with previous reports on UHV-grown graphene on SiC(0001).

The research has been carried out with the equipment purchased thanks to European Regional Development Fund (POIG.02.01.00-12-023/08).

INVITED LECTURES

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Electronic Density Redistribution in the Excited State of Quercetin–Metal Complexes

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Quercetin is one of the most common flavonoid compounds that are highly investigated because of their antioxidant, antibacterial and antimutagenic activity. The characteristic feature of flavonoids is related to their ability to make complexes with metal ions, so the research of complexation mechanism is of crucial significance [1,2]. The studies allow better understanding of reactions occurring in transport, reactivity as well as bioavailability and toxicity of metal ions. Numerous experimental and computational investigations of stoichiometry of the complexes and the modes of metal binding show different chelating power of quercetin with respect to Al, Zn, Fe, Pb, Cu ions.

The presented research is a continuation of our previous study on adsorption of morin [3] and quercetin (submitted) with TiO₂ nanoparticles. The main experimental method applied in previous investigations and in this work is the Stark spectroscopy (electroabsorption) allowing to determine the changes in permanent dipole moment and in polarizability, that characterize electronic density redistribution between the ground and excited state of the system. Our results show different modes of quercetin molecule binding to metal ions and provide quantitative measure of charge transfer contribution in electronic transitions.

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