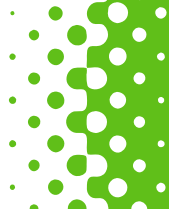


IWSP-2017



Uniwersytet
Wrocławski

8th International Workshop on Surface Physics
26–30 June 2017

Trzebnica, Poland

PROGRAM & ABSTRACTS

*Surface is Alive:
Atoms
Molecules
Functional Materials
etc.*

8th International Workshop on Surface Physics

Surface is Alive: Atoms, Molecules, Functional Materials etc.

26–30 June 2017
Trzebnica, Poland

organized by

The Institute of Experimental Physics
University of Wrocław



Uniwersytet
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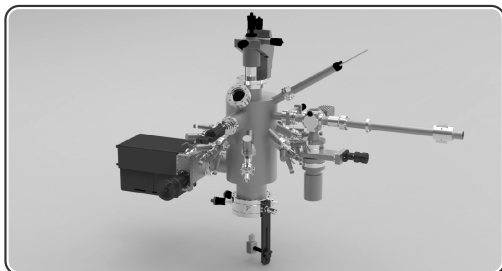
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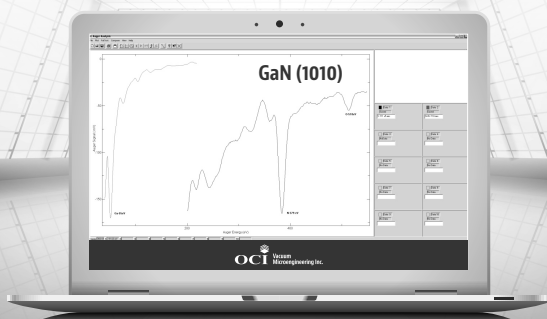
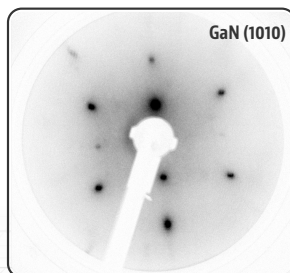
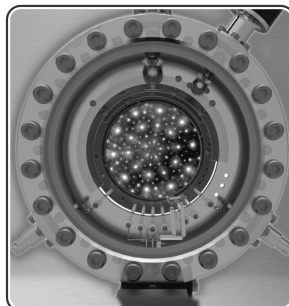
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Light-Matter Interaction at Surfaces and Interfaces Explored by *Ab Initio* Spectroscopy

Claudia Draxl

Institut für Physik and IRIS Adlershof, Humboldt-Universität zu Berlin, 12489 Berlin, Germany

Adsorbate systems and interfaces are most exciting since one can expect new properties that are absent in either of their building blocks. They open new perspectives towards the design and tailoring of materials with desired features and functions. Prerequisite for real progress is, however, the in-depth understanding of what happens on the atomic and electronic scale. In this respect, interfaces and, in particular, organic/inorganic hybrid materials pose a challenge for electronic-structure theory.

Based on selected examples I will discuss our recent progress in understanding level alignment and light-matter interaction of molecules adsorbed on surfaces and at interfaces between 2D materials.

Abstracts: Invited Lectures

Predictive Atomistic-Level Modeling of Diffusion-Mediated Self-Assembly and Catalytic Reaction Processes on Metal Surfaces

Jim Evans^{1,2}, Yong Han¹, Da-Jiang Liu²

¹Department of Physics & Astronomy, Iowa State University, Ames IA 50011, USA

²Ames Laboratory – USDOE, Iowa State University, Ames IA 50011, USA

We describe predictive stochastic atomistic-level modeling for non-equilibrium processes on crystalline metal surfaces. Of particular interest is the self-assembly during deposition of bimetallic nanoclusters, and also the analysis of catalytic surface reactions involving at least two reactant species. The multi-component nature of these systems produces significant challenges for the precise description of the underlying diffusion processes. Furthermore, predictive modeling requires ab-initio quality energetic input on both system thermodynamics and kinetics for the stochastic model, analysis of which on the appropriate time- and length scales is achieved by Kinetic Monte Carlo (KMC) simulation.

For self-assembly on metal nanoclusters during deposition, we highlight the need for a precise description on periphery diffusion and intermixing kinetics of aggregated atoms. We illustrate model predictions for core-shell and intermixed Ni-Al nanoclusters on NiAl(110) and Ag-Au nanoclusters on Ag(100) [1].

For catalytic reaction under flow conditions, modeling must describe the subtle ordering of mixed reactant adlayers, but also the kinetics of adsorption, desorption, diffusion, and reaction. These control steady-state reaction yield and bifurcation behavior, as well as spatiotemporal pattern formation [2]. Model predictions are shown for CO-oxidation.

[1] Y. Han et al., Nano Lett. 14 (2014) 4646; Y. Han et al., Phys. Rev. Lett. 108 (2012) 216201; J.W. Evans et al., Surf. Sci. Rep. 61 (2006) 1.

[2] D.-J. Liu et al., Chem. Rev. 115 (2015) 5979; D.J. Liu and J.W. Evans, Prog. Surf. Sci. 88 (2013) 393.

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Surface Science of Reactive Aromatic Molecules

J. Michael Gottfried*Department of Chemistry, University of Marburg, Germany*

Reactive aromatic molecules play an important role for surface functionalization, in model systems for contacts between metals and organic semiconductors, and for the generation of one- and two-dimensional covalent nanostructures. This contribution covers aspects of their surface and interface science, with particular focus on aryl halides and tetrapyrroles. Depending on the surface reactivity and temperature regime, these molecules undergo a wide range of different processes and form products ranging from periodic and fractal supramolecular assemblies to metal complexes and covalent nanostructures.

The first part focuses on tetrapyrrole macrocycles such as porphyrins, phthalocyanines, and corroles [1]. Phthalocyanine complexes form by on-surface tetramerization of dicarbonitrile precursors in the presence of metal atoms. Well-defined monolayers and multilayers of tetrapyrrole metal complexes are also synthesized by reaction of the metal-free tetrapyrroles with coadsorbed metal atoms (or metal atoms from the substrate), sometimes followed by the attachment of another ligand on the metal center. Tetrapyrroles with suitable peripheral functional groups form 2D metal-organic coordination networks. Mechanistic details and properties of the resulting complexes will be discussed [1].

The second part deals with structure formation and reaction of aryl bromides, which engage in Ullmann type reactions [2]. In the low-temperature regime, the intact molecules form complex supramolecular structures with periodic or fractal arrangement of the building blocks. At medium temperatures, dissociation of the carbon-halogen bonds results in the formation of cyclic and linear organometallic intermediates with carbon-metal-carbon bonds. Template effects of different surface structures and of the Cu(110)-(2×1)O piano-keyboard pattern are used to control the structure of the organometallic species. At high temperatures, elimination of the metal atom from the organometallic bond results in covalent nanostructures of different geometries. The hexagonal honeycombenes are prominent examples for a class of macrocyclic hydrocarbons that can only be obtained by on-surface synthesis. Strategies that control the competition between cyclic and open-chain products are discussed.

Support by the Collaborative Research Center (SFB) 1083 "Structure and Dynamics of Internal Interfaces" is gratefully acknowledged.

[1] J.M. Gottfried, Surf. Sci. Rep. 70 (2015) 259.

[2] Q. Fan, J.M. Gottfried, J.F. Zhu, Acc. Chem. Res. 48 (2015) 2484.

Abstracts: Invited Lectures

From Attoseconds to Picoseconds – Dynamics in Surfaces Studied by Photoemission

Matthias Hengsberger

Department of Physics, University of Zurich, Zurich, Switzerland

Dynamics in solid surfaces occur on atto-, femto- and picosecond timescales. ARPES spectra and angular intensity distributions contain a wealth of information about the electronic and atomic structure in surfaces. When used with pulsed light in a pump-probe setup the electronic and structural dynamics can be studied. The intrinsic timescales of the photoelectric effect and many-body effects like screening are faster than typical lifetimes of excited valence states in metals, which are of the order of femtoseconds. In order to obtain sub-femtosecond time resolution, the probe scheme must rely on the phase of the probing light field rather than on the intensity envelope. In a first part and after a general introduction into phase-sensitive measurement techniques, I will present attosecond measurements of electronic transitions in solid surfaces using the examples of noble metal surfaces [1,2].

In a second part, we extend ARPES to so-called photoelectron diffraction by recording the angular intensity distribution of photoelectrons emitted from well-defined states. Similar to holographic imaging, interference of the direct and scattered electron waves produces a complex pattern from which the atomic environment of the emitter can be deduced. Experiments on ultrafast electron dynamics and concomitant coherent structural dynamics will be presented from Bi(111) and Bi(111) [3,4].

[1] R. Locher et al., *Optica* 2 (2015) 405.

[2] M. Lucchini et al., *Phys. Rev. Lett.* 115 (2015) 137401.

[3] D. Leuenberger et al., *Phys. Rev. Lett.* 110 (2013) 136806.

[4] M. Greif et al., *Phys. Rev. B* 94 (2016) 054309.

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Self-Assembly and Surface Alloying of Group-14 Elements on Ruthenium

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As has been recently revealed, group-14 adatoms exhibit distinct growth characteristics on Ru(0001) at submonolayer coverages, despite a similar configuration of valence electrons. More specifically, Pb and Sn atoms tend to agglomerate and form dense islands of the $c(2\times 4)$ or $c(2\times 8)$ symmetry, respectively, with local coverage of 1/2 ML already for much lower deposition doses [1–3]. In contrast, Ge atoms self-assemble into the dilute $(\sqrt{21}\times\sqrt{21})$ structure with adatom density of 1/7 ML [4]. Si adatoms, in turn, at increasing deposition form a long-range-ordered herringbone structure with adatom density of 1/2 ML [5]. To trace the observed differences, we employed *ab-initio* DFT simulations and followed the early stages of growth of all group-14 elements on Ru(0001) in a systematic manner by examining the potential energy surfaces for successive adsorption of up to several atoms within a large surface unit cell. This way the effective lateral interactions between adatoms were recognized in the low-deposition regime and the most favorable dimer and trimer configurations of adatoms were identified. Interpreting them as initial building blocks of the resultant adsorbate structure helps understand the distinct overlayer properties of group-14 elements on Ru(0001) at low nominal coverages, in particular their tendency towards forming an ordered or not, dense or dilute adlayer. An attempt to follow the nucleation process of various group-14 elements on Ru(0001) by means of large-scale kMC simulations implementing the DFT-derived many-body interaction energy terms between adatoms will also be addressed.

In addition, we investigated the co-adsorption of immiscible Sn and Pb metals on Ru(0001), so as to establish conditions for the existence of their two-dimensional ordered alloys reported experimentally [1]. Several models of binary film formation, reflecting the experimental procedure of subsequent deposition of fixed doses of compositionally minor and major elements, were considered. We found the general preference for mixing of Sn and Pb atoms within the first wetting adlayer, and identified the favorable morphology of Sn–Pb surface alloys in terms of their stoichiometry, lateral symmetry, as well as the optimal adatom arrangement within the surface unit cell [5]. In particular, the hexagonal-like $(\sqrt{7}\times\sqrt{7})$ alloy structure with Sn:Pb = 3:1 composition ratio was predicted to occur at nominal Sn and Pb coverages of around 0.40 ML and 0.15 ML, respectively, in accordance with experiment [1].

[1] J. Yuhara et al., *Surf. Sci.* 616 (2013) 131.

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

[3] R. Topolnicki and R. Kucharczyk, *Appl. Surf. Sci.* 329 (2015) 376.

[4] Y.H. Lu et al., *Appl. Surf. Sci.* 254 (2007) 431.

[5] L. Huang et al., *Nano Lett.* 17 (2017) 1161.

[6] R. Topolnicki and R. Kucharczyk, *J. Alloys Compd.* 672 (2016) 317.

Abstracts: Invited Lectures

Probing Emergent Phenomena Through Large-Scale Atom Manipulation

Sander Otte

Delft University of Technology, Kavli Institute of Nanoscience, Department of Quantum Nanoscience, The Netherlands

The magnetic and electronic properties of materials often find their origin in basic atomic-scale interactions. Yet, due to the large number of atoms involved, many phenomena can be very difficult to predict: we call these 'emergent'. The ability to build structures atom-by-atom by means of scanning tunneling microscopy (STM) may provide an excellent platform to explore emergence as a function of system size. For example, by properly tuning the anisotropy of magnetic atoms a thin insulator, we have been able to engineer finite spin chains hosting spin waves [1] as well as the beginnings of a quantum phase transition at a critical magnetic field [2]. Unfortunately, the maximum size of such assembled structures is often limited due to e.g. crystal impurity, crystal strain, and general uncontrollability of the STM tip shape, hampering the reliability with which atoms can be manipulated. In this talk, I will demonstrate how atomic assembly can be enhanced dramatically by switching to manipulation of atomic vacancies, rather than adatoms, on a chlorine-terminated copper surface [3]. The resulting structures, comprising thousands of vacancies positioned on an exactly defined grid, are found to be stable at temperatures up to 77 K. We use this new technique to construct two-dimensional artificial crystals of various size and atomic spacing, and investigate their collective electronic properties through local tunneling spectroscopy.

[1] A. Spinelli et al., *Nature Mater.* 13 (2014) 782.

[2] R. Toskovic et al., *Nature Phys.* 12 (2016) 656.

[3] F. Kalff et al., *Nature Nano.* 11 (2016) 926.

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	8 th INTERNATIONAL WORKSHOP ON SURFACE PHYSICS (IWSP-2017)	
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PROGRAM OVERVIEW	Molecular Binding and Adsorption: Van der Waals Density Functional Study <u>Elsebeth Schröder</u> <i>Department of Microtechnology and Nanoscience (MC2), Chalmers University of Technology, Gothenburg, Sweden</i> The van der Waals (vdW) density functional (vdW-DF) method is a systematic extension of traditional semilocal density functional theory (DFT). It captures vdW forces such that they act on the same level as other binding forces. In my talk I introduce and summarize the method as well as our recent extensions to include spin effects and our construction of vdW-DF hybrids. I will also show a number of results for molecular binding and adsorption on graphene, and will contrast physisorption of for example n-alkanes and polycyclic aromatic hydrocarbon (PAH) molecules.	
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Abstracts: Invited Lectures

Long-Range Boundary Effects in Oxide-Supported Model Catalysts

Yuri Suchorski

Institut für Materialchemie, Technische Universität Wien, Vienna, Austria

The metal-oxide boundary and its role in the efficiency of supported catalysts have been discussed intensely in last decades [1]. However, up to now the discussion was mainly focused on the effects confined by the nm-sized surface region along the metal-oxide interface [2]. The present contribution demonstrates that the metal-oxide boundary interaction may also result in a long ranging effect, reaching on the metal side many μm far away from the metal-oxide boundary. Using photoemission electron microscopy (PEEM) it can be directly observed how the presence of the metal-oxide boundary modifies the catalytic behaviour of μm -sized Pd particles supported by non-reducible oxides such as Al_2O_3 and ZrO_2 , as compared to similar, but unsupported Pd particles.

Particularly, the kinetic transitions from the active to inactive state and vice versa, relevant for the catalytic ignition (cold-start problem, [3]) are influenced by such long ranging boundary effect: the oxide-supported Pd reveals a much higher tolerance to CO (lower ignition temperature) than the unsupported Pd. The detailed analysis of the nucleation and propagation of the reaction fronts allows to assign the observed effect to the pacemaker role of the metal-oxide boundary sites which they play in the activation/deactivation of the catalyst. Using the *kinetics by imaging* approach [4], the local kinetics for individual (supported and unsupported) Pd particles has been studied: the resulting local kinetic phase diagrams illustrate the details of the PEEM observations. The observed long-ranging effects are attributed to the locally modified adsorption kinetics along the metal-oxide boundary, which influences, rather unexpectedly, surface sites which are hundreds and thousands nanometers away.

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

[1] C.T. Campbell, Nature Chem. 4 (2012) 597, and references therein.

[2] Q. Pan, et al., Chem. Cat. Chem. 7 (2015) 2620, and references therein.

[3] M.V. Twigg, Cat. Today 163 (2011) 33.

[4] Y. Suchorski, G. Rupprechter, Surf. Sci. 643 (2016) 52.

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Metal Growth on and Under Graphene: Morphology, Growth Mode and Intercalation

M.C. Tringides¹, P.A. Thiel, M. Hupalo, M.T. Hershberger, D. McDougall

Department of Physics and Chemistry Iowa State University Ames Laboratory – USDOE, USA

Graphene based electronic and spintronic devices require understanding of the growth of metals on graphene. Several metals (Gd, Dy, Eu, Fe, Pb) deposited on epitaxial graphene were studied with STM, SPA-LEED and DFT. The grown morphology (island density and domain size distributions) was used to extract the metal diffusion and adsorption barriers [1,2]. For practically all metals the grown mode is 3-d as a result of (i) the low ratio of the metal adsorption to metal cohesive energy and (ii) the repulsive interaction of unscreened charges at the metal-graphene interface that favors islands of small “footprint”. These experimental results are fully supported with DFT calculations. It is essential to find ways to modify the growth to layer-by-layer for high quality metal contacts and for using graphene as a spin filter. By growing Dy at low temperatures or high flux rates it is found that upward adatom transfer is kinetically suppressed and layer-by-layer is possible [3].

Graphene intercalation provides a novel way to tune its properties. Experiments on graphene partially intercalated with Dy show that nucleation is preferred on the intercalated than on the pristine areas. Difference in doping between the two areas generates an electric field that transforms random to directional diffusion and accounts for the guided nucleation [4]. This can be a general method to control patterning of metallic films on graphene.

Many issues related to the intercalation process itself are poorly understood, i.e., the temperature where atoms move below graphene, different intercalation phases, their coverage, the entry points for atoms to move below, the intercalation time etc. SPA-LEED has been used to study these questions for Dy intercalation in graphene. Spot profiles of several spots (specular, $\sqrt{3}$, graphene) are studied as function of temperature and electron energy to deduce the kinetics of intercalation and the layer where atoms reside. This information is essential to tune the emerging properties of intercalated graphene.

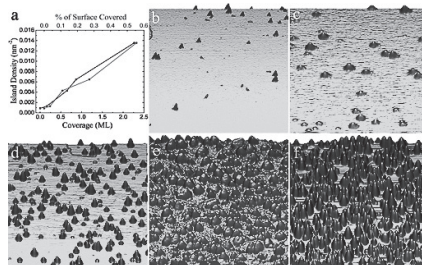


Figure: Fe nucleation on graphene shows increasing island density with Fe deposited amount; $200 \times 200 \text{ nm}^2$.

- [1] M. Hupalo et al., *Advanc. Mater.* 23 (2011) 2082.
- [2] X. Liu et al., *Progr. Surf. Sci.* 90 (2015) 397.
- [3] D. McDougall et al., *Carbon* 108 (2016) 283.
- [4] X. Liu et al., *Nano Res.* 9(5) (2016) 1434.

Abstracts: Invited Lectures

In-Situ Studies of Organic Thin Films

Th. Wagner, E. Ghanbari, A. Navarro Quezada, P. Zeppenfeld*Institute of Experimental Physics, Johannes Kepler University, Linz, Austria*

The Stranski-Krastanov growth mode is often observed during deposition of organic molecules. To study this evolution from 2D to 3D growth we apply Photoelectron Emission Microscopy (PEEM) and Differential Reflectance Spectroscopy (DRS) in situ and in real-time during the deposition of organic thin films. PEEM provides local information on the wetting layer and on μm sized crystallites. In spectroscopic mode, the electronic density of states is accessible like in traditional UPS but with a much better lateral resolution [1]. By using linear polarized light for the excitation of the photoelectrons, an additional image contrast can be achieved making the PEEM not only sensible to the morphology of the sample but also to the different orientations of the molecules with respect to the surface [2,3]. DRS compares the reflectance of the bare surface with the one of the surface after deposition of molecules. The different environment of the molecules in the first, the second and higher layers leads to unique spectral fingerprints of these layers [4]. The synchronized application of both techniques in a single experiment, turns out to be a very powerful tool to make a direct correlation between the morphology and the optical properties of the sample. As an example, we will discuss the deposition of α -sexithiophene on different silver surfaces.

[1] Th. Wagner et al., Org. Electron. 12 (2011) 442.

[2] Th. Wagner et al., Appl. Surf. Sci. 267 (2013) 26.

[3] Th. Wagner et al., Ultramicroscopy 159 (2015) 464.

[4] E. Ghanbari et al., J. Phys. Chem. C 119 (2015) 24174.

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	8 th INTERNATIONAL WORKSHOP ON SURFACE PHYSICS (IWSP-2017)	
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PROGRAM OVERVIEW	Rashba Effect in One-Dimensional Structures on Silicon Surface <u>Ryszard Zdyb</u> <i>Institute of Physics, Maria Curie-Skłodowska University, Lublin, Poland</i> Since its theoretical prediction in the 80's and experimental verification in the 90's of the last century the Rashba effect became important topic in the field of spintronics. The effect is due to a broken inversion symmetry at surfaces or interfaces of crystals. If in addition crystal experiences enough strong spin-orbit coupling then the Rashba effect can be observed in experiments as spin-split surface states [1].	
INVITED LECTURES	The spin-split electronic structure has also been found in various 1D systems e.g. Si(557)-Au, Si(553)-Au, Si(557)-Pb and Si(553)-Pb. It has been shown that each of these systems reveal interesting features associated with the spin-split surface states: Fermi surface nesting, exotic spin-orbit density waves, giant spin-splitting, unusual spin texture and others [2–5]. The observed diversity of new phenomena associated with the Rashba effect encouraged us to study one-dimensional structures prepared on other highly anisotropic surfaces. In this contribution we present results of studies of (quasi) 1D Pb and Bi structures formed on the Si(553), Si(331) and Si(110) surfaces. In particular, the crystallographic and electronic structures studied with reflection high energy electron diffraction, scanning tunneling microscopy, spin and angle-resolved photoemission spectroscopy and density functional theory calculations are reported.	
ORAL PRESENTATIONS	This work has been supported by the National Science Center under Grant No. 2013/11/B/ST3/04003. [1] S. LaShell et al., Phys. Rev. Lett. 77 (1996) 3419. [2] T. Okuda et al., Phys. Rev. B 82 (2010) 161410. [3] H.W. Yeom et al., New J. Phys. 16 (2014) 093030. [4] C. Tegenkamp et al., Phys. Rev. Lett. 109 (2012) 266401. [5] M. Kopciuszynski et al., Sci. Rep. 7 (2017) 46215.	
POSTER PRESENTATIONS		



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

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	8 th INTERNATIONAL WORKSHOP ON SURFACE PHYSICS (IWSP-2017)	
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PROGRAM OVERVIEW	Structure and Energetics of Cu Adlayers on Ru(10$\bar{1}$0) J. Brona, R. Kucharczyk, I. Morawski, R. Wasielewski, M. Nowicki, A. Ciszewski <i>Institute of Experimental Physics, University of Wrocław, Wrocław, Poland</i> Growth mode of ultrathin Cu epitaxial layer on Ru(10$\bar{1}$0) substrate was investigated. In the beginning, Cu grows layer by layer, like in the Frank–van der Merwe mode. However, these are not monolayers (MLs), but bilayers (BLs). Low energy electron diffraction revealed that structure of the adlayer is (1×1), and scanning tunneling microscopy showed that the layers are flat. Ab-initio density functional theory (DFT) simulations combined with directional elastic peak electron spectroscopy experiments determined the configuration of Cu adatoms with respect to the underlying substrate. Auger electron spectroscopy complemented the research. DFT revealed the energetic preference of deposited Cu atoms to form instantly the first BL than to wet the substrate with a single ML, and the analogous tendency was found for the second BL, confirming experimental findings. For the nominal coverage higher than 2 BL, Cu deposited at elevated temperatures forms three-dimensional islands in a mesa shape. Flat tops of mesas have Cu(111) structure.	
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Plasmonic Nanolayers Wetted with Semiconductor Films – Crystallinity and Dispersion Engineering

A. Ciesielski¹, Ł. Skowronski², M. Trzcinski², E. Górecka³, W. Pacuski¹, T. Szoplik¹

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Plasmonic metal nanolayers are used in biosensing and metamaterial wavefront shaping devices. For optimal performance, the surface of those nanolayers is required to be as smooth as possible. However, the implementation of semiconductor wetting layers, among which germanium has been most excessively tested, results not only in smoothening of the surface but also in changes in the crystallinity of the metal layer. This non-uniform crystallinity leads to segregation of the atoms of the wetting film into the metal structure [1]. Segregation results in significant modification of permittivity of noble metal films, where additional resonances originating from volumetric plasmons can be observed [2]. Apart from Ge, also Se and Te exhibit segregation in bulk plasmonic metals [3], however, to the best of our knowledge no research on segregation of those elements in plasmonic thin films has yet been performed.

Here we report on ellipsometric, XPS, XRD and XRR measurement results of Ag and Au nanolayers deposited on SiO₂ with Ge, Si, Se and Te wetting films. Our research shows, that each of the investigated wetting materials influences the crystallinity of the metal film in a unique way, then segregates at a different rate. This modifies dispersion characteristics and leads to additional plasmonic contributions to the metal permittivity at different wavelengths for each wetting material. Combining multiple wetting materials, temperature of substrates and annealing allows for engineering of crystallinity and thus for manipulating the additional contributions in the permittivity. This may lead to acquiring near-zero-index material.

[1] P. Wróbel et al., ACS Appl. Mater. Interf. 7 (2015) 8999.

[2] A. Ciesielski et al., Appl. Surf. Sci. (2017) in press.

[3] P. Lejcek, *Grain Boundary Segregation in Metals*, Springer, 2010, p. 196.

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	8 th INTERNATIONAL WORKSHOP ON SURFACE PHYSICS (IWSP-2017)	
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PROGRAM OVERVIEW	Field Emission Techniques to Study the Local Activity of Au-Ag Alloys During N₂O+H₂ Reaction <u>L. Jacobs</u>, N. Gilis, C. Barroo, S.V. Lambeets, E. Genty, T. Visart de Bocarmé <i>Chemical Physics of Materials and Catalysis, Université Libre de Bruxelles, Faculty of Sciences, CP 243, 1050, Brussels, Belgium</i>	
INVITED LECTURES	AuAg catalysts exhibit remarkable properties for low temperature selective oxidation of small organic molecules. The ability to supply oxygen species, the key step for the activity and selectivity on gold surfaces, is studied via N₂O+H₂ reaction. In our case, Ag allows the formation of O(ads) species on the nanoparticle, and the selectivity is driven by Au. Field Emission Microscopy (FEM) allows studying reaction dynamics, during the ongoing processes, with nanoscale resolution. When all the control parameters are fixed, local changes in the FE pattern reflect changes of the surface composition. Here, FEM is used to study the interaction of N₂O with AuAg samples, as well as the N₂O+H₂ reaction. In reactive conditions, we observed a FE pattern with the same symmetry as the underlying surface indicating a structure-sensitivity of the reaction. Using selected N₂O/H₂ mixtures, we observed that the pressure ratio does not affect the emission pattern, suggesting a localized dissociative adsorption phenomenon for N₂O and H₂. The formation of a reactive interface between O(ads) and H(ads) around the {210} facets is indeed observed. Considering the poor activity of bare Au, it is supposed that surface segregation induced by O-species leads to a localized silver enrichment of the {210} facets.	
ORAL PRESENTATIONS	This work contributes to a better determination of the alloy surface composition during its catalytic activity. This general idea fits within a further challenge to optimize the surface composition by well-chosen reaction conditions so as to keep catalysts most active and/or selective.	
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Abstracts: Oral Presentations

Antimonene on Metallic Quantum Well

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Bulk antimony surface bands are connected to the conduction band and the valence band separately. It has a small negative band gap that avoids the Topological Insulator (TI) phase to occur. However, theoretical studies have shown that the Quantum Spin Hall (QSE) phase could be realized by reducing the dimensionality of 3DTI in 2D. Although theoretical studies show that free standing single bilayer (BL) is stable [1], an experimental verification must consider an unavoidable interaction with a substrate.

Here we first present experimental and theoretical study of antimonene (single BL of antimony) and double BL of antimony on metallic quantum well. Antimonene was prepared on Pb ultrathin films deposited on Si(111)-(6×6)Au substrates. Crystal structure of growing films was examined with Reflection High Energy Electron Diffraction (RHEED) whereas Local Density of States (LDOS) was determined using STS methods. The experimental results were complemented with DFT calculations of atomic structure, STM topography and LDOS.

Experiments show that 1 BL and 2 BL of antimony on 4 monoatomic layer (ML) Pb quantum well form epitaxial layer with well-ordered flat hexagonal structure, with the same orientation as the under-laying Pb(111) ultrathin film. The present work would uniquely make it possible to investigate an engineering of antimonene band structure via tuning the Pb quantum well states.

This work was supported by National Science Centre, Poland, under grant OPUS No. 2014/13/B/ST5/04442.

[1] O. Üzengi Aktürk, V. Ongun Özçelik, S. Ciraci, Phys. Rev. B 91 (2015) 235446.

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	8 th INTERNATIONAL WORKSHOP ON SURFACE PHYSICS (IWSP-2017)	
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PROGRAM OVERVIEW	Mechanism of Molecular Photo-Switch Adsorbed on Si(100) <u>Leszek Jurczyszyn</u> <i>Institute of Experimental Physics, University of Wrocław, Wrocław, Poland</i> We present experimental and theoretical study of the adsorption of 4-anilio-4'-nitroazobenzene molecule on Si(100). It was shown that this molecule can be bonded with silicon substrate in vertical configuration via the phenyl ring. The experimental and theoretical data demonstrate that the adsorbed molecule has two stable isomers: <i>trans</i>-upright and <i>cis</i> -upright configuration. The obtained results indicate that the photoisomerization between <i>trans</i>- and <i>cis</i>-conformation can take place. We have shown in this way that the considered system can work as a molecular photoswitch which is feasible for incorporation with other nanostructures such as wires. In our opinion this opens a novel approach aiming at combining molecular electronics with the state-of-the-art silicon-based technology.	
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Controlling Spin Interactions in Metallo-Molecule/Au(111) Studied Using Scanning Tunneling Microscopy and Spectroscopy

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²Graduate School of Nanoscience and Technology, KAIST, 34141, Daejeon, Republic of Korea

Metal-centered organometallic complexes form 6 coordinated structures having two out-of-plane bonds that competes each other; one of the two out-of-plane bonds that formed earlier than the other is weakened with an increased bond length by the formation of the other. This well-known trans-effect in chemistry, appeared recently on metal surfaces in spin versions in regard to the coordination reactions between small molecules and metallo-porphyrin. Here, we present that spin interactions in Co-porphyrin/Au(111) can be controlled by coordination and de-coordination of small molecules using scanning tunneling microscopy and spectroscopy (STM and STS) [1–4]. With small molecule coordination, we observed that a zero-bias peak at Co-porphyrin, a signature of Kondo resonance in STS, switched off or remained but with a reduced width, i.e., Kondo temperature, and that it could be reversibly retrieved by single molecular STM manipulations. Based on our density functional theory calculation results, the reduced Kondo temperature is explained with the change in the unpaired spins in d_z orbitals of Co-porphyrin by small molecule coordination. Our study shows that a spin version of trans-effect can be directly probed through Kondo resonance with STS at the single molecule level.

[1] H. Kim et al., ACS Nano 7 (2013) 9312.

[2] H. Kim, et al., Chem. Sci. 5 (2014) 2224.

[3] H. Kim, et al., ACS Nano 9 (2015) 7722.

[4] Y. H. Chang et al., Dalton Trans. 45 (2016) 16673.

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	8th INTERNATIONAL WORKSHOP ON SURFACE PHYSICS (IWSP-2017)	
PROGRAM OVERVIEW	Abstracts: Oral Presentations	
INVITED LECTURES	Self-Assembly of Phthalocyanine Molecules on Metal-Passivated Si Surface: Influence of the Electric Field of an STM Tip P. Matvija¹, P. Sobotík¹, B. Pieczyrak², L. Jurczyszyn², F. Rozbořil¹, I. Ošťádal¹, P. Kocán¹ ¹Charles University, Prague, Czech Republic ²Institute of Experimental Physics, University of Wrocław, Wrocław, Poland Ordered layers of organic molecules are usually grown on weakly interacting surfaces, typically those of metal mono-crystals. An interesting alternative, consistent with silicon technologies, is represented by silicon surfaces passivated by metal mono-layers. Such surfaces carry exotic electronic properties, e.g. the Rashba-type spin-split bands in the case of $\text{Ti/Si}(111)-(1 \times 1)$ [1]. We use the scanning tunneling microscopy (STM) to study field-dependent assembly of copper phthalocyanine (CuPc) molecules on the $\text{Ti/Si}(111)-(1 \times 1)$ surface. Previously we reported that the surface is inert to adsorbates [2]. We demonstrate that the electric force can be used to control the assembly of molecules and switch between phases on areas of hundreds of nm^2 with a switching time of less than 1 ms. With help of ab-initio calculations and kinetic Monte Carlo simulations we explain the mechanism of the STM tip influence on assembly of the molecules by means of electrostatic interactions. Two aspects are important for explanation of observed morphologies and dynamic behavior: (1) molecular assembly as a result of high density and steric repulsion, and (2) the charge rearrangement induced by adsorption of the molecules on the substrate. [1] K. Sakamoto et al., J. Electron. Spectrosc. Relat. Phenom. 201 (2015) 88. [2] P. Matvija et al., Appl. Surf. Sci. 331 (2015) 339.	
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Abstracts: Oral Presentations

Electronic Structure of the Si(110) Surface with (3×2)Bi Reconstruction

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Spin polarized electron bands in nonmagnetic, silicon based systems are of particular interest in spintronics as a possible source of spin current. Lifting of the spin degeneracy may be induced by the spin-orbit coupling in low dimensional structures with a broken inversion symmetry (Rashba effect). The magnitude of band splitting is proportional to the potential gradient and implicitly to the Z number of atoms. Pb and Bi are among elements with the highest Z number and therefore surfaces modified by these atoms are expected to give a large spin splitting of surface state bands.

In this report we show a crystallographic and electronic structure of the Si(110)-(3×2)Bi surface measured by means of reflection high energy electron diffraction (RHEED), scanning tunneling microscopy (STM) and angle-resolved photoelectron spectroscopy (ARPES). The (3×2) Bi-induced reconstruction is formed by deposition of about 0.25 ML Bi and annealing at about 500 °C [1]. The STM images show a zig-zag shaped structures running along the [-110] direction and elongated in two equivalent <11-2> directions. Photoemission maps reveal two sets of electron bands. One group has nondispersive character and may be considered as localized states. The second group is placed around the X point of the surface Brillouin zone and show parabolic-like dispersion. Nonetheless, those bands do not cross the Fermi level what makes the surface semiconducting.

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

[1] A.K.R. Ang, S.N. Takeda, H. Daimon, J. Vac. Sci. Technol. A, 34 (2016) 51401.

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	8 th INTERNATIONAL WORKSHOP ON SURFACE PHYSICS (IWSP-2017)	
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PROGRAM OVERVIEW	Ab Initio Theory of Scattering Resonances in Electron Diffraction from Surfaces and Ultrathin Films Eugene Krasovskii^{1,2,3} ¹Departamento de Física de Materiales, Universidad del País Vasco (UPV-EHU) ²Donostia International Physics Center (DIPC), San Sebastián/Donostia, Spain ³IKERBASQUE, Basque Foundation for Science, Bilbao, Spain Unoccupied electronic structure of surfaces and 2D films is important in electron diffraction and photoemission: unambiguous interpretation of spectroscopic experiments depends on a knowledge of the behavior of the outgoing or reflected electron. Here, the scattering of electrons by surfaces and thin films at low energies is considered within a Bloch-waves based ab initio theory [1]. Scattering states in semi-infinite crystals are analyzed for clean surfaces of Al(111) and Ru(0001) and for oxidized Ru(0001), and the sharp features in the reflection spectra are traced to critical points in the complex band structure of the substrate and to scattering properties of the overlayer [2]. Scattering from ultrathin films is represented by stand-alone graphene [3] and hexagonal boron nitride [4]. The unbound electronic structure of a graphene is discussed in the context of discrete states immersed in a 3D continuum. Here, scattering resonances originate from the coupling of the in-plane and perpendicular electron motions, as elucidated by an exactly solvable model [3]. Ab initio scattering theory [1] confirms the existence of the resonances in realistic graphene and shows that they lead to a total reflection below and total transmission above the resonance energy. Scattering by few-layer films is discussed for hexagonal boron nitride [4]. [1] E.E. Krasovskii, Phys. Rev. B 70 (2004) 245322. [2] E.E. Krasovskii et al., J. Phys.: Cond. Matter 27 (2015) 035501. [3] V.U. Nazarov, E.E. Krasovskii, V.M. Silkin, Phys. Rev. B 87 (2013) 041405. [4] J. Jobst et al., Nat. Commun. 7 (2016) 13621.	
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Multilayer Silicene on Si(111)- $\sqrt{3}\times\sqrt{3}$ Ag Surface

Mariusz Krawiec¹, Haifeng Feng², Jincheng Zhuang², Zhi Li², Amanda Generosi³, Barbara Paci³, Carlo Ottaviani³, Claudio Quaresima³, Bruno Olivieri³, Marek Kopciuszynski¹, Ryszard Zdyb¹, Paola De Padova³, Yi Du²

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Silicene, a graphene-like two-dimensional material, has recently attracted an increasing attention due to its outstanding electronic properties and compatibility with the present Si-based electronics. Due to the preferred sp^3 bonding of Si atoms, silicene must be grown on a substrate [1], and the interaction between silicene and the substrate must be considered [2]. Beyond monolayer, multilayer silicene has also been synthesized on Ag(111) surface [3].

In the present work we report on the formation of multilayer silicene on Ag-induced $\sqrt{3}\times\sqrt{3}$ of Si(111) surface. Auger electron spectroscopy, low energy electron diffraction, scanning tunnelling microscopy/spectroscopy, *in-situ* Raman spectroscopy, energy dispersive in-plane x-ray diffraction techniques, angle resolved photoelectron spectroscopy and density functional theory calculations demonstrate that the synthesized system is quite different from the diamond-like silicon, showing its physical properties similar to those of the multilayer silicene obtained on the Ag(111) substrate.

This work has been supported by the National Science Centre (Poland) under Grant No. DEC-2014/15/B/ST5/04244, Australian Research Council (ARC) Discovery Project (DP140102581), and the Project for International Scientific Cooperation, CNR short-term mobility 2014, Italy/Australia.

[1] P. Vogt et al., Phys. Rev. Lett. 108 (2012) 155501.

[2] A. Podsiadły-Paszkowska, M. Krawiec, Phys. Rev. B 92 (2015) 165411.

[3] P. De Padova et al., Appl. Phys. Lett. 102 (2013) 163106.

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	8 th INTERNATIONAL WORKSHOP ON SURFACE PHYSICS (IWSP-2017)	
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PROGRAM OVERVIEW	Real-Space Visualization of the Pair Correlation Function in a 2D Molecular Gas P. Matvija¹, F. Rozbořil, P. Sobotík, I. Ošťádal, P. Kocán <i>Faculty of Mathematics and Physics, Charles University, Prague, Czech Republic</i> Properties of matter in fluid phases, determined by the interactions between particles, can be described by the pair correlation function. The function is defined as ensemble-averaged particle density $\bar{\theta}$ at a given position relative to a reference molecule. We demonstrate that the scanning tunneling microscope (STM) is capable to directly visualize the $\bar{\theta}$ in the real space in the case of two-dimensional (2D) molecular gas on weakly interacting surfaces.	
INVITED LECTURES	We use the STM to study highly mobile molecules of fluorinated copper phthalocyanine on the Si(111)/Ti-(1×1) surface. A slow mechanism of STM imaging results in the time-averaging of molecular occurrence under the STM tip. The obtained image represents a map of local density of the 2D gas $\bar{\theta}(x, y)$. We show that in the proximity of fixed molecules the images represent directly the pair correlation function. We support the data interpretation by lattice-gas kinetic simulations and we use the method to analyze interactions between the molecules and surface defects.	
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Segregation of Chromium in Mechanically Synthesized Iron Based Alloys Studied by ⁵⁷Fe Mössbauer and Auger Electron Spectroscopy

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The room temperature ⁵⁷Fe Mössbauer and Auger electron spectra were measured for mechanically synthesized iron-based Fe-Cr alloys, where Cr contributed from 2% to 8% of the total weight. This combination of experimental techniques allows to get chemical composition from: the surface by the Auger Electron Spectroscopy, from the 300 nm pre-surface region by the Conversion Electron Mössbauer Spectroscopy (CEMS) and from the bulk by the Transmission Mössbauer Spectroscopy (TMS).

Many previous experiments performed on Fe-Cr alloys obtained from melting in an arc furnace [1–6] show Cr segregation to the surface occurring at elevated temperatures. This effect plays important role in a passivation of the surface. In our work, mechanical synthesis leads to creation of the Fe-Cr alloy with Cr bulk concentration equals to its weight contribution, which is proved by CEMS and TMS results. Short annealing at elevated temperature leads to a segregation of the Cr to the “surface”, confirmed by AES results, although such samples contain of the different size particles (from few to ~20 μm). It enables novel way of the preparation iron-based alloys, which avoids high temperatures.

[1] M. Levesque, Phys. Rev. B 87 (2013) 075409.

[2] W. E. Delpont, J. P. Roux, Corros. Sci. 26 (1986) 407.

[3] P. A. Dowben et al., Surf. Sci. 134 (1983) L524.

[4] C. Leygraf et al., Surf. Sci. 46 (1974) 157.

[5] S. Suzuki et al., Appl. Surf. Sci. 103 (1996) 495.

[6] R. Idczak, K. Idczak, R. Konieczny, J. Nucl. Mater. 452 (2014) 141.

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	8 th INTERNATIONAL WORKSHOP ON SURFACE PHYSICS (IWSP-2017)	
PROGRAM OVERVIEW	Abstracts: Oral Presentations	
INVITED LECTURES	Adsorption of Anthracene and Pentacene on Coinage Metal Surfaces: Coverage Effects and the Role of the van der Waals Interactions <u>Juliana M. Morbec, Peter Kratzer</u> <i>Faculty of Physics, University of Duisburg-Essen, Duisburg, Germany</i> Understanding the interactions between metal surfaces and organic molecules—such as anthracene and pentacene, which have great potential for optoelectronic applications—is essential for electric contacts in organic electronics. In this work we use first-principles calculations to investigate the adsorption of anthracene and pentacene on coinage metal surfaces (especially Ag(111)), examining the effects of the van der Waals (vdW) interactions on the structural and electronic properties of these systems. We consider different coverages to disentangle the energy contributions to the molecule-molecule and molecule-surface interactions. Our results show, for example, that vdW interactions strongly affect the stability and structural properties of both anthracene/Ag(111) and pentacene/Ag(111), but have little effect on the electronic properties of these systems once the correct geometry has been obtained [1]. We found, in particular, that the inclusion of vdW interactions is crucial to correctly describe the flat adsorption geometry of anthracene/Ag(111) observed in experiments [2]. Moreover, we found that the adsorption of anthracene induces a larger reduction in the work function of the Ag(111) surface than pentacene, which is consistent with the stronger physisorption character observed in anthracene/Ag(111) [1]. We will additionally discuss the change in the work function and adsorption energy as function of the coverage. [1] J.M. Morbec and P. Kratzer, J. Chem. Phys. 146 (2017) 034702. [2] T. Shimooka et al., Langmuir 17 (2001) 6380.	
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Abstracts: Oral Presentations

Copper Deposition on Au(111) in Sulfuric Acid: New Insights

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

Electrochemical scanning tunneling microscopy (EC-STM) and cyclic voltammetry (CV) were used to investigate the co-adsorption of sulfate anions and copper cations on Au(111) in 0.1 mM CuSO₄ + 0.1 M H₂SO₄ in under- and overpotential deposition regions. The well known ($\sqrt{3} \times \sqrt{3}$) sulfate structure [1] was observed at 2/3 ML of Cu. On the first completed pseudomorphic Cu monolayer a disordered sulfate layer was found, which at more negative potentials gradually transforms into a ($\sqrt{3} \times \sqrt{7}$) sulfate structure [2], as it was observed for sulfate on unreconstructed Au(111). Further deposition of Cu from solution results in the formation of a ($\sqrt{3} \times \sqrt{3}$)-like structure on the incomplete second Cu layer at 5/3 ML local coverage. The formation of this structure is rationalized by the adsorption of sulfate anions in atomic vacancies within the second Cu layer, as it was also observed at 2/3 ML. Cu islands, which exhibit multilayer thickness show the characteristic sulfate induced Moiré structure [3]. The detailed analysis of STM images and height profiles across different terraces show that the formation of the Moiré structure characterises Cu layers at local coverage equal and higher than 5 ML [4]. The comparison of the results with the data obtained for Cu(111) [5] is presented. The adsorption of large organic molecules on sulfate covered Cu layers deposited on Au(111) is discussed.

[1] O.M. Magnussen et al., Phys. Rev. Lett. 64 (1990) 2929.

[2] B. Madry, K. Wandelt, M. Nowicki, Electrochim. Acta 217 (2016) 249.

[3] B. Madry, K. Wandelt, M. Nowicki, Surf. Sci. 637-638 (2015) 77.

[4] B. Madry, K. Wandelt, M. Nowicki, Appl. Surf. Sci. 388 (2016) 678.

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

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	8 th INTERNATIONAL WORKSHOP ON SURFACE PHYSICS (IWSP-2017)	
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PROGRAM OVERVIEW	DFT Study of Water at the Stoichiometric and Defected Fe(1 1 0) Surfaces <u>Tomasz Ossowski</u>¹, Juarez L.F. Da Silva^{1,2}, Adam Kiejna¹ ¹<i>Institute of Experimental Physics, University of Wrocław, Wrocław, Poland</i> ²<i>São Carlos Institute of Chemistry, University of São Paulo, SP, Brazil</i> Water adsorption on iron surfaces is important in understanding of corrosion and reduction of iron oxides by hydrogen. Density functional theory (DFT) with the van der Waals correction is applied to study molecular water adsorption on stoichiometric and defected Fe(1 1 0) surfaces. Structural and electronic properties of the H₂O/Fe(1 1 0) system, and a role of the vacancies are analyzed. Results show that vacancy prefers sites at the topmost atomic layer, without energy barrier for its diffusion from the interior. The vacancies cause decreasing of the work function and local change the geometry with larger effects for higher vacancy density. At stoichiometric surface water adsorbs flat on top the Fe atoms with the H–O–H plane almost parallel to the surface, with a binding energy of about 0.3 eV/molecule. Moreover, the adsorption energy of flat lying water is degenerated for few different orientation. It suggests possibility of H₂O rotation around direction perpendicular to the surface. At the defected surface, H₂O prefers sites near the vacancy. The binding of water to defected surface is by more than 0.2 eV stronger than to the stoichiometric one. Moreover, the adsorption of H₂O at stoichiometric region of the defected surface is by about 0.2 eV less preferable. It means that water is stronger bound to defected Fe(110) surface and vacancy can be considered as an adsorption centre for H₂O.	
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DFT+*U* Investigation of FeO(111) Films on Ag(111) Surface**Tomasz Pabisiak, Adam Kiejna***Institute of Experimental Physics, University of Wrocław, Wrocław, Poland*

In recent years metal-supported ultrathin oxide films have attracted significant interest for their unique electronic, magnetic and catalytic properties, governed by low-dimensionality and interaction with the support. In this work the adsorption of monolayer and bilayer FeO (111) films on Ag(111) surface is investigated using density functional theory (DFT) with Hubbard correction *U* (DFT+*U*). Relaxed oxide films adopt the structural parameters of silver support, and despite small lattice mismatch between Ag(111) and FeO(111) the perfect structural order is preserved. It excludes formation of Moiré superstructure, which was reported previously for monolayer FeO(111) grown on various metal single crystal supports. On Ag(111) surface FeO(111) monolayer of oxygen termination is the most stable one with Fe and O atoms sitting in the threefold coordinated *fcc* and *hcp* hollow sites of Ag(111), respectively. For FeO(111) bilayer both ferromagnetic and antiferromagnetic ordering in layers was considered, and the latter appeared to be more stable. The relatively large Fe-Ag distance suggests weak interaction of the oxide bilayer with the silver support. The structure, energetics, and electronic properties of the stable FeO (111) films on Ag(111) are discussed. Our calculations are in fair agreement with recent experimental results for ultrathin FeO(111) film grown on Ag(111) surface [1].

[1] M. Lewandowski et al., submitted for publication.

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First-Principles-Based Simulation of STM: From Magnetic Surfaces to Molecular Structures

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²*Department of Theoretical Physics, Budapest University of Technology and Economics, Budapest, Hungary*

Understanding of scanning tunneling microscopy (STM) image contrasts is of crucial importance in wide areas of surface science, ranging from magnetic surfaces to molecular structures. In my talk, two new developments of STM theories are presented: (i) a combined charge and vector spin tunneling transport theory, which provides the first steps towards the theoretical modeling of high resolution spin transfer torque imaging [1]; (ii) an extension of Chen's derivative rule [2] for STM simulations including tip-orbital interference effects with demonstrated importance of such effects on the STM contrast for two surface structures: N-doped graphene and a magnetic Mn₂H complex on the Ag(111) surface [3]. The latter method has recently been applied to validate a newly proposed structural model for the magnetite, Fe₃O₄(110) surface with two-fold oxygen vacancies [4], and to study surface defects in an organic perovskite, CH₃NH₃PbBr₃ [5]. Taking the highly oriented pyrolytic graphite, HOPG(0001) surface, by comparing STM topographic data between experiment and large scale simulations based on the 3D-WKB tunneling theory [6], a statistical analysis of the tip apex structure is demonstrated for the first time [7]. Finally, a combination of STM, X-ray photodiffraction (XPD) and density functional theory (DFT) helps the understanding of chirality transfer from molecules to crystal surfaces [8].

[1] K. Palotás et al., Phys. Rev. B 94 (2016) 064434.

[2] C.J. Chen, Phys. Rev. B 42 (1990) 8841.

[3] G. Mándi, K. Palotás, Phys. Rev. B 91 (2015) 165406.

[4] B. Walls et al., Phys. Rev. B 94 (2016) 165424.

[5] Y. Liu et al., ACS Nano 11 (2017) 2060.

[6] G. Mándi et al., J. Phys.: Condens. Matter 25 (2013) 445009; K. Palotás et al., Front. Phys. 9 (2014) 711.

[7] G. Mándi et al., J. Phys.: Condens. Matter 26 (2014) 485007; Prog. Surf. Sci. 90 (2015) 223.

[8] W. Xiao et al., Nature Chem. 8 (2016) 326.

Abstracts: Oral Presentations

Long-Range Corrugated Silicene

A. Podsiadły-Paszkowska, M. Krawiec*Institute of Physics, Maria Curie-Skłodowska University, Lublin, Poland*

Silicene, a two-dimensional material featuring a single sheet of Si atoms arranged in a honey-comb lattice, shares many of the remarkable properties of graphene. However, due to mixed sp^2 and sp^3 hybridization it has the low-buckled structure and cannot be easily produced as a free-standing layer [1]. Silicene has been successfully grown on a few different substrates and the experiments have indicated that interaction with a substrate modifies its atomic and electronic structure [2–6]. Moreover, this interaction can be controlled using metallic quantum wells of different thicknesses as substrates [7].

We discuss the properties of long-range corrugated silicene, which can be produced on vicinal (stepped) surfaces. We show that such modification of its structure leads to anisotropy of electron group velocity and opening of a small energy gap, which grows and oscillates with increasing of the corrugation. It also induces charge density oscillations which follows the structural deformation of silicene and features opposite phases in different sublattices. The emerging charge density oscillations phase is related to the σ - π rehybridization and the low-buckled structure of silicene, thus a similar behavior is expected also for other graphene-like materials, which prefer sp^3 bonding, like germanene or stanene.

This work has been supported by the National Science Centre (Poland) under Grant No. DEC-2014/15/B/ST5/04244.

- [1] S. Cahangirov et al. Phys. Rev. Lett. 102 (2009) 236804.
- [2] P. Vogt et al., Phys. Rev. Lett. 108 (2012) 155501.
- [3] A. Fleurence et al., Phys. Rev. Lett. 108 (2012) 245501.
- [4] L. Meng et al., Nano Lett. 13 (2013) 685.
- [5] T. Morishita et al., J. Phys. Chem. C 117 (2013) 22142.
- [6] T. Aizawa et al., J. Phys. Chem. C 118 (2014) 23049.
- [7] A. Podsiadły-Paszkowska, M. Krawiec, Phys. Rev. B 92 (2015) 165411.

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	8th INTERNATIONAL WORKSHOP ON SURFACE PHYSICS (IWSP-2017)	
PROGRAM OVERVIEW	Abstracts: Oral Presentations	
INVITED LECTURES	Revealing the Phthalocyanine Arrangements on Ag(100): From Pure Overlayer of CoPc and F₁₆CuPc to Bimolecular Heterostructures A. Sabik, P. Mazur, F. Golek, G. Antczak <i>Institute of Experimental Physics, University of Wrocław, Wrocław, Poland</i> Metal phthalocyanines (MPc) are macrocyclic coordinative compounds with remarkable chemical and thermal stability which have been widely studied as the suitable candidates for organic electronic devices. Variety of molecular compositions provide broad array of MPc (opto)electronic and magnetic properties. It is also possible to tune material properties by preparation of the layer which consists of MPc blend. The commonly performed fundamental studies on the adsorption of MPc on monocrystalline metal and semiconductor surfaces are indirect way to get better insight into organic nanotechnology. In this work we have utilized scanning tunneling microscopy (STM) and low energy electron diffraction (LEED) to determine the structural properties of cobalt phthalocyanine (CoPc) and prefluorinated copper phthalocyanine (F₁₆CuPc) on the Ag(100) surface. For coverages close to monolayer both studied systems form long-range ordered structures which are characterized by LEED. Their alignments (with respect to the [110] silver crystallographic direction) as well as the local lateral molecular arrangements, investigated by STM, depend on the molecule composition. Finally, we co-adsorb CoPc and F₁₆CuPc on the Ag(100) surface with various amounts of components. We demonstrate that adsorption of CoPc-F₁₆CuPc blends leads to new arrangement of ordered structure, visible in both STM and LEED. The difference in the STM appearance of central part of the molecule allows us to distinguish each MPc in the bimolecular heterostructure. This work has been supported by National Science Center, Poland within the project number 2015/19/N/ST3/01044.	
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Optical and Microstructural Properties of Al/Ti/TiO₂ Interference Systems

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Dielectric layers can protect the surface against corrosion as well as can be used as a decorative coatings. A TiO₂/Ti system, which is widely used in these applications, can be produced by laser oxidation, thermal oxidation and (also in the industrial scale) by using electrolytic oxidation (anodizing) as well as the magnetron sputtering method. In this case a color of the coating is an effect of the interference of light in the thin dielectric layer (titanium dioxide is a non-absorbing material in the visible spectral range). Aluminum is a highly reflective metal therefore aluminum oxide (Al₂O₃) formed on the aluminum plate does not produce saturated colors in contrast to the Ti/TiO₂ system. Saturated colors of the Al₂O₃-based coatings are prepared by adding an organic or inorganic dye to the highly porous aluminum oxide layer or as multilayer structures with oxides included (SiO₂, TiO₂, Fe₂O₃, Cr₂O₃, Bi₂O₃). Both methods are widely used in the industry. In this study, an alternative method for the preparation of color coatings is demonstrated which can be deposited on aluminum by the use of the Ti/TiO₂ double layer (the Al/Ti/TiO₂ structure).

The TiO₂/Ti/Al systems are produced using the industrial magnetron line in the Bohamet company using the pulsed gas injection magnetron sputtering technique (GIMS). Series of samples with varied thicknesses of TiO₂ layers (20–50 nm) and Ti films (5–125 nm) are prepared and examined by means of spectroscopic ellipsometry (SE), spectrophotometry (R) and atomic force microscopy (AFM). A Ti layer between Al and TiO₂ causes decrease in the luminance and increase in the color saturation. The luminance and the saturation of Al/Ti/TiO₂ systems depend on the thickness of the metallic film. The most significant changes are observed for thickness of Ti ranging from 0 nm to 20 nm.

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PROGRAM OVERVIEW	Effects of Acceptor Doping on a Metalorganic Switch <u>Tomasz Ślusarski</u>, Tomasz Kostyrko <i>Faculty of Physics, A. Mickiewicz University, Poznań, Poland</i> A copper dioxolene molecule with valence tautomeric properties [1,2] as a molecular switch is analysed with the density functional theory within GGA + <i>U</i> approach. We compute the transmission function of the junction with the Cu-dioxolene unit in the nonequilibrium case and show that it depends on the spin state of the molecule. We study effects of doping with ICl₂ acceptor molecules on the magnetic and electronic features of the device. In the absence of dopants the Cu-dioxolene unit is nearly charge neutral in <i>S</i>=1/2 spin state. The acceptors increase charge state of molecule and make possible high-spin (<i>S</i>=1) triplet to low-spin (<i>S</i>=0) singlet transition. The <i>I</i>–<i>V</i> dependence shows a manifestation of a negative differential resistance effect which is controllable by the acceptor doping. Our findings can be useful in the field of molecular spintronics for development of memory storage devices and resonance tunneling diodes [3]. Prof. Bogdan Bułka is gratefully acknowledged for a helpful discussion. This work has been supported by the National Science Centre under the contract DEC-2012/07/B/ST3/03412. The computations were performed at the Poznań's Supercomputing and Networking Center. [1] P. Dapporto et al., Chem. Eur. J. 14 (2008) 10915. [2] T. Kostyrko, T. Ślusarski, Appl. Surf. Sci. 373 (2016) 19. [3] S.J. van der Molen, P. Liljeroth, J. Phys.: Condens. Matter 22 (2010) 133001.	
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Molecular Size/Shape Effects in the Self-Assembly of Functional Units on Solid Surfaces

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³Supramolecular Chemistry Laboratory, University of Warsaw, Warsaw, Poland

Functional organic molecules are promising building blocks for the surface-confined fabrication of low-dimensional structures with predefined structural properties. The outcome of the self-assembly is often largely affected by the shape/size of molecular units at play and interactions between them. In this contribution, based on the Monte Carlo computer simulations, we discuss the effect of these factors on the pattern formation in adsorbed systems sustained by short-range directional interactions such as hydrogen bonding or metal-ligand coordination. Our results demonstrate how subtle modifications of the geometry and distribution of interaction centers within the building block can induce significant changes in the morphology of the resulting superstructures. In particular, we present molecular architectures ranging from achiral and chiral porous networks, strings, clusters and other structures formed by star-shaped molecules with different size and aspect ratio [1,2].

This work was supported by the Polish National Science Centre research grant 2015/17/B/ST4/03616.

[1] P. Szabelski, W. Rżysko, D. Nieckarz, J. Phys. Chem. C 120 (2016) 13139.

[2] W. Rżysko, D. Nieckarz, P. Szabelski, J. Phys. Chem. C 121 (2017) 410.

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	8 th INTERNATIONAL WORKSHOP ON SURFACE PHYSICS (IWSP-2017)	
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PROGRAM OVERVIEW	DFT Study of Stepped 4H-SiC{0001} Surfaces E. Wachowicz^{1,2}, T. Ossowski¹, A. Kiejna¹ ¹<i>Institute of Experimental Physics, University of Wrocław, Wrocław, Poland</i> ²<i>Interdisciplinary Centre for Mathematical and Computational Modelling, University of Warsaw, Warsaw, Poland</i> The growth of hexagonal crystals of the 4H-SiC and 6H-SiC polytypes occurs in the $\langle 0001 \rangle$ direction. The exposed crystal surface is composed of terraces of the {0001} oriented crystal planes separated by atomic steps of half-unit-cell or single-unit-cell height. We present results of density functional theory (DFT) study of the atomic structure and morphology of the atomic steps formed in the $[10\bar{1}0]$ and $[11\bar{2}0]$ directions on the Si-terminated 4H-SiC{0001} and the C-terminated 4H-SiC{0001} surfaces. On the latter surface atomic and electronic structure is modified only in the nearest neighbourhood of the step whereas the structure of the terrace is almost unchanged compared to that of the smooth stoichiometric surface. In contrast, on the Si terminated surface for both types of the applied model steps and on the widest terraces considered a substantial surface buckling is observed in the regions between steps. We calculated ledge energy and found that $[11\bar{2}0]$ step with C atom on the edge at Si-terminated surface is the most favourable energetically of all examined cases.	
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	8 th INTERNATIONAL WORKSHOP ON SURFACE PHYSICS (IWSP-2017)	
PROGRAM OVERVIEW	Abstracts: Poster Presentations Synthesized and Characterization of Nickel-Silicide Thin Film by Low Temperature Microwave Anneal Mohamed Salah Benlatreche¹, Ouafa Boukhemis², Kacem Smaili¹, Boudjma Bouaoina¹ ¹University of Boumerdés, Boumerdés, Algeria ²University of Constantine, Constantine, Algeria In this paper we proposed the formation of nickel-silicide thin film by using a physical vapor deposition (PVD). We are prepared metallic by PVD and annealed at temperatures from 250 to 350 °C using microwave-annealed silicidation. Thin film nickel deposition on a Si(111) wafer, the pressure was adjusted at 2×10^{-4} mbar, SEM and XRD profiles results showed that as-resulted NiSi thin film were almost thicker with size between 90 nm to 110 nm. The composition profile of the structure was investigated by scanning electron microscopy (SEM) with energy dispersive X-ray spectroscopy (EDS) however the XRD profiles shows the formation of structure NiSi and the presence of NiO. [1] T. Jarmar, <i>High-Resolution Studies of Silicide for Nano IC-Componenets</i>, ACTA Universitatis Upsaliensis, Uppsala, 2005. [2] L.J.Chen, <i>Silicide Technology for Integrated Circuits</i>, London: Institution of Electrical Engineers, 2004. [3] L. Christian, M.D. Francois, Z. Shi-Li, Silicides, <i>Handbook of Semiconductor Manufacturing Technology</i>, 2nd ed. (Boca Roton, FL: CRC Press, 2007) pp. 10–52.	
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Abstracts: Poster Presentations

Oxygen Adsorption and Reaction with Hydrogen on Pt-Rh Alloy Nanocrystals Studied by Field Emission Techniques

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Platinum group metals are widely used as catalysts, particularly in the form of alloys. The combination of features of each element may lead to an enhancement of the efficiency, selectivity and stability of catalytic reactions. Pt–Rh based catalysts present interesting properties in three-way catalytic converters: simultaneous oxidation of CO and unburned hydrocarbons (to form CO₂ and H₂O) and reduction of NO_x into N₂.

This contribution presents results of the Field Emission and Ion Microscopy studies of adsorption and interaction of oxygen with surfaces of nanosized Pt–Rh crystals, as well as catalytic oxygen reduction by hydrogen. The experimental method enabled us to study adsorption and reactions of adsorbates on the model particle of Pt–Rh catalyst: the hemispherical apex of the field emitter. Adsorption of oxygen on the sample at 600–700 K led to formation of subsurface oxygen in {113} regions (for O₂ exposure of ~3 L at 700 K, what corresponds to hypothetical oxygen coverage of 0.55 ML) and further formation of subsurface oxygen in more rough, high indexes areas between {012} and {011} poles of the hemispherical sample (for O₂ exposures ~100 L and hypothetical oxygen coverage of 0.91–0.94 ML). The oxygen, both adsorbed on the surface and subsurface can be effectively removed from the sample surface in the course of its catalytical reaction with hydrogen. During this reaction a sudden, eruptive change of the emission pattern brightness was observed.

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PROGRAM OVERVIEW	Abstracts: Poster Presentations	
INVITED LECTURES	H₂ Oxidation on Rh: Mapping the nm- and μm-Sized Reaction Fronts S. Buhr, J. Zeininger, M. Datler, C. Freytag, P. Winkler, G. Rupprechter, Y. Suchorski <i>Institut für Materialchemie, Technische Universität Wien, Vienna, Austria</i> Catalytic ignition and kinetic phase transitions are phenomena which can occur in heterogeneously catalyzed reaction systems and thus are of significant technological and scientific interest. In analogy to real thermodynamic phase transitions, the kinetic behavior of a system changes qualitatively during the kinetic transition when a control parameter (e.g. temperature or pressure) passes through a critical point [1]. A peculiarity of this phenomenon in a catalytic system is that it can be accompanied by reaction fronts which propagate over the surface during the transition. Studying the reaction front propagation allows to get interesting insights into the mechanism of the particular reaction [2]. In the present contribution, the propagation of reaction fronts during the ongoing H₂ oxidation reaction on Rh was studied <i>in situ</i> on the μm-scale by photoemission electron microscopy (PEEM) and on the nm-scale by field emission microscopy (FEM). Two differently sized Rh samples were used, a polycrystalline foil containing several μm-sized domains and a sharp nanotip consisting of nm-sized facets, both exhibiting a plenty of high-Miller-index surfaces with similar surface structure [3]. By comparing the anisotropy of the front propagation on samples of two different size scales (μm versus nm), the role of steps and kinks in the reaction front propagation and in the spatial coupling of the H₂ oxidation reaction on heterogeneous surfaces was studied. The role of such coupling in the oscillating behavior of H₂ oxidation on Rh is discussed.	
ORAL PRESENTATIONS	This work was supported by the Austrian Science Fund (FWF) [SFB F45 FOXSI]. [1] V.P. Zhdanov, B. Kasemo, Surf. Sci. Rep. 20 (1994) 111. [2] G. Ertl, Nobel Lecture, Angew. Chem. Int. Ed. 47 (2008) 3524. [3] M. Datler et al., Catal. Lett. 146 (2016) 1867.	
POSTER PRESENTATIONS		

Abstracts: Poster Presentations

Chemometrics Approach to the Spatially-Resolved XPS Studies of Heterogeneous Surfaces

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Spatially-resolved XPS studies of heterogeneous surfaces, such as e.g. polycrystalline foils or model systems for catalytic studies designed on a μm -scale result usually in a big number of complex spectra. The biggest problem is the handling of data is the assignment of the spectra and of their evolution to the corresponding spatial coordinates on the surface. "Mapping" the heterogeneous surface by optical microscopy can be of great help for the rapid localization of different regions (e.g. differently oriented domains of a polycrystalline surface). Such dual instrumental monitoring of the sample requires data handling techniques which can utilize the natural inter-correlations between observed optical picture and XPS signal. Multivariate statistical analysis methods (commonly known as chemometrics [1]) can significantly simplify extraction of the information obtained from large data sets.

In the present contribution, polycrystalline Rh foil consisting of several μm -sized domains of different crystallographic orientations was used as a test model for application of such approach. Surface oxidation of Rh was chosen as a process to study: subsurface oxygen and surface oxides of Rh play significant role during the catalytic oxidation reactions on Rh containing catalysts [2]. It might be supposed, that incorporation of oxygen atoms depends on the crystallographic orientation of individual domains, thus a polycrystalline Rh foil provides a possibility to study such a process in the exactly the same conditions for each particular orientation. Revealed peculiarities of the orientation dependent surface oxidation of Rh(*hkl*) are discussed.

[1] S. Wold, Chemom. Intell. Lab. Syst. 30 (1995) 1.

[2] M. Shelef, G.W. Graham, Cat. Rev. Sci. Eng. 36 (1994) 433.

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	8 th INTERNATIONAL WORKSHOP ON SURFACE PHYSICS (IWSP-2017)	
PROGRAM OVERVIEW	Abstracts: Poster Presentations	
INVITED LECTURES	Growth Model and Time Evolution of Ag Films Deposited on Ge A. Ciesielski¹, Ł. Skowronski², E. Górecka³, T.Szoplík¹ ¹<i>Faculty of Physics, University of Warsaw, Warsaw, Poland</i> ²<i>Institute of Mathematics and Physics, UTP University of Science and Technology, Bydgoszcz, Poland</i> ³<i>Department of Chemistry, University of Warsaw, Warsaw, Poland</i> Noble metal nanofilms constitute one of basic structures used in functional plasmonic devices. The range of surface plasmon polariton wave on metal/dielectric interface depends on ohmic losses in the metal skin depth and scattering losses on surface roughness. Because of the lowest ohmic losses, silver is typically employed for application in plasmonics [1]. Since the adhesion of silver to most oxides is low, depositing Ag films even on polished oxide substrates may results in a high surface roughness, hence in high scattering losses. Recently, it has been reported, that Ge wetting film, despite smoothening Ag surface, increases ohmic plasmon losses due to segregation [2]. Moreover, a hypothesis has been stated, that the segregation is intrinsically connected to changes in crystallinity [3]. Here we report on time-dependent ellipsometry and transmission measurements supported by XRR and XRD analysis which describe the growth and evolution of Ag nanocrystal layers deposited on Ge at different temperatures. We connect the kinetics of the segregation process with the crystallinity of the silver films. The results show, that Ge atoms imply a grain size gradient in the Ag layer (with largest grains on the bottom and smallest on top), then lower their energy by migrating from points on single grains boundaries to points on multiple grain boundaries. [1] T. Stefaniuk et al., Appl. Opt. 53 (2014) B237. [2] P. Wróbel et al., ACS Appl. Mater. Interfaces 7 (2015) 8999. [3] A. Ciesielski et al., Appl. Surf. Sci. (2017) in press.	
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Alternately Aligned Pb and Sb Atomic Chains on Si(553)**M. Dachniewicz, M. Jałochowski***Institute of Physics, Maria Curie-Skłodowska University, Lublin, Poland*

According to theoretical studies antimony atomic layers and nanoribbons are predicted to exhibit a variety of novel properties [1]. Among them edge states are particularly interesting due to their relevance to the Sb topological insulator properties. Existence of the edge states in ultrathin (2D) Sb(111) layers was recently confirmed experimentally [2]. It is known, that in sufficiently narrow nanoribbons the edge state functions overlap and their topological character changes. In order to overcome this difficulty it is demanding to study more complicated systems, like hybrid nanoribbons with enhanced spin-orbit interaction.

We present STM and RHEED experimental study of antimony atomic chains alternately aligned with Pb atomic nanoribbons on vicinal Si(553). For production of Pb-Sb hybrid nanoribbons the self-assembling method previously utilized in study of Pb nanoribbons was employed [3]. A single Pb-Sb nanoribbon was 1.48 nm wide and consisted of 5 Pb atomic chains and single Sb chain. On Si substrate the nanoribbons were aligned parallel to Si(553) step edges and, according to electron diffraction study, they formed spatially coherent system of nanostructures. We believe that our finding opens a new route in engineering of hybrid metallic nanoribbons.

We acknowledge financial support by National Science Centre by grant OPUS No. 2014/13/B/ST5/04442.

[1] O. Üzengi Aktürk, V. Ongun Özçelik, S. Ciraci, Phys. Rev. B 91 (2015) 235446.

[2] S.H. Kim et al., Sci. Rep. 6 (2016) 33193.

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

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H₂ Oxidation on Rh: Guiding Reaction Instabilities Through Surface Geometry

M. Datler, J. Zeininger, C. Freytag, S. Buhr, P. Winkler, G. Rupprechter, Y. Suchorski

Institut für Materialchemie, Technische Universität Wien, Vienna, Austria

Heterogeneous catalytic reactions, such as CO oxidation, may exhibit self-sustaining oscillations under stationary conditions [1]. The non-steady-state operation modes are promising for the possible improving of overall yield and selectivity of a catalyst, e.g. through the local actuation of reaction dynamics [2]. The attempts to guide the reaction oscillations through geometry by designing the reactive domains, using e.g. microlithography, were until now undertaken mainly for the CO oxidation [3].

The increased importance of hydrogen based energy conversion has enhanced interest in studying the catalytic hydrogen oxidation, including its oscillating modes. Until now, the oscillating behavior of the catalytic H₂ oxidation was observed on polycrystalline Pt or Pd wires [4,5] and on supported Pd catalysts [6]. In the case of Rh, the oscillating H₂ oxidation was solely observed on sharp Rh nanotips under high field conditions (FIM, $F > 10$ V/nm, [7]) and on bimetallic Rh/Ni catalysts [8].

We demonstrate an oscillation mode of the H₂ oxidation on confined pure Rh surfaces. The oscillations were studied within a slit-like mesoscopic defect on a Rh(111) single crystal using photoemission electron microscopy (PEEM) and on two differently curved Rh nanotips using field-emission microscopy (FEM, $F < 5$ V/nm). Structure related requirements for oscillations as well as a suggested feedback mechanism are discussed.

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

- [1] G. Ertl, Nobel lecture, Angew. Chem. Int. Ed. 47 (2008) 3524, and references therein.
- [2] J. Wolff et al., Science 294 (2001) 134.
- [3] L. Qiao et al., Phys. Rev. E 73 (2006) 036219.
- [4] J.E. Zuniga, D. Luss, J.Catal. 53 (1978) 312.
- [5] K. Rajagopalan, M. Sheintuch, D. Luss, Chem. Eng. Commun. 7 (1980) 335.
- [6] E. Lalik et al., Ind. Eng. Chem. Res. 54 (2015) 7047.
- [7] T. Visart de Bocarme, T. Bär, N. Kruse, Ultramicroscopy 89 (2001) 75.
- [8] F. Lovis et al., J. Phys. Chem. C 116 (2012) 4083.

Abstracts: Poster Presentations

Annealing Treatment of Polycrystalline Diamond Surfaces, Photoemission Results

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³*Faculty of Technical Physics, Poznań University of Technology, Poznań, Poland*

The effect of annealing temperature on the morphology, crystalline quality, and bonding character of continuous polycrystalline diamond are reported. Diamond films were deposited using Hot Filament Chemical Vapor Deposition (HF CVD) technique on a silicon substrate that was pretreated using an optimized, standard procedure. In this investigation, diamond thin films with different grain sizes ranging from 0.50 μm to 1.5 μm have been analyzed by X-ray photoelectron spectroscopy (XPS) and ultraviolet photoelectron spectroscopy (UPS).

The diamond microcrystalline films are highly defective, due to grain boundaries or intra-grain dislocations, intergranular amorphous or graphitic regions and hydrogen is supposed to be trapped on these intra- or intergranular defects. The presence of disordered hydrogenated sp^2 carbon in grain boundaries, a high density of dislocations which may trap hydrogen, together with the presence of H_2^* dimers, are supposed to explain the high hydrogen concentration which can be observed in polycrystalline diamond [1,2].

Some of the mechanisms of the behavior of diamond films during annealing and XPS carbon peak evolution was reported in terms of the change of the diamond-like sp^3 bonding relative to non-diamond sp^2 [3]. On the other hand the observations may be explained by surface chemical reactions (carboxylic, different carbonyl groups and hydrogen).

The main goal of this work is to discuss the results of thermal treatment in terms of hydrogen remove from the samples and possible surface reactions.

[1] A.T. Blumenau et al., Phys. Rev. B 65 (2002) 2052051.

[2] J.P. Goss et al., Phys. Rev. B 65 (2002) 1152071.

[3] D.G. McCulloch et al., Phys. Rev. B 70 (2004) 085406.

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	8th INTERNATIONAL WORKSHOP ON SURFACE PHYSICS (IWSP-2017)	
PROGRAM OVERVIEW	Abstracts: Poster Presentations	
INVITED LECTURES	Graphene Phonons in Inelastic Electron Tunnelling Spectroscopy Johannes Halle¹, Nicolas Néel¹, Mads Brandbyge², Jörg Kröger¹ ¹<i>Institute of Physics, Technical University of Ilmenau, Ilmenau, Germany</i> ²<i>DTU Nanotech, Technical University of Denmark, Lyngby, Denmark</i> Graphene on Ir(111) was intercalated by Li, Cs, and Ni. Inelastic electron tunnelling spectroscopy (IETS) unraveled remarkably strong signatures of graphene phonons for Li and Cs intercalants. For Ni-intercalated graphene, in contrast, phonon signals stayed below the detection limit of the low-temperature scanning tunnelling microscope (STM). On the basis of previously determined phonon dispersion branches the IETS features were assigned to acoustic and optical graphene phonons at the M point of the surface Brillouin zone. Additional experiments unveiled that the IETS signal increased with increasing Li coverage. Moreover, decreasing the separation between STM tip and graphene from the tunnelling to contact ranges led to a significant lowering of the phonon spectroscopic signatures. Combining these results, and comparing to transport calculations based on density functional theory, we discuss possible mechanisms that appropriately describe inelastic excitations with non-zero wave vectors via electron injection from an STM tip. Financial support by the Deutsche Forschungsgemeinschaft through Grant No. KR 2912/10-1 is acknowledged.	
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Formation of In/Alq₃ Films on Mo(100), W(110) and HOPG Substrates Studied by XPS and UPS**T. Hiller, A. Dittmar–Wituski, M. Trzcinski, A. Bukaluk***Institute of Mathematics and Physics, UTP University of Science and Technology, Bydgoszcz, Poland*

The results of thin layers of In, on a tris(8-hydroxyquinolino)aluminium – Alq₃(Al(C₉H₆NO)₃) films are presented. Alq₃ layers were formed by vacuum evaporation on the surface of metal single crystals (Mo(100), W(110) and graphite (HOPG)). 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 Alq₃ film was observed. The growth of indium film on Alq₃ was studied by XPS and UPS technique. The Growth was tracked by indium 4*d* valence band levels in HeII UPS spectra.

Additionally we present preliminary results from these layers using STM and optical techniques (ellipsometry).

[1] W. Song et al., Surf. Interface Anal. 32 (2001) 70.

[2] A. Droghetti et al., Phys. Rev. B 89 (2014) 094412.

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PROGRAM OVERVIEW	Growth of Thin Zn Films on 4H-SiC(0001) Studied by XPS and LEED K. Idczak, A. Próchnicka, L. Markowski <i>Institute of Experimental Physics, University of Wrocław, Wrocław, Poland</i> Silicon carbide (SiC) is an extremely hard and inert IV–IV group compound semiconductor material which has been drawing special attention in recent years because of its high suitability for high-temperature, high-power, high-frequency semiconductor devices, whereas conventional semiconductors such as Si, GaAs etc. are reaching their limits [1]. On the other hand, there is another important wide-bandgap semiconductor which has many potential applications, especially due to its unique physical properties. It is zinc oxide (ZnO) which is a pressure-sensing ceramic and can be used as nonlinear varistor or surface and bulk acoustic wave devices [2]. Due to its high thermal and chemical stability, wide tuneable bandgap and thus large exciton energy ZnO is a promising optoelectronic material. For example, thin films of ZnO show high transmittance and conductivity and can be used on solar cells as functionalized energy-efficient window. It is well known that every thin film physical, chemical and structural properties strongly depend on growth condition and growth techniques used. Until now, many techniques have been employed to prepare ZnO films, including chemical vapor deposition, sol–gel, molecular beam epitaxy, pulsed laser deposition, vacuum arc deposition, magnetron sputtering or thermal oxidation of metallic Zn [3,4]. In this work, we present results of growth of thin Zn films on 4H-SiC(0001) surface studied by X-ray Photoelectron Spectroscopy (XPS) and Low Energy Electron Diffraction (LEED). The properties of as deposited films, chemical composition and surface structure are explored. Obtained results designate further direction in oxidation of metallic Zn films experiments. [1] B. Pécz, Appl. Surf. Sci. 184 (2001) 287. [2] A.B. Djurisić, Y. Chan, E.H. Li, Mater. Sci. Eng. 38R (2002) 237. [3] T. Schuler, M.A. Aegerter, Thin Solid Films 351 (1999) 125. [4] S. Singh, P. Chakrabarti, Superlattices Microstruct. 64 (2013) 283.	
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A Study of Oxidation and Surface Segregation of Silicon and Chromium in Fe-Cr-Si Alloys by Mössbauer and X-ray Photoelectron Spectroscopies

R. Idczak, K. Idczak, R. Konieczny

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The addition of silicon or chromium has a significant effect on the oxidation resistance of iron. As it was shown, in our previous works [1–3], alloying a small amount of Cr or Si into iron do not prevent corrosion, during exposure to air at elevated temperatures, however significantly reduce the oxidation rate. These results are important due to fact that iron alloys are still ones of the most important materials for the modern industry. For example, the nuclear energy sector is looking for a new structural materials which could be able to keep their design parameters for a long time during the exposure to factors such as high temperature, high-energy neutron bombardment and corrosion [4]. These conditions will exist in new types of advanced fission reactors (Generation IV) and fusion reactors (ITER, DEMO).

In this work, the room temperature ^{57}Fe Mössbauer and XPS spectra were measured for polycrystalline iron-based Fe-Cr-Si alloys. Before measurements, the samples were annealed in the vacuum and then exposed to air at 870 K for several hours. 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 to take data simultaneously from the surface of studied alloys by the X-ray photoelectron spectroscopy (XPS), from the 300 nm subsurface region by the conversion electron Mössbauer spectroscopy (CEMS) and from the bulk by the transmission Mössbauer spectroscopy (TMS). The observed differences in Cr and Si concentration on the surface, in the subsurface region and the bulk should give the answer about segregation process in Fe-Cr-Si alloys. The second part of our study concerns the oxidation process in Fe-Cr-Si alloys. The experimental techniques used in this study are very sensitive to the presence of iron oxides (TMS, CEMS, XPS) as well as chromium and silicon oxides (XPS).

[1] K. Idczak et al., Phys. B 491 (2016) 37.

[2] R. Idczak, Appl. Phys. A 122 (2016) 1009.

[3] R. Idczak, Oxid. Met. 87 (2017) 75.

[4] I. Cook, Nat. Mater. 5 (2006) 77.

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2D Supramolecular Organization of Electroactive Flavanthrone-Thiophene Derivatives on HOPG – STM Studies

T. Jaroch¹, R. Nowakowski¹, P. Bujak², K. Kotwica², M. Zagórska², A. Proń²

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²*Faculty of Chemistry, Warsaw University of Technology, Warsaw, Poland*

A family of organic semiconductors based on the azaacene group represent hot topic of intensive research interest due to their satisfying electrical transport properties. These materials are commonly used in FET's and other organic electronic devices. It is well known that semiconducting properties of applied thin layers of such compounds, in general, and the charge carriers mobility, in particular, are very sensitive to several factors of molecular and supramolecular nature. Among them, very often molecular ordering plays a crucial role.

This communication presents recent combined studies of supramolecular structure and additionally electrochemical properties of series of three freshly synthesized solution-processable flavanthrone-alkyl-thiophene derivatives, namely (8,16-bis(n-octylthiopheno-2-yl)benzo[h]benz[5,6]acridino[2,1,9,8-klmna]acridine) [1]. The monomolecular monolayers prepared by drop-casting method on a freshly cleaved HOPG were imaged at molecular resolution by scanning tunneling microscopy in ambient conditions. Especially, the influence of the position of octyl group substituted to the thiophene ring (n=3, 4, 5; C β , C γ , C δ) being connected to the flavanthrone core is comparatively analyzed. Careful discussion of registered dissimilarities in structural properties of monolayers is undertaken in the light of molecular structure and resulted distribution of intermolecular interactions. The structural studies additionally have been extended to electrochemical analysis for studied derivatives.

[1] K. Kotwica et al., Chem. Eur. J. 22 (2016) 7978.

Abstracts: Poster Presentations

Impact of Embedded Dipole on Transport Properties of Single Molecular Junction

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In the molecular electronics it is essential to design the structure of molecules to achieve specific functions. In particular, diode (or rectification) behaviour [1,2] of single molecules is one of the most exciting device characteristics.

In this work we study the charge transport through symmetric and non-symmetric (with embedded dipole) benzene-based molecules covalently bound via sulfur linkers to the (111)-oriented Au electrodes. First-principle calculations are performed based on density functional theory (DFT) using the FIREBALL code [3], whereas calculations of the transport properties employ the nonequilibrium Green function (NEGF) technique [4]. Electron transport is studied in detail by analysing the transmission spectra, density of states distributions, current–voltage characteristics and eigenchannel decomposition [5].

We show that energy level alignment within a single molecular junction can be tuned by the presence of a dipole moment in the molecule without altering any other properties of the junction. More specifically, we investigate the influence of embedded dipoles in non-symmetric molecules on their rectification characteristics.

[1] A. Kovalchuk et al., Chem. Sci. 7 (2016) 781.

[2] I. Díez-Pérez et al., Nat. Chem. 1 (2009) 635.

[3] G. Rocha et al., Phys. Rev. B 73 (2006) 085414.

[4] M. Paulsson et al., Phys. Rev. B 76 (2007) 115117.

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

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PROGRAM OVERVIEW	Surface Segregation of Chromium in Mechanosynthesized Fe-Cr Alloys Studied by Mössbauer and Directional Auger Electron Spectroscopy	
INVITED LECTURES	R. Konieczny, I. Morawski <i>Institute of Experimental Physics, University of Wrocław, Wrocław, Poland</i> The room temperature ^{57}Fe Mössbauer and Auger electron spectra were measured for iron-based solid solutions $\text{Fe}_{1-x}\text{Cr}_x$, prepared by mechanical alloying with x in the range $0.02 \leq x \leq 0.08$. The spectra were collected using three techniques: the transmission Mössbauer spectroscopy (TMS), the conversion electron Mössbauer spectroscopy (CEMS) and the Auger Electron Spectroscopy (AES). This unique combination of experimental techniques allows to take data simultaneously from the surface of studied mechanically synthesized alloys by the Auger Electron Spectroscopy (AES), 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 Cr concentration on the surface, in the pre-surface region and bulk should give the answer about segregation process in mechanosynthesized Fe-Cr alloys. Worth noting is fact that the majority of previous experimental studies on surface segregation of Fe-Cr alloys were performed on single crystals or samples which were obtained by melting in an arc furnace [1–6]. Taking into account that iron alloys are one of the most important engineering materials [7], it seems appropriate to investigate polycrystalline samples which were obtained in mechanical synthesis.	
ORAL PRESENTATIONS	[1] W.E. Delport, J.P. Roux, Corros. Sci. 26 (1986) 407. [2] P.A. Dowben et al., Surf. Sci. 134 (1983) L524. [3] C. Leygraf et al., Surf. Sci. 46 (1974) 157. [4] S. Suzuki et al., Appl. Surf. Sci. 103 (1996) 495. [5] R. Idczak, K. Idczak, R. Konieczny, J. Nucl. Mater. 452 (2014) 141. [6] M. Levesque, Phys. Rev. B 87 (2013) 075409. [7] I. Cook, Nat. Mater. 5 (2006) 77.	
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Spin-Orbit Effects in Atomic Ribbons on Different Substrates

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The transport properties of low-dimensional conductors are particularly interesting due to their possible applications in nanoelectronics – atomic chains or ribbons of metallic atoms are the ultimate small conductors. Such systems are often sensitive to the electron spin and orbital degrees of freedom which lead to the spin-orbit effects. The Rashba term in the tight-binding Hamiltonian is responsible for the spin-flip processes between neighboring atomic sites in the central system [1].

In our work we concentrate on the electrical properties of single-row and multi-row atomic structures on different substrates. Such quasi-one-dimensional systems can be fabricated on modified vicinal surfaces, e.g. Si(553) with Pb chains [2,3] or Pb-Sb nonoribbons. In our numerical calculations we consider finite-length atomic ribbons and investigate the role of the system geometry in the electron transport. In particular, we analyze the influence of spin-orbit couplings on the local density of states (DOS) along the system. Also the modifications of DOS due to electron localization in the substrate are studied – we consider insulator, semiconductor and metallic substrates. We have found that in the presence of the spin-flip couplings the local DOS at the Fermi level oscillates with different periods along the ribbon.

This work is supported by National Science Centre, Poland, under Grant No. 2014/13/B/ST5/04442.

[1] F. Mireles, G. Kirczenow, Phys. Rev. B 64 (2001) 024426.

[2] P. Nita et al., Phys. Rev. B 84 (2011) 085453.

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

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	8 th INTERNATIONAL WORKSHOP ON SURFACE PHYSICS (IWSP-2017)	
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PROGRAM OVERVIEW	Structural and Electronic Properties of 6H-SiC(0001)–(3×3) Surface Reconstruction: Theoretical Study G. Miłkaszewicz, L. Jurczyszyn <i>Institute of Experimental Physics, University of Wrocław, Wrocław, Poland</i> Silicon carbide polytypes represent different crystallographic structures, namely the most common 2H, 4H, 6H and 3C. The difference comes from the stereometry of bonding between bilayers of SiC; synperiplanar or antiperiplanar. The 6H-SiC(0001) surface has been investigated experimentally by the of STM and LEED measurements. Depending on silicone concentration at the surface it exhibits different reconstructions, most common are Si(3×3) and Si($\sqrt{3}\times\sqrt{3}$). A variety of different models have been discussed in literature for the atomic structure of 6H-SiC(0001)–(3×3) surface reconstruction. In our theoretical study we have analyzed the atomic and electronic properties of the surface reconstruction models proposed Kulakov [1], Tsong [2], and Starke [3]. Our investigation is based on DFT ab-initio calculations. [1] M.A. Kulakov, G. Henn, B. Bullemer, Surf. Sci. 246 (1996) 49. [2] L. Li, I.S.T. Tsong, Surf. Sci. 351 (1996) 141. [3] U. Starke et al., Phys. Rev. Lett. 80 (1998) 758.	
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h-BN Layer Induced Chiral Decomposition in the Electronic Properties of Multilayer Graphene

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The so called Klein tunneling effect is known, and outstanding electronic properties of graphene sheets. Previous research on this effect focused on the cases of single-layer, and two-band approximation of bi-layer. Our work is a purely theoretical description of chiral tunneling or Klein-like tunneling effect in the multilayer stockings. We consider the cases of multilayer graphene systems within many-band approximation as well as systems consisting of graphene and hexagonal boron nitride. In the last case, we introduce the chiral decomposition procedure of the tight-binding Hamiltonian which leads to the effective Hamiltonian composed of the isolated bi-layer systems with some effective interlayer hoppings and one monolayer system if number of layers is odd. Similar procedure has been used previously for multilayer graphene systems [1,2]. The results consist of band structures and transmission probabilities in exemplar systems of homo- and heterogeneous structures. We also reveal the similarities in the band structures, and transmission probability which can be found between the bilayer, and multilayer structures.

[1] M. Koshino, T. Ando, Phys. Rev. B 76 (2007) 085425.

[2] M. Nakamura, L. Hirasawa, Phys. Rev. B 77 (2008) 045429.

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	8th INTERNATIONAL WORKSHOP ON SURFACE PHYSICS (IWSP-2017)	
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INVITED LECTURES	Segregation of Chromium in Mechanically Synthesized Iron Based Alloys Revealed by Auger Electron Spectroscopy and Directional Auger Electron Spectroscopy I. Morawski, R. Konieczny, M. Nowicki <i>Institute of Experimental Physics, University of Wrocław, Wrocław, Poland</i> The Cr segregation to the surface occurring at elevated temperatures in Fe-Cr samples, obtained from melting in an arc furnace, is well established knowledge [1–6]. This effect plays an important role in a passivation of the surface against oxidation of Fe. In this work we use Auger Electron Spectroscopy (AES) and Directional Auger Electron Spectroscopy (DAES) [7] to investigate mechanically synthesized iron-based $\text{Fe}_{1-x}\text{Cr}_x$ alloys, where x was in the range of 2% – 8%. We show that the segregation of Cr also occurs in polycrystalline samples, which consist of grains of different size (from few to $\sim 20\text{ }\mu\text{m}$). AES investigations proved that the amount of segregated chromium is approximately proportional to its concentration in the bulk. DAES measurements show the formation of crystalline phase after the temperature treatment of the polycrystalline sample. [1] W.E. Delport, J. P. Roux, Corros. Sci. 26 (1986) 407. [2] P.A. Dowben et al., Surf. Sci. 134 (1983) L524. [3] C. Leygraf et al., Surf. Sci. 46 (1974) 157. [4] S. Suzuki et al., Appl. Surf. Sci. 103 (1996) 495. [5] R. Idczak, K. Idczak, R. Konieczny, J. Nucl. Mater. 452 (2014) 141. [6] M. Levesque, Phys. Rev. B 87 (2013) 075409. [7] S. Mróz, M. Nowicki, Surf. Sci. 297 (1993) 66.	
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Optical and Microstructural Characterization of the Annealed TiO₂ Layers

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²Faculty of Chemistry, Nicolaus Copernicus University in Toruń, Toruń, Poland

³Faculty of Physics, University of Warsaw, Warsaw, Poland

In the last few decades titanium oxides have been intensively studied because of their exceptional properties. These oxides are used in such high-tech applications as electrochromic devices and dye-sensitized solar cells as well as protective and antireflective coatings. Moreover, titanium oxides and (oxy)nitrides can be applied as a decorative material for architecture, the automotive industry, electronics and jewellery. The main crystallite phases of titanium dioxide are anatase and rutile, however, in certain deposition conditions a mixture of both phases or amorphous TiO₂ can be fabricated. Part of the aforementioned properties of TiO₂ strongly depend on the crystallite structure therefore the control of the phase composition of the dielectric film is required during the layer formation.

TiO₂ layers with a thickness 160–260 nm were deposited at room temperature and at 500 K using the PVD technique then annealed at 1073 K in a UHV conditions as well as in the presence of O₂ (10⁻⁵ mbar). The prepared layers were examined by means of powder X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), UV-photoelectron spectroscopy (UPS), atomic force microscopy (AFM), scanning electron microscopy (SEM), spectroscopic ellipsometry (SE) and Raman spectroscopy techniques.

The used experimental techniques allow for detailed analysis of both microstructural and optical properties of the prepared dielectric films. The TiO₂ films deposited on the unheated substrates are amorphous while those prepared at 500 K exhibit anatase nature. In the annealed samples both anatase and rutile crystallites were found.

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PROGRAM OVERVIEW	Properties of Pt on Cu(111) Revealed by AES, LEED, and DEPES A. Miszczuk, I. Morawski, M. Jurczyszyn, <u>M. Nowicki</u> <i>Institute of Experimental Physics, University of Wrocław, Wrocław, Poland</i> The investigations of Pt on Cu(111) were performed to reveal the growth mode and structure of adsorbate with the use of Auger Electron Spectroscopy (AES), Low Energy Electron Diffraction (LEED), and Directional Elastic Peak Electron Spectroscopy (DEPES) [1]. Auger signal recorded during the continuous Pt adsorption on Cu(111) at 330 K confirms the layer by layer growth mode. LEED patterns observed at 1ML show the formation of compressed Pt monolayer. At higher coverages such as 3 ML and 6 ML the increase of the lattice constant of the topmost Pt layer, which approaches the bulk value of Pt(111), is observed. DEPES investigations performed for 1 ML of platinum indicate the nucleation of adsorbate domains characterized by A/CBA and B/CBA stacking sequences at the Pt/Cu interface, which at higher coverages lead to the nucleation of mutually rotated by 180° Pt domains. Experimental DEPES data were compared to theoretical results obtained with the use of the multiple scattering (MS) calculations [2]. The quantitative analysis of the data made by an <i>R</i>-factor calculations enabled the determination of Pt domain populations. The data indicate the formation of intermixing layer at the Pt/Cu interface at 330 K. [1] M. Jurczyszyn, A. Miszczuk, I. Morawski, M. Nowicki, <i>Structural Investigations by Means of Directional Elastic Peak Electron Spectroscopy</i>. In: Reedijk, J. (Ed.) Elsevier Reference Module in Chemistry, Molecular Sciences and Chemical Engineering. Waltham, MA: Elsevier. 18-Dec-2015, doi:10.1016/B978-0-12-409547-2.11459-3. [2] I. Morawski, M. Nowicki, Phys. Rev. B 75 (2007) 155412.	
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Ultra-Thin In Films on the Si(111)- $\alpha(\sqrt{3} \times \sqrt{3})$ -Pb Reconstructed Surface

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In and Pb on Si(111) surface are still of interest because of exhibiting a variety of phases with interesting and unique properties. In particular, interest stems from the self-assembled 3D nanostructures based on quantum size effects resulted in uniform height islands, which were observed for Pb/Si(111) and In/Pb/Si(111) systems at low temperature. However the “magic” heights and a bulk structure of the nano-islands strongly depend on an interfacial structure, i.e. surface reconstruction and metallic surfactant (for example, recent studies have shown that FCC structure of In islands converts to BCT structure when the coverage of indium increases [1]).

This work presents experimental results obtained for the system of In deposited on Si(111)- $\alpha(\sqrt{3} \times \sqrt{3})$ -Pb reconstructed surfaces and annealed in the temperature range 25–700 °C. Low Energy Electron Diffraction and X-ray Photoelectron Spectroscopy have been used as our basic techniques. The aim of the present study is to gain knowledge of the surface structure and thermal stability of thin layers of indium in dependence on the original surface reconstruction and annealing temperature. Particular interest stems from the fact that among various Pb 2D phases Si(111)- $\alpha(\sqrt{3} \times \sqrt{3})$ -Pb phase is extremely smooth and commensurate with silicon substrate lattice underneath, which implies a very low diffusion barrier and high mobility of adsorbed atoms [2]. Hence, it is expected that it may effectively influence on adsorbed metal, showing its new behavior.

[1] J. Chen et al., Phys. Rev. B 77 (2008) 233302.

[2] M. Hupalo et al., Phys. Rev. B 71 (2005) 193408.

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PROGRAM OVERVIEW	Abstracts: Poster Presentations	
INVITED LECTURES	Metastable Magnetic Skyrmionic Spin Structures in an Ultrathin Film and their Electron Charge/Spin Transport Properties Krisztián Palotás^{1,2}, Levente Rózsa^{3,4}, Eszter Simon², László Udvardi², László Szunyogh² ¹<i>Institute of Physics, Slovak Academy of Sciences, Bratislava, Slovakia</i> ²<i>Department of Theoretical Physics, Budapest University of Technology and Economics, Budapest, Hungary</i> ³<i>Institute of Applied Physics and Interdisciplinary Nanoscience Center, University of Hamburg, Germany</i> ⁴<i>Wigner Research Centre for Physics, Hungarian Academy of Sciences, Budapest, Hungary</i> Metastable localized spin configurations with topological charges ranging from $Q = -3$ to $Q = 2$ are observed in a $(\text{Pt}_{0.95}\text{Ir}_{0.05})/\text{Fe}$ bilayer on $\text{Pd}(111)$ surface [1] by performing spin dynamics simulations, using a classical Hamiltonian parametrized by ab initio calculations [2]. It is demonstrated that the frustration of the isotropic exchange interactions is responsible for the creation of these various types of skyrmionic structures. The Dzyaloshinsky-Moriya interaction, present due to the breaking of inversion symmetry at the surface, energetically favors skyrmions with $Q = -1$, distorts the shape of the other skyrmionic objects, and defines a preferred orientation for them with respect to the underlying lattice. By performing spin-polarized scanning tunneling microscopy (SP-STM) calculations, a direct connection between experimentally measurable SP-STM contrasts and different topologies of skyrmionic systems is established in an isotropic environment of skyrmion formation [3]. Moreover, the first results on high resolution scanning tunneling spin transfer torque (STT) microscopy simulations of the skyrmionic structures are also presented, employing a recently developed calculation method for tunneling STT [4]. [1] L. Rózsa et al., Phys. Rev. B 95 (2017) 094423. [2] L. Rózsa et al., Phys. Rev. Lett. 117 (2016) 157205. [3] K. Palotás et al., arXiv:1609.07016 (2016). [4] K. Palotás et al., Phys. Rev. B 94 (2016) 064434.	
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Microstructural, Electrical and Optical Properties of Sn Thin Layers – Effect of the Deposition Rate

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³*Faculty of Chemistry, Nicolaus Copernicus University in Toruń, Toruń, Poland*

Microstructural, electrical and optical properties of thin films strongly depend on the deposition conditions (e.g. temperature, deposition rate). The 30 nm tin (Sn) layers were prepared using the physical vapor deposition (PVD) method. These tin layers were deposited on the Al₂O₃ – coated Si substrates at six different deposition rates (0.05 Å/s, 0.15 Å/s, 0.25 Å/s, 0.50 Å/s, 2.50 Å/s, 5.00 Å/s) at room temperature.

The microstructural, electrical and optical properties of obtained samples were investigated by means of atomic force microscopy (AFM), scanning electron microscopy (SEM), powder X-ray diffraction (XRD), spectroscopy ellipsometry (SE) techniques and the four-point probe (4P) method.

The AFM and SEM results reveal that lateral grain size increases with the increase in the deposition rate. Additionally, for deposition rates higher than 0.5 Å/s, large and flat microstructures can be observed. The XRD patterns show the strong texture (preferred grown orientation of Sn grain is (002)). The results of four-point probe indicate that resistivity decreases with the increase in the deposition rate. Moreover, for deposition rates lower than 0.25 Å/s the sheet resistance is at the level of MΩ. The determined dielectric functions of the Sn film exhibit the largest differences for photon energies lower than 2.5 eV. This fact is associated with varied formation of metallic layers (their microstructure), thereby with different response of free electrons on the incident light – with different contribution of the Drude term to the complex dielectric function of the Sn layers.

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PROGRAM OVERVIEW	Monte Carlo Study of the Self-Assembly of Tripod Molecules in Two-Dimensional Systems W. Rżysko¹, P. Szabelski², D. Nieckarz³ ¹<i>Department for the Modeling of Physico-Chemical Processes, Maria Curie–Sklodowska University, Lublin, Poland</i> ²<i>Department of Theoretical Chemistry, Maria Curie–Sklodowska University, Lublin, Poland</i> ³<i>Supramolecular Chemistry Laboratory, University of Warsaw, Warsaw, Poland</i> We present the results of simulations carried out for off-lattice model of monolayers which contain tripod molecules. The molecule is modeled as a star particle with three arms of different lengths (numbers of segments). Molecules interact only through the last segments of arms. The interactions are highly directional, they act exclusively along axes of the arms. Our calculations were performed for selected parameters characterizing the architecture of molecules with different lengths of particular arms and different angles between the arms. At different temperatures and densities of the fluid we have calculated the association degrees, the correlation functions and structure factors. Depending on thermodynamical conditions we found hexagonal or square phases. This work was supported by the Polish National Science Centre research grant 2015/17/B/ST4/03616.	
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Thermal Desorption and Stability of Cobalt Phthalocyanine on Ag(100)

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

The studies on the adsorption, thermal stability and desorption of π conjugated organic molecular layers on metal surfaces are important with respect to their potential application in organic electronic. In contrast to widely reported and studied electronic and structural properties of metal-organic interfaces, the description of desorption phenomenon is scanty and complicated. During desorption of such complex systems the various degrees of freedom as well as dissociation may be activated. [1, 2]

Utilizing work function change ($\Delta\phi$) measurements and low energy electron diffraction, we have characterized adsorption, thermal stability and desorption of cobalt phthalocyanine (CoPc) molecules on the Ag(100) surface from sub-monolayer to multilayer regimes. [3, 4] We probed temperature evolutions of $\Delta\phi$ for three different initial molecular states which correspond to 0.3 ML (2D molecular gas phase), 1.0 ML (ordered structure) and 2.0 ML (multilayer). Based on these results we have estimated the desorption temperature ranges. Then we investigated the time evolutions of $\Delta\phi$ during sample annealing at fixed temperatures and determined the activation energies and frequency prefactors for desorption. Surprisingly, desorption activation energies for all studied coverages are comparable whereas the frequency prefactors differ by eleven orders of magnitude. We will also show the indications of thermal re-ordering and decomposition of the molecules which remained in direct contact with the Ag(100) surface.

[1] J. Hwang, A. Wan, A. Kahn, Mater. Sci. Eng. R-Rep. 64 (2009) 1.

[2] J.M. Gottfried, Surf. Sci. Rep. 70 (2015) 259.

[3] A. Sabik, F. Gólek, G. Antczak, J. Phys. Chem. C 120 (2016) 396.

[4] A. Sabik, F. Gólek, G. Antczak, Rev. Sci. Instrum. 86 (2015) 056111.

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PROGRAM OVERVIEW	Interface Potentials, Intrinsic Defects, and Passivation Mechanisms in Al₂O₃, HfO₂, and TiO₂ Ultrathin ALD Films <u>Dieter Schmeißer</u>, Małgorzata Kot, Karsten Henkel <i>Angewandte Physik-Sensorik, BTU Cottbus–Senftenberg, Cottbus, Germany</i> We study the electronic structure of ultrathin Al₂O₃, HfO₂, and TiO₂ ALD films by resonant photoelectron spectroscopy (resPES) and by electrical measurements (capacitance-voltage). For all films investigated intrinsic defect states within the electronic band gap were observed including excitonic, polaronic, and charge-transfer defect states, where their relative abundance is subject of the choice of ALD parameters and of the used substrate. The spectroscopic assigned in-gap defect states are related with electronic charges as determined in the electrical measurements. The defect states are responsible for the active sites in interface reactions, for the incorporation of intrinsic charges, and for the formation of local dipole momenta. All of these features determine the surface potentials and the reactivity of the surface of the ALD coated systems. We give examples of charges and dipoles in Al₂O₃, on a study of the surface potentials in HfO₂, and relate the intrinsic defects in TiO₂ to their electrochemical relevance.	
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Ionicity Factors, Charge-Neutrality Levels, and Multiple-Atom Processes in ZnO, HfO₂, and TiO₂

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²Institut f r Physik, Humboldt-Universit t zu Berlin, Berlin, Germany

We study the electronic structure of ZnO single crystals and ultrathin a-ZnO [1], HfO₂ [2], and TiO₂ [3] films by resonant photoelectron spectroscopy (resPES). We derive the ionicity factors of the individual metal-oxygen bonds in a procedure based on the original concepts of Pauling [4] and Phillips [5]. The charge-neutrality level (CNL) is determined following a description of Robertson [6]. Both, ionicity factors and CNL are based on the differences in the respective electronegativities [4–6]. For the systems investigated here we find values between 0.6 and 0.8 for the ionicity factors. These are consistently derived from the resonant PES data at the O1s absorption edge as well as from non-resonant O1s core level data. The CNL for all systems investigated is significantly different from earlier findings [3] and in all systems is well separated from the Fermi energy.

Our results suggest that the bonding in the three oxidic systems involves a phase separation of the charge density to yield the ionic and the covalent contributions. For the ionic contributions the charge density is fixed between the metal and oxygen atoms and localized by the direct Coulomb interaction. However, the valence states may form multi-atomic hybrids which enable the formation of polarons, excitons, and ligand-to-metal charge-transfer (CT) states. Thus, the strict localization is reduced as the wave-functions now are extended over several atomic distances. The covalent contributions are not localized and may be considered as free charges. Thereby the energy separation between CNL and Fermi energy can be rationalized. However, they can be trapped by polaronic states or by the local dipole momenta of the CT states. We give a quantitative charge density distribution based on the plasma frequency of the individual system.

[1] J. Haeberle et al., Mater. Res. Express 3 (2016) 106302.

[2] S. Alberton Corr a, S. Brizzi, D. Schmeisser, J. Vac. Sci. Tech. A 34 (2016) 01A117.

[3] C. Das, M. Richter, M. Tallarida, D. Schmei er, J. Phys. D: Appl. Phys. 49 (2016) 275304.

[4] L. Pauling, *The nature of the chemical bond*, Cornell Univ. Press, New York (1960).

[5] J.C. Phillips, Rev. Mod. Phys. 42 (1979) 317.

[6] J. Robertson, J. Vac. Sci. Technol. A31 (2013) 050821.

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PROGRAM OVERVIEW	Abstracts: Poster Presentations	
INVITED LECTURES	Structural and Optical Properties of In-doped ZnO Films Synthesized by Spin-Coating Technique P. Sedzicki¹, R. Szczesny², L. Skowronski³, A. Apostoluk⁴, A. Bouaine⁵, S. Abed⁶, B. Derkowska-Zielinska¹ ¹<i>Institute of Physics, Faculty of Physics, Astronomy and Informatics, Nicolaus Copernicus University in Toruń, Toruń, Poland</i> ²<i>Faculty of Chemistry, Nicolaus Copernicus University in Toruń, Toruń, Poland</i> ³<i>Institute of Mathematics and Physics, UTP University of Science and Technology, Bydgoszcz, Poland</i> ⁴<i>Université de Lyon, Lyon, France</i> ⁵<i>Laboratoire de Physique de la Matière Condensée et Nanomatériaux (LPMCN), Département de Physique, Faculté des Sciences Exactes et Informatique, Université Abdelhak Benhamouda de Jijel, Jijel, Algeria</i> ⁶<i>Faculty of Technology, Department of Technology, 20 Aout 1955 University, Skikda, Algeria</i> ZnO is an optically transparent II–VI oxide semiconductor used in solar cells (as conductive oxide), varistors, piezoelectric and optoacoustic sensors, UV diodes and lasers devices, thin-film transistors as well as data storage and gas sensors. On the other hand, ZnO doping with the elements of group III may be beneficial for modify and control optical, electrical and luminescence properties of material. In this paper, we were focused on indium-doped ZnO thin films deposited by spin-coating method. The morphology of ZnO:In layers were examined with AFM to investigate surface topography. The produced layers were also measured using spectroscopic ellipsometry to determine dielectric function and thickness of the layers. The thickness of the films were estimated at 200–300 nm. The room temperature photoluminescence (PL) of the fabricated layers doped with In at various atomic % was studied. PL measurement was carried out with a continuous laser excitation at 266 nm. The emission from the layers was collected by an optic fiber located close to the sample, dispersed by a spectrometer and detected by a liquid-nitrogen cooled Si CCD detector. The steady-state PL spectra of all layers has two distinct peaks with the excitonic one in UV range at around 380 nm and the other wide emission band in the visible range from blue to infrared.	
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STM and NC-AFM Investigations of Graphene on Ir(111)

V. Simić-Milosevic¹, Y. Dedkov², E. N. Voloshina³, A. Thissen¹¹SPECS Surface Nano Analysis GmbH, Berlin, Germany²Universität Konstanz, Konstanz, Germany³Humboldt-Universität zu Berlin, Institut für Chemie, Berlin, Germany

We present the systematic investigations of the geometry, electronic structure and their effects on the observed imaging contrast during STM and AFM experiments on graphene/Ir(111). Microscopy experiments were performed in constant current /constant frequency shift (CC/CFS) and constant height (CH) modes, exploiting a combination of the STM and NC-AFM capabilities of the SPM Aarhus 150 system. We found that in STM imaging the electronic contribution is prevailing compared to the topographic one and the inversion of the contrast can be assigned to the particular features in the electronic structure of graphene on Ir(111). Contrast changes observed in constant height AFM measurements are analyzed on the basis of the energy, force, and frequency shift curves, obtained in DFT calculations, reflecting the interaction of the W-tip with the surface and are attributed to the difference in the height and the different interaction strength for high-symmetry sites within the moiré unit cell of graphene on Ir(111).

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PROGRAM OVERVIEW	Molecular Self-Assembly of Porphyrin Layers at Metal/Metal-Electrolyte Interfaces B. Madry¹, K. Skorupski¹, K. Wandelt^{1,2}, M. Nowicki¹ ¹<i>Institute of Experimental Physics, University of Wrocław, Wrocław, Poland</i> ²<i>Institute of Physical and Theoretical Chemistry, University of Bonn, Bonn, Germany</i> The spontaneous self-assembly of organic molecules is a promising “bottom-up” approach in nanotechnology to create surface patterns and molecular electronic devices. Porphyrins, for example, are important organic compounds for potential applications as catalysts and sensors. In this work we have studied the selforganization of redox-active Tetra (N-methyl-1-pyridyl) porphyrin molecules (TMPyP) on over potentially deposited Cu layers on Au(111) surface in sulfuric acid solution using cyclic voltammetry (CV) and in situ scanning tunneling microscopy (STM) with submolecular resolution. This enables unprecedented insight into such self-assembly phenomena at solid-liquid interfaces in the presence of anions and organic molecules as a function of electrode potential. The Cu/Au(111) surface with coadsorbed sulfate was found to be a good substrate for the self-assembly of highly ordered layers of porphyrin cations. Furthermore Cu/Au(111) show several phase transitions of sulfate anions dependent on the thickness of Cu layer correlated with electrode potential [1–3]. Results of the investigations of TMPyP molecules on Cu/Au(111) show long-range periodic superstructures, which depend on the thickness of Cu layers. [1] B. Madry, K. Wandelt, M. Nowicki, <i>Surf. Sci.</i> 637–638 (2015) 77. [2] B. Madry, K. Wandelt, M. Nowicki, <i>Appl. Surf. Sci.</i> 388 (2016) 678. [3] B. Madry, K. Wandelt, M. Nowicki, <i>Electrochim. Acta</i> 217 (2016) 249.	
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The Process of Dissociative Adsorption of Bromine and Iodine on the Ge(001) Surface

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²*Nokia, Wrocław, Poland*

The process of dissociation of bromine and iodine 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 discussed process on molecule orientation with respect to the substrate is shown.

The atomic and electronic structure, including spatial distributions of electron density of the adsorbate/substrate system are presented. The results are compared with a similar process of dissociative adsorption of shorter halide molecules at the Ge(001)-p(1 × 2) surface [1, 2].

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

[2] B. Stankiewicz, P. Mikołajczyk, Appl. Surf. Sci. 384 (2016) 263.

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Surface is Alive		8 th INTERNATIONAL WORKSHOP ON SURFACE PHYSICS (IWSP-2017)	
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PROGRAM OVERVIEW		Formation of Silicene Nanostructures on Si(111)-√3×√3-Pb Surface A. Stępniaś-Dybala¹, M. Jałochowski, M. Krawiec Institute of Physics, Maria Curie-Skłodowska University, Lublin, Poland Recently silicene, a silicon counterpart of graphene, has attracted increasing attention due to its outstanding electronic properties. Therefore numerous experimental and theoretical studies have been devoted to fabrication of silicene, but still its synthesis remains a big challenge. So far silicene has been faricated with success, mostly in epitaxial process, e.g. on Ag(111) [1], Ir(111) [2] or on graphite [3]. Here we discuss the growth of Si nanostructures on the Si(111)-√3×√3-Pb surface [4]. Our combined scanning tunneling microscopy and density functional theory calculations reveal formation of silicene nanoribbons (SiNRs), directly bonded to the Si(111) substrate. Pb atoms dope SiNRs with electrons and stabilize the system. The proposed structural model features deformed honey-comb structure, and reproduce well the experimental data. This work has been supported by the National Science Centre (Poland) under Grant No. DEC-2014/15/B/ST5/04244. [1] P. Vogt et al., Phys. Rev. Lett. 108 (2012) 155501. [2] A. Fleurence et al., Phys. Rev. Lett. 108 (2012) 245501. [3] M. de Crescenti et al., ACS Nano 10 (2016) 11163. [4] A. Stępniaś-Dybala, M. Jałochowski, M. Krawiec, Condens. Matter 1 (2016) 8.	
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Bi Nanostructures on the Si(331) Surface**M. Stróżak, M. Dachniewicz, R. Zdyb***Institute of Physics, Maria Curie-Skłodowska University, Lublin, Poland*

One dimensional metallic structures prepared on vicinal silicon surfaces attracted considerable attention during last years because of diversity of novel phenomena and relative simplicity in their preparation. The most often studied nanostructures are prepared on the Si(557) and Si(553) surfaces [1–4]. Motivated by their reach physics we are looking for other one dimensional structures prepared on various highly anisotropic silicon surfaces.

In this contribution we investigate morphology and crystallographic structure of the Si(331) surface covered with Bi. Changes in the surface morphology and structure induced by the presence of Bi in the thickness range up to about 2 ML are studied with reflection high energy electron diffraction and scanning tunneling microscopy techniques. Depending on the Bi coverage and annealing temperature the surface develops either regular distribution of steps over macroscopic scale with one dimensional structures or forms additional facets like (553). Similar behavior has been observed for Bi-induced changes of the morphology of the Si(553) surface where regular distribution of steps or (331) facets have been found [5].

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

- [1] M. Kopciuszynski et al., Sci. Rep. 7 (2017) 46215.
- [2] C. Tegenkamp et al., Phys. Rev. Lett. 95 (2005) 176804.
- [3] C. Brand et al., Nature Comm. 6 (2015) 8118.
- [4] C. Tegenkamp et al., Phys. Rev. Lett. 109 (2012) 266401.
- [5] M. Kopciuszynski et al., Thin Solid Films 631 (2017) 80.

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	8th INTERNATIONAL WORKSHOP ON SURFACE PHYSICS (IWSP-2017)	
PROGRAM OVERVIEW	Abstracts: Poster Presentations	
INVITED LECTURES	Van der Waals Corrections Applied to Metallic Surfaces R. Topolnicki, R. Kucharczyk Surface Theory Group, Institute of Experimental Physics, University of Wrocław, Wrocław, Poland Long-range electron correlations, which are essential to characterize interactions in a number of relevant systems, such as organic and layered materials or molecules adsorbed on surfaces, are not included in GGA and hybrid functionals. Hence, incorporation of van der Waals (vdW) forces to DFT becomes a method of choice for many surface-science-related problems. Several encouraging approaches have been proposed to include both dispersive and repulsive long-range interactions in the standard DFT framework [1,2], however, there is no agreement on the reliability of particular methods. Moreover, most studies are focused solely on the proper description of adsorbate–substrate interactions. The influence of vdW corrections on the main characteristics of clean surfaces—such as surface energy, work function, structural relaxations and electronic structure of the topmost layers—is investigated in a systematic manner for a series of (100), (110) and (111)-oriented metallic substrates. The corresponding effect on bulk parameters [3] is also addressed. We focus on fcc and bcc transition and noble metals (V, Cu, Mo, Rh, Pd, Ag, W, Pt, Au), but some free-electron-like metals (Al and Ca) are examined for comparison. Several commonly used vdW corrections, including DFT-D2, DFT-D3, revPBE-vdW, optB86b, DF2 and family of DFT-TS methods, are employed. Results are contrasted with the corresponding PBE and LDA computations as well as available experimental data. Some statistical analysis is performed in order to demonstrate performance of various vdW-DFT approaches.	
ORAL PRESENTATIONS	[1] A. Tkatchenko et al., Phys. Rev. Lett. 108 (2012) 236402. [2] K. Berland et al., Rep. Prog. Phys. 78 (2015) 066501. [3] J. Park et al., Curr. Appl. Phys. 15 (2015) 885.	
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Abstracts: Poster Presentations

Unique Monodefects on Reconstructed Au(100) Surface

B. Pieczyrak, A. Trembulowicz, G. Antczak, L. Jurczyszyn*Institute of Experimental Physics, University of Wrocław, Wrocław, Poland*

We perform scanning tunneling microscope (STM) studies combined with density functional theory (DFT) calculations as implemented in the Vienna Ab-initio Simulation Package to unravel details of massive reconstruction of Au(100) [1]. The surface has a buckled quasi-hexagonal reconstructed top-most layer on a square, weakly reconstructed, second layer. The reconstruction can be described by a huge $c(28 \times 48)$ unit cell, which is a challenge for modeling. In our DFT study, we have modeled only short range arrangement described by the (5×20) unit cell. We probe how such complex surface changes due to the presence of surface monovacancies.

The surface monovacancies are imaged in the STM as monodepressions with the depth of around $0.4 \text{ \AA}$. That depth is smaller than one can expected for a regular surface monovacancy. To understand that we utilized DFT and explored the surface reaction to the creation of such defect at various characteristic sites of the surface. We found that the created defects are either spontaneously or with some energy cost healed by the upward shift of the subsurface atom into the vacant position.

[1] B. Pieczyrak et al., Appl. Surf. Sci. 407 (2017) 345.

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PROGRAM OVERVIEW	Formation and Study of Basic Physicochemical and Structural Properties of Au@SnO₂ Core-Shell Particles M. Trzcinski¹, Ł. Skowroński¹, R. Szczęsny² ¹<i>Institute of Mathematics and Physics, UTP University of Science and Technology, Bydgoszcz, Poland</i> ²<i>Faculty of Chemistry, Nicolaus Copernicus University in Toruń, Toruń, Poland</i> Gold particles and nanoparticles are good candidates for low temperature catalysts of CO oxidation. It has been shown that Au catalytic properties increase with the decrease of its particle size and is much higher as compared with that of bulk. Recently so-called core-shell structures based on gold particles became the subject of intensive research due to the improvement of catalytic behaviour, since the interface around the gold particles can modify significantly their chemical properties. In present contribution we investigate the process of fabrication of Au@SnO₂ core-shell particles on Si(100) substrate. The structure of the samples have been characterized by Powder X-Ray Diffraction (XRD), the chemical state have been analysed by means of X-Ray Photoelectron Spectroscopy (XPS) and Raman Spectroscopy. The topography of samples have been studied by Confocal Optical Microscopy (COM) and Scanning Electron Microscopy (SEM). The Au-Sn intermetallic compound is formed directly during the deposition of gold and tin thin films. After pre-heating process the presence of Au-Sn small islands and particles is observed. The oxidation causes the formation of SnO₂ shells around the gold particles. The influence of the deposition process and oxidation conditions on the shape and size of synthesized particles have been studied as well as their physicochemical properties.	
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Growth of Perfluoro-Pentacene on Ag(110) Studied with PEEM and DRS

Th. Wagner, E. Ghanbari, A. Navarro-Quezada, P. Zeppenfeld

Institute of Experimental Physics, Johannes Kepler University Linz, Austria

Ultrathin films of organic molecules on metal surfaces usually exhibit quite different physical behavior compared to their bulk counterparts. Upon deposition of the first layer, a surface dipole is formed, which leads to a change of the work function. On the other hand, the optical transitions of the molecules are modified due to hybridization with the electronic states of the surface. The influence of the substrate will decrease with increasing layer thickness until, eventually, the bulk properties of the organic material are reached.

We have studied the evolution of ultrathin films of perfluoro-pentacene on Ag(110) by means of photoelectron emission microscopy (PEEM) and differential (optical) reflectance spectroscopy (DRS). PEEM and DRS yield complementary information on the surface morphology, the electronic and the optical properties during the thermal deposition of the organic material in an ultrahigh vacuum system [1]. The setup allows recording PEEM images and DRS spectra simultaneously, providing the unique opportunity to correlate the morphology and electronic structure (PEEM) with the associated optical response (DRS). We will demonstrate how linearly polarized light can be used in PEEM to differentiate between changes of the work function and effects related to the density of electronic states and their particular symmetry. In parallel, the reflectance of linearly polarized light in the DRS experiments can be used to follow the evolution of the optical anisotropy of the organic thin film.

[1] A. Navarro-Quezada et al., Rev. Sci. Instr. 86 (2015) 113108.

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	8 th INTERNATIONAL WORKSHOP ON SURFACE PHYSICS (IWSP-2017)	
	Abstracts: Poster Presentations	
PROGRAM OVERVIEW	Effect of Annealing on the Properties of ZnO:Al Films Prepared by RF Magnetron Sputtering A. Zdyb, E. Krawczak, S. Gułkowski <i>Faculty of Environmental Engineering, Lublin University of Technology, Lublin, Poland</i> Numerous studies have been devoted to deposition as well as characterization of transparent conductive oxides (TCOs) due to their unique optical and electronic properties combination that makes them useful in wide application area. Among many oxides that are good candidates to substitute ITO, Al doped ZnO is considered as viable alternative because it is non-toxic and non-expensive material [1–3].	
INVITED LECTURES	In this contribution we present research on structural, electrical and optical properties of ZnO:Al layers obtained in RF magnetron sputtering system, in which varying of deposition parameters allows to improve the quality of the films. We focused on the optimization of cathode power, pressure in the chamber and flow rate of Ar as a process gas during the grow of layers on glass substrates in RT. Different methods such as XRD, SEM, UV-VIS spectrophotometry and four point probe resistance measurements were applied to characterize the obtained films. Post-annealing treatment in the temperature ranging from 100 °C to 500 °C leads to the increase of crystallite size, better conductivity and improvement of transparency. [1] M. Saad, A. Kassis, Mat. Chem. Phys. 136 (2012) 205. [2] S. Rahmane et al., Superlattices Microstruct. 79 (2015) 148. [3] P. Prepelita et al., Appl. Surf. Sci. 352 (2015) 23.	
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Exploring from Ab Initio Calculations the Structural and Electronic Properties of Supported Metal Linear Atomic Chains on the NiAl (1 10) Surface

B.F. Zornio¹, E.Z. da Silva², M.A. San-Miguel¹

¹*Institute of Chemistry, University of Campinas, Campinas, Brazil*

²*Institute of Physics "Gleb Wataghin", University of Campinas, Campinas, Brazil*

First principles calculations based on periodic DFT have been carried out to gain insight into the structural, energetic and electronic structure of linear atomic chains grown on the NiAl (1 10) surface. A large (5 × 3) supercell was built (more representative model than a previous one [1,2]) allowing allocation of 3 or 5 atoms along the three different surface directions.

STM simulated images demonstrate that a real LAC is formed only along the [001] direction. The decomposition of the binding energy into metal-metal and metal-surface contributions was useful to verify that the interaction between the adatoms is negligible for the 3 atoms models, being quite significant for the 5 atoms model.

The analysis of the PDOS and electron charge differences indicate that the chemical bonding between the LAC and the substrate is mainly covalent for group 10 metals involving strong d orbital coupling between the LAC atoms and surface Ni atoms, meanwhile for group 11 metals the ionic interaction with surface Al atoms is more significant, except for Cu, which shows an intermediate behavior. On the other hand, the interaction between metals within the LAC is mainly contributed by d orbital coupling.

Pt LACs show an intriguing behavior with respect to the other transition metals. This fact might involve singular conductance properties in the fabrication of LACs as wires in nanodevices.

[1] M.A. San-Miguel, E.P.M. Amorim, E.Z. da Silva J. Phys. Chem. C 119 (2015) 2456.

[2] M.A. San-Miguel, E.P.M. Amorim, E.Z. da Silva J. Phys. Chem. A 118 (2013) 5748.

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 The logo consists of a green circle with the text "Surface is Alive" inside, set against a background of a hexagonal molecular lattice.	8 th INTERNATIONAL WORKSHOP ON SURFACE PHYSICS (IWSP-2017)	
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 The logo consists of a green circle with the text "Surface is Alive" inside, set against a background of a hexagonal molecular lattice pattern.	8 th INTERNATIONAL WORKSHOP ON SURFACE PHYSICS (IWSP-2017)	
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Notes

Monday, 26 June 2017	
16:00	Bus to Trzebnica
16:00	Registration
18:00	Supper
20:00	Get-together

Tuesday, 27 June 2017	
7:30	Breakfast
8:45	Workshop Opening
9:00	Orte 7
9:50	Ślusarski 34
10:15	Morbec 26
10:40	Coffee Break
11:15	Schröder 8
12:05	Wachowicz 36
13:00	Lunch
14:30	Evans 3
15:20	Palotás 30
15:45	Coffee Break
16:20	Pabisiaak 25
16:45	Ossowski 29
18:00	Supper
19:00	Poster Session

Wednesday, 28 June 2017	
7:30	Breakfast
9:00	Hengsberger 5
9:50	Ciesielski 15
10:15	Skowroński 33
10:40	Coffee Break
11:15	Kucharczyk 6
12:05	Jurczyszyn 18
13:00	Lunch
14:30	Zdyb 12
15:20	Kopciuszynski 21
15:45	Coffee Break
16:20	Morawski
16:45	Jacobs
19:00	

Thursday, 29 June 2017	
7:30	Breakfast
9:00	Tringides 10
9:50	Jalochowski 17
10:15	Brona 14
10:40	Coffee Break
11:15	Suchorski 9
12:05	Krasovskii 22
13:00	Lunch
14:30	Wagner 11
15:20	Kahng 19
15:45	Coffee Break
16:20	Krawiec 23
16:45	Podsiadły-Paszowska31
18:30	Barbeque Supper

Friday, 30 June 2017	
7:30	Breakfast
9:00	Gottfried 4
9:50	Sabik 32
10:15	Szabelski 35
10:40	Coffee Break
11:15	Kocán 20
11:40	Matvija 24
12:05	Nowicki 27
13:00	Lunch
14:00	Bus to Wrocław