9th International Workshop on Surface Physics

organized by

Institute of Experimental Physics University of Wrocław



Uniwersytet Wrocławski

24 – 28 June 2019 Trzebnica, Poland

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ii



TECHNIKA PRÓŻNIOWA



IWSP-2019

M			Program Overview	
Program Overvie			MONDAY, 24 JUNE	
Invited Lectures				
Oral Presentations				
ons	16:00		Bus to Trzebnica	
	17:00		Registration	
	18:00		Supper	
Poster Pr	20:00		Get together	
	iv	• •	• • • • •	• •

	🔹 🕻 🚺 🔹 Program Overview 🔮 化 📢	
	TUESDAY, 25 JUNE	
7.30	Breakfast	
9.1E	Workshop Oppning	
9:00	Francess M. Ross PATTERNING NANOSTRUCTURES ON 2D MATERIALS VIA IN SITU TEM GROWTH EXPERIMENTS	12
9:50 10:15	Adam Busiakiewicz TiO ₂ : FROM REVERSIBLE SEGREGATION OF TRANSITION METAL NANOSTRUCTURES FOR PHOTOCATALYSIS TO MODIFICATION OF GRAPHENE FOR OLED TECHNOLOGY Marcin Pisarek APPLICATION OF IN-SITU XPS SPECTROSCOPY FOR ANALYSIS THE CHEMISTRY OF PLASMA NITRIDED TiO ₂ NANOTUBES	■19 ■33
10:40	Coffee Break	
11:15	Takashi Kumagai 🖙 PLASMON-INDUCED PHOTOPHYSICS AND PHOTOCHEMISTRY IN NANOCAVITY	≣7
12:05 12:30	Mikołaj Lewandowski 🖙 TUNING THE STRUCTURE OF ULTRATHIN FEO ISLANDS ON Ru(0001) B OXIDATION/REDUCTION Ying Wang 🖙 ON THE STRUCTURE OF ULTRATHIN FEO FILMS ON Ag(111)	■25 SY ■38
13:00	Lunch	
L4:30	Gareth Parkinson C "SINGLE ATOM" CATALYSIS: AN ATOMIC-SCALE VIEW	∎10
15:20	Nika Spiridis ☞ REDUCTION OF Fe ₃ O ₄ FILMS ON Pt(111) - SURFACE STRUCTURE VS. COMPOSITION	35
15:45	Coffee Break	
16:20	Nian Lin METAL-ORGANIC π-CONJUGATED COORDINATION FRAMEWORKS SYNTHESIZED ON SURFACE	8
17:10	Anna Mandziak S STRUCTURAL AND MAGNETIC PROPERTIES OF TRANSITION METAL O	≣26 KIDE
	THIN FILMS GROWN ON Ru(0001)	
18:00	THIN FILMS GROWN ON Ru(0001) Supper	

	• • • • Program Overview • • •
	WEDNESDAY, 26 JUNE
7:30	Breakfast
9:00	Alessandro Fortunelli C COMPUTATIONAL MODELING OF NANOSTRUCTURED METAL SURFACES AND THEIR ELECTRONIC AND CATALYTIC PROPERTIES
9:50 10:15	Leszek Jurczyszyn 🖙 🛛 🗍 MODIFICATION OF THE RELATIVISTIC SURFACE BAND STRUCTURE OF TI/Si(111) SYSTEM BY ADSORPTION OF O AND CI Tomasz Ossowski 🕼
	DFT STUDY ON THE STRUCTURE OF ULTRATHIN FEO FILMS ON Ru(0001)
10:40	Coffee Break
11:15	Talat S. Rahman IP Image: Comparison of the second state of
12:05 12:30	Elwira Wachowicz C HYDROGEN INFLUENCE ON SURFACE MORPHOLOGY OF 4H-SiC{0001} SURFACES Damian Nieckarz C S 2D SELF-ASSEMBLED NANOMATERIALS – COMPUTER SIMULATIONS AND EXPERIMENT
13:00	Lunch
14:30	Christian Tusche C NONLOCAL ELECTRON CORRELATIONS IN AN ITINERANT FERROMAGNE MAPPED BY SPIN-RESOLVED MOMENTUM MICROSCOPY
15:20	Jacek Kołodziej 🕼 🗐 🗐 🗐 ELECTRONIC STRUCTURE AND STM IMAGING OF THE KBr/InSb INTERFA
15:45	Coffee break
16:20	Martin Sterrer © I CONTROL OF CHARGE TRANSFER INTO ORGANIC MOLECULES ON ULTRATHIN MgO(001) FILMS
17:10 17:35	Szymon Godlewski 🖙 E HIGHER ACENES GENERATED BY ON-SURFACE DEHYDROGENATION Tomasz Rerek 🖙 E FORMATION AND OPTICAL PROPERTIES OF THIN TIN AND GOLD FILMS PRODUCED BY PVD METHOD
19:00	Workshop dinner

	🔹 🕻 🚺 🔹 Program Overview 🔮 🌒 🔹	
	THURSDAY, 27 JUNE	
7:30	Breakfast	
9:00	Moritz Sokolowski 🖙 ORGANIC MOLECULES OBSERVED ON SURFACES BY FLUORESCENE SPECTROSCOPY	13
9:50 10:15	Christine Brülke C INVESTIGATION OF THE VERTICAL STRUCTURE OF hBN ON Cu(111) VI. NIXSW AND SPA-LEED Krisztian Palotás C HEXAGONAL BORON NITRIDE NANOMESH STRUCTURE TUNED BY GO RHODIUM SURFACE ALLOY	■18 A ■32 LD-
10:40	Coffee break	
11:15	Mieczysław Jałochowski 🖙 ANTIMONENE ELECTRON BAND STRUCTURE ENGINEERING	≣6
12:05 12:30	Lucyna Żurawek 🖙 Pb NANOCHAINS ON THE Si(113) SURFACE Shiva L. Udachan 🖙 IMPACT OF SUBSTRATE TEMPERATURE ON OPTICAL CONSTANS OF CHROMIUM NANO-FILMS	≣ 39 ≣ 36
13:00	Lunch	
14:30	Olaf Magnussen 🕼 ADSORBATE DYNAMICS AT ELECTROCHEMICAL INTERFACES	
15:20	Bartosz Mądry S MOLECULAR SELF-ASSEMBLY OF PORPHYRINS ON Au(111) PRECOVER BY COPPER AND SULPHATE	≣27 ED
15:45	Coffee break	
16:20	Peter Broekmann © POWER-TO-VALUE: NOVEL CATALYSTS FOR THE ELECTROCHEMICAL CONVERSION OF CO ₂	≣3
17:10 17:35	Andrzej Miszczuk © PROPERTIES OF ULTRATHIN Pt LAYERS ON Cu(111) REVEALED BY AES, LEED AND DEPES Rafał Lewandków © THERMALLY INDUCED REACTIONS BETWEEN A GaN(0001) SUBSTRATI AND HAFNIUM LAYER	≣28 ≣24 Ξ
19:00	Barbeque supper	
	• • • • • • • • •	vii

	CONTRACTOR OVERVIEW
	FRIDAY, 28 JUNE
7:30	Breakfast
9:00	Gold (100) SURFACE: RECONSTRUCTION, DEFECTS AND SURFACE DIFFUSION
9:50	Karolina Idczak ☞ ■2 PHYSICOCHEMICAL PROPERTIES OF THIN Gd FILMS ON 4H- SiC(0001)—GRAPHENE
10:15	Pb INTERCALATION OF GRAPHENE ON Ru(0001) – AES, LEED AND DEPES STUDY
10:40	Coffee break
13:00	Lunch
14.00	Bus to Wrocław

•

•

viii

	🕐 🕻 🌔 Program Overview 🥤 🌓 🔍	
	POSTER SESSION OVERVIEW	
P-01	Abhijit Bera 🕼 FORMATION OF SODIUM BROMIDE LAYERS ON Ag(111) TO CHARACTERIZE CARBENE MOLECULES	≣42
9-02	Łukasz Bodek ☞ MICROSCOPIC VIEW OF TIN PHTHALOCYANINE ADSORPTION ON TH RUTILE TIO2 (011) SURFACE	≣43 E
9-03	Robert Bryl © OXYGEN ADSORPTION, SUBSURFACE OXYGEN LAYER FORMATION A REACTION WITH HYDROGEN AND CARBON OXIDE ON SURFACES OF Rh ALLOY NANOSIZED CRYSTAL	≣44 ND A Pt-
P-04	Grażyna Balcerowska-Czerniak INVESTIGATION OF INTERFACE FORMATION OF INDIUM ON AN ORO THIN FILMS DEPOSITED ON DIFFERENT SUBSTRATES USING PHOTOELECTRON SPECTROSCOPY COMBINED WITH CHEMOMETRIC METHODOLOGY	■45 GANIC
P-05	Marek Dachniewicz 🖙 STRUCTURAL AND ELECTRONIC PROPERTIES OF Sb ATOMIC CHAINS Si(553) WITH Pb NANORIBBONS	≣46 ON
P-06	Adam Dittmar-Wituski ☞ In/Alq₃/HOPG STUDIED BY UPS AND XPS	≣47
9-07	Pavlo V. Galiy ☞ USE OF NANOSTRUCTURED In₄Se₃ CRYSTAL (100) SURFACE AS A TEMPLATE FOR OBTAINING AN ARRAY OF NANOWIRES	≣48
9-08	Niklas Humberg 🕼 ONE-DIMENSIONAL MOLECULAR CHAINS OF QUINACRIDONE ON Ag STM AND SPA-LEED INVESTIGATIONS	≣49 g(100):
P-09	Wojciech Kamiński 🕼 THE MOLECULAR SWITCH ON METALLIC SURFACE	≣50
P-10	Marek Kopciuszyński 🖙 SILICENE ON ULTRATHIN GOLD LAYERS	≣51
2-11	Krzysztof Kopyściński 🕼 INVESTIGATION OF Pt AND Mn THIN FILMS ON Si(111) SURFACE	≣52

• • • • Program Overview

P-12	Serhii Kovalchuk C SURFACE TERMINATION REVEALED BY DIRECTIONAL ELASTIC PEAK ELECTRON SPECTROSCOPY	≣53
P-13	Monika Krawczyk 🕼 UNUSUAL STRUCTURAL PHASE TRANSITIONS IN THE CRYSTAL OF {[N2H5]3CdCl5}n	≣54
P-14	Karolina Kruk © APPLICATION OF THE MULTIPLE SCATTERING FORMALISM TO THE QUANTITATIVE ANALYSIS OF DEPES RESULTS FOR Ru(0001) AND Pt(1	≣55 11)
P-15	Marcin Kurzyna 🕼 DYNAMIC PROPERTIES OF TOPOLOGICAL ATOMIC CHAINS	≣56
P-16	Katarzyna Lament 🕼 EC-STM AND CV INVESTIGATIONS OF Au(110) IN ACID SOLUTIONS	≣57
P-17	Anna Mandziak C A NEW CUSTOM-MADE SAMPLE HOLDER FOR HIGH-TEMPERATURE A IN SITU APPLICATION OF MAGNETIC FIELDS IN A PHOTOEMISSION ELECTRON MICROSCOPE	≣58 AND
P-18	Katarzyna Pabianek © TITANIUM AND ITS OXIDES ON SELECTED SURFACES: SILICON(100), GRAPHITE(0001) AND GRAPHENE/4H-SIC(0001) FOR APPLICATIONS II OLED TECHNOLOGY	≣59 ∖
P-19	Marcin Pisarek 🕼 SURFACE CHARACTERIZATION OF THIN MoS2 FLAKES ON SI SUBSTRATES	≣60
P-20	Agnieszka Puchalska ☞ ELECTRONICS OF Ba ADSORBED ON Ge(001)	■61
P-24	Agata Sabik 🕼 THE Au(100) SURFACE AS A TEMPLATE FOR PENTACENE ADSORPTION	≣62 ∖
P-21	Kamil Skorupski 🖙 EC-STM AND CV INVESTIGATIONS OF Au(111) IN SULPHURIC ACID SOLUTION	■63
P-22	Łukasz Skowroński © MICROSTRUCTURE AND OPTICAL PROPERTIES OF THIN COPPER FILM PRODUCED BY THE PVD METHOD	≣64 S
x		

	🕐 🌔 🌔 Program Overview 🔰 🌓 🔍	
P-23	Piotr Staniorowski © SURFACE CHARACTERISATION BY THE X-RAY PHOTOELECTRON SPECTROSCOPY COMBINED WITH THE DIELECTRIC AND SPECIFIC HE STUDY IN DMAGAS CRYSTAL	≣65 AT
P-25	Artur Trembułowicz 🕼 MOLECULAR INSTABILITY OF CoPc IN ORDERED LAYER ON Ag(100) DURING STM MEASUREMENTS	
P-26	Marek Trzciński 🕼 STRUCTURE SENSITIVITY OF THE INITIAL OXIDATION OF RHODIUM: AND PEEM STUDIES	≣67 XPS
P-27	Ying Wang ☞ DETERMINING THE WORK FUNCTION OF ULTRATHIN FeO(111) FILM Ag(111)	≣68 IS ON
»-28	Marcin Wiejak THE GROWTH OF MANGANESE SULFIDE THIN FILM ON Ru(0001)	≣69



IWSP-2019





Invited Lectures

GOLD (100) SURFACE: RECONSTRUCTION, DEFECTS AND SURFACE DIFFUSION

A. Trembułowicz, B. Pieczyrak, L. Jurczyszyn, G. Antczak

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

The modifications of the surface due to e.g. ion bombardment has been widely studied due to technological importance. Stage of the surface (e.g. roughness, corrugation or presence of step benches) influences the adsorbatesurface interaction what can alter the performance of the electronic devices. Using scanning tunneling microscopy and density functional theory we explored structure developed after ion bombardment on quasi-hexagonal Au(100) surface. Coexistence of hex structure of quantized width in accord with (6n+1) formula, with (1×1) arrangement of atoms is observed. We show that both structures are part of the same topmost layer. The changes in relative proportions and shapes of phases as well as the arrangement of atoms within nano-wire-like structures will be discussed [1]. When the flux of incoming ions is small we are able to create the monovacancy-like defects on the surface [2]. Additionally, based on the nucleation's theory, we explored surface diffusion on gold quasi-hexagonal surface. We show that surface reconstruction induces preferential direction for surface diffusion. The characteristic parameters of surface diffusion will be presented [3].

[1] A. Trembułowicz et al., Nanotechnology **30** (2019) 045704.

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

[3] A. Trembulowicz, G. Ehrlich, G. Antczak, Phys. Rev. B 84 (2011) 245445.



Invited Lectures

POWER-TO-VALUE: NOVEL CATALYSTS FOR THE ELECTROCHEMICAL CONVERSION OF CO₂

A. Dutta¹, M. Rahaman¹, C. Morstein¹, Y. Hou¹, A. Cedeño Lopez¹,
P. Moreno¹, K. Kiran¹, V. Grozovski¹, N. Kovacs^{1,2}, S. Vesztergom^{1,2},
<u>P. Broekmann¹</u>

¹ Department of Chemistry and Biochemistry, University of Bern, Bern, Switzerland ² Department of Physical Chemistry, Eötvös Loránd University, Budapest, Hungary

The electrochemical conversion of CO_2 (denoted as CO_2RR) has attained significant interest in the catalysis research worldwide over the recent years as it provides means of transforming an environmentally harmful molecule back into products of higher value (e.g. high energy density fuels, chemical feedstock and useful commodity chemicals such as carbon monoxide). This process becomes particularly sustainable when using the surplus of electric power produced from renewable hydro, wind or solar sources (power-tovalue concept). Substantial progresses have already been made during the last decade in the tailored design of novel catalyst materials needed to increase the energy efficiency of the CO₂/water co-electrolysis and to guide the product distribution reaction into the desired direction. These progresses remained, however, restricted to the fundamental research whereas no technologically and economically feasible process could be established on an industrial scale so far. One key challenge left is related to the particular stability of the catalyst materials, a crucial pre-requisite for any industrial application of catalytic processes.

In this contribution, various concepts for the design of CO₂RR catalysts will be discussed that are based either on colloidal synthesis of nano-materials (shape- and size-selective particles, nanowires etc.) or on the additiveassisted electroplating of high-surface area metal foams. Main target products of the CO₂RR discussed herein are syngas (CO/H₂) as valuable chemical feedstock for a subsequent non-electrochemical conversion process (Fischer-Tropsch, Rheticus process/Siemens-Evonik) and high energy density fuels (e.g. ethanol, propanol). Advanced operando techniques utilizing synchrotron facilities (x-ray absorption spectroscopy, and x-ray diffraction) will be demonstrated to be useful for the identification of active catalyst species under electrolysis conditions.



Program Uverview

Invited Lectures

COMPUTATIONAL MODELING OF NANOSTRUCTURED METAL SURFACES AND THEIR ELECTRONIC AND CATALYTIC PROPERTIES

A. Fortunelli^{1,3}, L. Sementa¹, F. R. Negreiros², W. A. Goddard³, Q. An^{3,4}

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² Universidad Nacional de Córdoba, Córdoba, Argentina

³ California Institute of Technology, Pasadena, CA, USA

⁴ University of Nevada-Reno, Reno, NV, USA

I will present results of our work in two different topics in computational catalysis, whose underlying theme lies in the possibility of creating catalysts with rationally designed nanoscale surface features.

The former direction deals with nanoporous platinum structures obtained by electrochemical leaching Ni-Pt alloy and their extraordinary activity in the oxygen reduction reaction (ORR). We focus on nanoparticle and nanowires and show how it is possible to achieve insight into the relationships between nanoscale atomistic surface features and ORR performance via first-principles-based theory and simulations [1-3]. Enhanced ORR activity by a factor of 50 with respect to commercial platinum catalysts are achieved in the nanowire case. Comparison/validation with experiment is further pursued via operando vibrational frequencies and XPS shifts at the electrode-electrolyte interface (EEI).

Second, I will switch to regular metal nanoparticle catalysts. I will report an extensive study of ammonia synthesis via the Haber-Bosch (HB) process over Fe bcc(111) and bcc(211). Our computational protocol combines Density-Functional Theory plus dispersion to unveil the mechanistic steps at the atomic level with kinetic Monte Carlo (kMC) modeling to predict steady-state catalytic reaction rates under realistic conditions, thus allowing us to validate our predictions against experimental kinetic data from classic surface science literature [4]. We then use the detailed knowledge derived for this system to consider modifications of the catalyst such as alloying the first few surface layers. In order to span the largest possible set of catalyst modifications simultaneously minimizing computational effort, we derive a Hierarchical High-Throughput Screening (HHTS) approach to catalyst design. The HHTS approach singles out the most promising alloying elements and configurations as a function of catalyst structure and alloying site. In the case of HB over top-layer substitutional 0.25 ML alloyed Fe-bcc(111), HHTS indicates Rh as the most promising dopant. The approach is validated by reconstructing the complete free-energy diagram for the Rh-doped system, conducting a full kinetic analysis, and comparing the results from those



estimated on the basis of HHTS, finding very good agreement [5]. Other doping sites and strategies are discussed, enabling catalytic activity enhanced by up to 2 orders of magnitude with respect to the pure Fe case. This represents a new strategy that can be used to optimize catalyst performance for complex reactions involving 10 to 20 potential rate determining steps, where the simple Sabatier-principle-based volcano relationships in terms of a single controlling parameter no longer apply.

[1] A. Fortunelli, W. A. Goddard et al., Chem. Sci. 6 (2015) 3915-3925.

[2] M. Li et al., Science **354** (2016) 1414-1419.

[3] T. Cheng, A. Fortunelli, W. A. Goddard, PNAS (2019) 201821709.

[4] J. Qian et al., J. Am. Chem. Soc. 140 (2018) 6288-6297.

[5] Q. An et al., J. Am. Chem. Soc. 140 (2018) 17702-17710.

Invited Lectures

Invited Lectures

ANTIMONENE ELECTRON BAND STRUCTURE ENGINEERING

M. Jałochowski, M. Krawiec

Institute of Physics, Maria Curie-Skłodowska University, Lublin, Poland

Whereas bulk antimony is a semimetal with topological states screened by valence bands, the antimonene is ultimately thin, novel graphene-like buckled honeycomb-lattice two-dimensional material with trivial states. According to density functional theory (DFT) calculations Sb(111) film upon reduction of its thickness opens a gap and becomes a topological insulator, then converts into quantum spin Hall phase and finally becomes an ordinary semiconductor. Several theoretical studies attempted to find a method to tune the gap while preserving the topological states by applying stress, or by atomic adsorption. It is obvious, that also interaction with certain type of substrate can modify electronic structure of antimonene. In this study we propose a new method of engineering of antimonene electronic band structure by means of quantum size effect (QSE) of the substrate. Two-dimensional sheets of hexagonal (β form) antimonene have been epitaxially prepared on Pb(111) ultrathin films grown on $Si(111)(6\times 6)Au$. Scanning tunneling microscopy and spectroscopy of atimonene-covered Pb surface were analyzed within ab-initio density functional theory predictions. We found that the quantum states extend far away from the Pb surface, penetrate the antimonene and generate electronic states within adlayer energy gap. This result points to new purely electronic method of engineering electronic band structure of antimonene. The presented work reports on first experimental realization of β - antimonene on metallic ultrathin films.

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

 Invited Lectures

PLASMON-INDUCED PHOTOPHYSICS AND PHOTOCHEMISTRY IN NANOCAVITY

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Nanostructures made of coinage metals strongly interact with visible light through excitation of localized surface plasmon resonance, enabling efficient light-harvesting and concentrating light on the nanoscale. Plasmonic nanocavities are of particular interest due to the capability of extreme confinement and enhancement of electromagnetic fields, which can largely promote near-field-driven processes by optical excitation. However, the direct observation of local field enhancement and near-field-driven processes in plasmonic nanocavities remains a significant experimental challenge. I will talk about our recent progress on the direct observation of plasmon-induced photophysics and photochemistry in nanocavities using low-temperature photon scannig tunneling microscopy. First topic is plasmon-assisted resonant electron tunneling in the STM junction consisting of the Ag/Au tip and the Ag(111) surface [1]. Second topic is the direct observation of plasmonic photochemical reactions at the single-molecule level [2]. I will also discuss our latest results of vibrational "nano" spectroscopy using tipenhanced Raman spectroscopy.

S. Liu, M. Wolf, T. Kumagai, Phys. Rev. Lett. **121** (2018) 226802.
 H. Böckmann et al., Nano Lett. **18** (2018) 152.

Invited Lectures

METAL-ORGANIC π -CONJUGATED COORDINATION FRAMEWORKS SYNTHESIZED ON SURFACE

<u>N. Lin</u>

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

Recently, two-dimensional metal-organic frameworks with π -conjugated backbone (2D- π MOFs) have been proposed to exhibit interesting electronic and magnetic properties, including metallic, semi-metallic, topological insulating, quantum anomalous Hall, and even superconducting. In this presentation, I will discuss our efforts of employing on-surface coordination self-assembly to fabricate monolayer of 2D- π MOFs stabilized by dihydroxy and diimine ligands coordinated with Ni, Fe or Cu. Since such coordination provides effective pi-conjugation, the 2D- π MOFs feature strongly dispersive electronic bands. We investigate the electronic and magnetic properties of the 2D- π MOFs using low-temperature scanning tunneling spectroscopy and density-functional theory calculations.

 Invited Lectures

ADSORBATE DYNAMICS AT ELECTROCHEMICAL INTERFACES

O. M. Magnussen

Institute of Experimental and Applied Physics, Kiel University, Kiel, Germany

Electrochemical interfaces are the key to many current and emerging technologies, for example in energy storage or micro/nanofabrication. All of these applications involve atomic-scale processes on the electrode surface, such as the surface diffusion and mutual interactions of the atomic and molecular species, participating in the reactions. However, in contrast to adsorbate dynamics at solid surfaces under vacuum conditions, understanding of the surface dynamics at these complex interfaces is still rudimentary. Many aspects of the elementary dynamic events at electrochemical interface are unclear, for example: How is the motion of atoms across the surface affected by the presence of the electrolyte, in particular by coadsorbed species? Which role does the strong electric field at electro-chemical interfaces play? What kinds of interactions between adsorbed species on the electrode surface exist, how strong are they, and what is their distance dependence?

A direct and powerful way to clarify such phenomena are direct observations of the atomic motion at the interface, provided the employed technique has a sufficient high spatial and temporal resolution for such studies. In the talk, I will discuss in situ studies of surface transport at electrochemical interfaces by high-speed scanning tunneling microscopy (Video-STM), which allows direct observations of the atomic-scale dynamics. By detailed statistical analysis, quantitative data on the diffusion barriers and interaction energies is obtained from these video data, providing insight into the role of the electrode potential and coadsorbed species. As examples, I will discuss the diffusion of isolated anionic, cationic, and organic adsorbates on noble metal electrodes as well as the interactions between identical and different adsorbate species. These studies reveal a very strong dependence of the tracer diffusion of these adsorbates on the electrode potential, leading to changes in mobility over several orders of magnitude. Furthermore, coadsorbed anions can have a huge influence, leading to fundamentally different behavior even in systems, in which the adsorbate layers have identical structure.

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Invited Lectures

"SINGLE ATOM" CATALYSIS: AN ATOMIC-SCALE VIEW

G. S. Parkinson

Institute of Applied Physics, TU Wien, Vienna, Austria

The field of "single-atom" catalysis (SAC) [1-2] emerged as the ultimate limit of attempts to minimise the amount of precious metal used in heterogeneous catalysis. Over time, it has become clear that metal adatoms behave differently to supported nanoparticles [3-4], primarily because they form chemical bonds with the support and become charged. In this sense, SAC systems resemble the mononuclear coordination complexes used in homogeneous catalysis, and there is much excitement that SAC could achieve similar levels of selectivity, and even heterogenize problematic reactions currently performed in solution. It is important to note, however, that homogeneous catalysts are designed for purpose based on well-understood structure-function relationships, but the complexity of real SAC systems means that the structure of the active site is difficult to determine, never mind design. In this talk, I will describe how we are using $Fe_3O_4(001)$ as a precisely-defined model support [5] to unravel the fundamentals of SAC. I will show scanning probe microscopy, x-ray photoelectron spectroscopy (XPS) and temperature programmed desorption (TPD) data to show how the local structure of Ir₁/Fe₃O₄(001) and Rh₁/Fe₃O₄(001) single atom catalysts changes based on preparation and adsorption of reactants, and that CO oxidation activity in the Pt₁/Fe₃O₄(001) system results from Pt₂ dimers, not single atoms.

[1] B. Qiao et al., Nature Chemistry 3 (2011) 634-41.

[2] J. Liu, ACS Catalysis 7 (2016) 34-59.

[3] B.C. Gates et al., Catalysis Science & Technology 7 (2017) 4259-4275.

[4] G.S. Parkinson, Catalysis Letters 149 (2019) 1137-1146.

[5] R. Bliem et al., Science 346 (2014) 1215-8.

Invited Lectures

TUNING PROPERTIES OF 2D MATERIALS: FROM CATALYTIC ACTIVITY TO SINGLE PHOTON EMISSION

T. S. Rahman

Department of Physics, University of Central Florida, Orlando, USA

Single-layer of molvbdenum disulfide (MoS₂) and other transition metal dichalcogenides (TMDC) appear to be promising materials for next generation optoelectronic applications, because of their low-dimensionality and intrinsic direct band-gap which typically lies in the visible spectrum. MoS₂ is also known to be a leading hydrodesulphurization catalyst, for reasons that remain elusive. Another 2D material displaying novel chemical and optical properties is good old hexagonal boron nitride (h-BN). Efforts are underway to further tune these properties through alloying, defects, doping, coupling to a substrate, and formation of bilayer stacks (homo- and hetero-structures). In this talk, I will present some results which provide a framework for manipulating the functionality of these interesting van der Waals materials. With regard to optical properties, I will present our analysis of the quasiparticle energetics (excitons, trions, etc.) and ultrafast charge dynamics in both single- and bi-layer TMDCs obtained through the application of combined time-dependent density functional theory and manybody theory. With emphasis on chemical properties of defect-laden single layer MoS₂ and h-BN. I will examine modulations the local atomic environment under which these inert materials could serve as a catalyst for several technologically important reactions.

Invited Lectures

PATTERNING NANOSTRUCTURES ON 2D MATERIALS VIA IN SITU TEM GROWTH EXPERIMENTS

F. M. Ross

Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts, USA

Building functional nanostructures with atomic level precision requires a detailed understanding of self-assembly and crystal growth at the nanoscale. *In situ* imaging in the transmission electron microscope (TEM) can provide unique information about crystal growth by measuring individual nanostructures while they grow. Here we will describe the use of *in situ* TEM to explore growth mechanisms and suggest strategies to build new types of structure. We will focus on the epitaxial growth of 3D nanocrystal arrays on 2D materials, since controlled integration of 2D and 3D materials is helpful for applications involving quantum computation and electronic and opto-electronic device concepts.

The experiments involve deposition of metals and semiconductors onto freestanding 2D membranes during observation in the TEM. It is well known that Au evaporated onto graphene or hexagonal boron nitride forms flat, triangular, epitaxial nanocrystals. However, chemical vapor deposition of Ge or Si, using digermane or disilane, does not lead to epitaxy. Using concepts borrowed from the growth of semiconductor nanowires, we show that Au can act as a catalyst to nucleate epitaxial Ge. The solid catalyst has interacted with both the 2D material and the growing 3D crystal, resulting in alignment of all three lattices. *In situ* TEM helps to establish the relationship between the crystals, explore the reaction pathways and optimize the catalyst and growth conditions.

We suggest that a strategy involving solid catalysts, that brings together the benefits of catalytic growth and van der Waals epitaxy, can be extended to other materials and we discuss the prospects for patterned 3D-on-2D nanostructure arrays and single crystal thin films. We conclude with a perspective on the exciting recent advances in electron microscopy and how these developments will impact future *in situ* growth experiments.



Invited Lectures

ORGANIC MOLECULES OBSERVED ON SURFACES BY FLUORESCENE SPECTROSCOPY

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The adsorption of large π -conjugated organic molecules on well-defined surfaces has been a topic of large interest during the last years, because the surface has significant impact on their structural ordering and their electronic excitations. Here, fluorescence spectroscopy is a very valuable method, although it is not very commonly used in surface science, yet. We will report on two topics related to the optical transitions of molecules on surfaces that were investigated by high resolution laser spectroscopy [1]. The first topic, concerns the self-organization of molecules on surfaces which can lead to well-defined two-dimensional ordered molecular aggregates that are different to those known for the respective bulk materials. Thus, the intermolecular delocalization of the excitation can lead to new interesting optical phenomena not present in 3D structures [2]. Further, we report on the detection of single molecules on surfaces by fluorescence excitation spectroscopy. Here, it is possible to separate the excitations of single molecules in the frequency range using the high resolution of laser spectroscopy. This yields insight into the interactions of the molecules with their individual local environment on the surface.

A. Paulheim et al., The Journal of Physical Chemistry C 120 (2016) 11926.
 A. Eisfeld et al., Physical Review Letters 119 (2017) 097402.

Invited Lectures

CONTROL OF CHARGE TRANSFER INTO ORGANIC MOLECULES ON ULTRATHIN MgO(001) FILMS

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Charge transfer processes on ultrathin, supported oxide films have received increasing attention in recent years because of the possibility to control the charge state of adsorbates or the direction of catalytic reactions. The main driving forces for the occurrence of charge transfer in these systems is the reduction of the substrate work function induced by deposition of the oxide film in combination with an adsorbate with high electron affinity. While previous studies have focused on the charging of metal atoms (e.g. Au) or small molecules (e.g. O₂, NO₂), we have recently extended these investigations into charge transfer processes to large organic molecules. In this contribution, we present results on the adsorption and charging of pentacene (5A) and tetraphenylporphyrin (2H-TPP) on ultrathin MgO(001) films supported on Ag(001). By combing scanning tunneling microscopy and photoemission spectroscopy and tomography, we are able to identify and quantify charge transfer into the organic monolayer film. In addition, we show that by variation of the work function and the MgO thickness it is possible to drive the system into a state where no charge transfer occurs. In the case of 2H-TPP charge transfer also appears to strongly influence the selfmetalation of 2H-TPP to Mg-TPP. Thus, our investigations lay the basis for the ultimate control of charge transfer, and the related chemistry, on ultrathin oxide film systems.

Invited Lectures

NONLOCAL ELECTRON CORRELATIONS IN AN ITINERANT FERROMAGNET MAPPED BY SPIN-RESOLVED MOMENTUM MICROSCOPY

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A fundamental concept in solid state physics describes the degrees of freedom of electrons in a solid by the relation of the energy E vs. the crystal momentum k in a band structure of independent quasi particles. In a real electron system, exchange- and correlation interaction are collective phenomena that lead, for instance, to effects like ferromagnetism. Consequently, for the 3d ferromagnets Fe, Ni, and Co, a description of the band structure in the widely used local density approximation (LDA) is of limited use, as seen by the fact that predicted well defined electronic bands are not observed experimentally. Only recently, experimental access to the spin resolved band structure at every point in the Brillouin zone became feasible by spin-resolved momentum microscopy [1]. This novel concept combines high resolution imaging of photoelectrons in two-dimensional (k_x , k_y) maps with a highly efficient imaging spin filter [2].

Our comprehensive measurements of the spectral-function by spin-resolved momentum microscopy give evidence that in itinerant ferromagnets like cobalt electron correlations are of nonlocal origin. This manifests in a complex self-energy that disperses as function of spin, energy, and momentum. Together with one-step photoemission calculations, we quantify the dispersion of the self-energy over the whole Brillouin zone [3]. The observation of nonlocal electron correlations in cobalt substantially affects our understanding of electron interactions, and makes itinerant ferromagnets a paradigmatic test case for the interplay between band structure, magnetism, and correlations.

Despite a pronounced lifetime broadening, direct optical inter-band excitations can be highly spin selective. This leads to the creation of nearly 100% polarized hot carriers in ferromagnetic cobalt, and might serve as a source of spin-polarized electron currents in spintronics applications [4].

- [1] C. Tusche, A. Krasyuk, J. Kirschner, Ultramicroscopy 159 (2015) 520.
- [2] C. Tusche, et al., Appl. Phys. Lett. 99 (2011) 032505.
- [3] C. Tusche et al., Nat. Commun. 9 (2018) 3727.
- [4] M. Ellguth, C. Tusche, J. Kirschner, Phys. Rev. Lett. 115 (2015) 266801.





IWSP-2019



Oral Presentation

INVESTIGATION OF THE VERTICAL STRUCTURE OF hBN ON Cu(111) VIA NIXSW AND SPA-LEED

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In the recent emergence of two-dimensional materials, hexagonal boron nitride (hBN) has been investigated in great detail both as a template for the growth of organic layers as well as the subject of interest itself since it displays a wide variety of different structures depending on the supporting metal substrate. The interaction strength between hBN and the metal determines both the lateral structure (lattice matching) and the vertical structure (adsorption height and corrugation) of the layer [1].

Here, we are presenting a study of the structure of an hBN layer weakly bonded to the Cu(111) surface including the determination of its vertical structure. The x-ray standing waves technique (XSW) gives insight into the average height of the different atoms in the layer [1] while an analysis of the intensities of satellite reflexes around the (00)-spot as a function of the electron energy observed via SPA-LEED allows conclusions concerning a possible buckling of the layer [2].

C. Brülke et al., J. Phys. Chem. C **121** (2017) 23964.
 M. Horn-von Hoegen et al., Surf. Sci. **298** (1993) 29.

Oral Presentation

TiO₂: FROM REVERSIBLE SEGREGATION OF TRANSITION METAL NANOSTRUCTURES FOR PHOTOCATALYSIS TO MODIFICATION OF GRAPHENE FOR OLED TECHNOLOGY

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Nowadays TiO_2 is often considered as a base material for advanced functionalities. For example, it is photocatalytically active itself but can be also improved by deposition of metal nanostructures on its surface. In the present work a method based on thin film deposition and thermally-induced formation of transition metal nanostructures is shown. The size and concentration of nanostructures on (001) surface of TiO₂ can be reversibly controlled simply by annealing at selected temperatures in vacuum. A few transition metals are compared in the context of nanostructures' morphology and reversible segregation [1-3]. The Fe/TiO₂(001) system is also tested to find out the influence of Fe nanostructures on photocatalytical growth of Ag nanoparticles [4].

In the second part Ti/TiO_2 is applied to modify electronic properties of graphene on SiC. Ti layers are deposited by ion sputtering method and vacuum thermal evaporation method and then oxidized in air. Two model substrates, i.e. Si(100) and graphite (HOPG), are at first used to compare the interaction of Ti/TiO_2 layers with various substrates. Morphology and chemical composition of the interfaces are monitored using AFM and XPS techniques. The work function of interfaces is determined using UPS to find out their usefulness as OLED cathode.

[1] A. Busiakiewicz, Thin Solid Films 550 (2014) 347.

[2] A. Busiakiewicz et al., Mater. Res. Express 3 (2016) 085004.

[3] A. Busiakiewicz et al., Vacuum 163 (2019) 248.

[4] A. Busiakiewicz et al., Appl. Surf. Sci. 401 (2017) 378.

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Oral Presentation

HIGHER ACENES GENERATED BY ON-SURFACE DEHYDROGENATION

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In recent years we observe rapid development of organic electronics. This has prompted the researcher attention toward detailed characterization of single molecules, which are the building blocks of novel devices. Among different families of organic species, the members of the acene family, linearly fused benzene rings, hold the special position being one of the most often studied families in the context of the organic semiconductor applications [1-5].

Herein we present the on-surface generation of long acenes as well as the detailed study of their electronic structure on Au(111) surface. Our method is based on the two-step dehydrogenation of a stable and easily handled tetrahydroacene precursors, assisted by the tip of a combined STM/AFM instrument. High-resolution NC-AFM imaging was applied for the detailed visualization of the internal structure of the generated long acenes. Details on the electronic structure of final molecules, as well as the intermediate dihydroacenes, were revealed using high resolution dI/dV mapping, which allowed the spatial visualization of the electron density cloud. Our measurements showed that not only frontier molecular orbitals (i.e., HOMO and LUMO) but also deeper lying ones could be imaged with submolecular resolution.

[1] J. E. Anthony, Chem. Rev. 106 (2006) 5028-5048.

[2] H. F. Bettinger, C. Tönshoff, Chem. Rec. 15 (2015) 364-369.

[3] R. Zuzak, et al., ACS Nano 11 (2017) 9321–9329.

[4] J. Krüger, et al., Angew.Chem. Int.Ed. 56 (2017) 11945–11948.

[5] R. Zuzak, et al., Angew.Chem. Int.Ed. 57 (2018) 10500–10505.

Oral Presentation

PHYSICOCHEMICAL PROPERTIES OF THIN Gd FILMS ON 4H-SiC(0001)–GRAPHENE

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Graphene is the most promising electronic material discovered in the past decade. This material exhibits a number of interesting properties such as high electron mobility at room temperature, remarkable optical transparency, high thermal conductivity and exceptional mechanical properties. Moreover, the peculiar band structure of graphene makes it different from any other compounds. A crucial goal in ongoing research is to characterise various graphene growth techniques along with their potential application (e.g. flexible electronics, optoelectronics, energy storage devices). One of the most well known technique to obtain graphene is high temperature thermal decomposition of silicon carbide - semiconductor characterised by a wide band gap (more than 3 eV), high electric breakdown field, high-saturation electron velocity and tolerance to high temperature. Another important issue is to find the way to control graphene physical properties. One of the possibility is the intercalation - process, in which atoms interject between the graphene and the substrate.

In this work, the growth of gadolinium (Gd) on 4H-SiC(0001)–graphene have been investigated. The properties of as deposited films and after annealing system at various temperatures were studied using X-ray Photoelectron Spectroscopy and Low Energy Electron Diffraction. Analyses of chemical composition and obtained surface structures for Gd/4H-SiC(0001)–graphene system allow to characterise parameters for gadolinium intercalation, which in this case is initial coverage and temperature of annealing.

Oral Presentation

MODIFICATION OF THE RELATIVISTIC SURFACE BAND STRUCTURE OF TI/Si(111) SYSTEM BY ADSORPTION OF O AND CI

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The influence of the adsorption of chemically active atoms as oxygen and chlorine on surface band structure of Tl/Si(111) system has been studied theoretically with the use of fully relativistic DFT calculations. The obtained results indicate the incorporation of oxygen atoms into the Tl layer. It was found that the adsorption of oxygen adatoms leads to the formation of the band composed almost solely of the electronic states associated with topmost silicon atoms – this band is located inside the bulk band gap around 0.4 eV below the Fermi level. The s-orbitals of Tl atoms are inactive in the bonding with silicon substrate in Tl/Si(111), however, in the presence of oxygen adatoms these states are involved in the strong bonding between Tl and O atoms - the band with these states lies deeply below the Fermi level (around 6 eV). On the other hand, 0.7 eV above E_F the calculated band structure indicates the presence of band with anti-bonding states between Tl and O atoms. The obtained band structure indicates the lack of the spin splitting of the electronic bands inside the energy gap. The corresponding system with chlorine adatoms also shows the lack of spin splitting for the bands inside the gap. However, contrary to adsorption system with oxygen adatoms, chlorine adatoms are not incorporated into Tl atomic layer.

Oral Presentation

ELECTRONIC STRUCTURE AND STM IMAGING OF THE KBr/InSb INTERFACE

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Using scanning tunneling microscopy (STM) and angle-resolved photoelectron spectroscopy (ARPES) we study the KBr/InSb(001) epitaxial system, for ultrathin KBr films of a thickness 1–4 ML. It is found that KBr overlayer formation does not perturb the crystallographic structure of the InSb surface and its electronic structure is mostly unaffected as well. Thus the film-substrate binding is concluded to be almost purely ionic and the electronic systems of the substrate and the overlayer are decoupled.

A simple model of the studied system is proposed for the electron tunneling, in which the ultrathin KBr film is treated as a dielectric layer, modifying the tunneling potential barrier. Apparent step heights on the KBr film surface, measured using STM, agree well with predictions of such a model.

Interestingly the atomically-resolved STM images show patterns strongly resembling In and Sb sublattices at the KBr-InSb interface. We think that this is a result of the fact that, at the considered scales, the atomic scale structure of the tunneling barrier can not be neglected. The barrier is spatially modulated (in the sample plane) in register with the KBr film Madelung potential. We observe tunneling current maxima (electrons flowing out of the sample) when the STM tip is over Br⁻ ions. These ions are located over In atoms for the odd number of KBr layers, and over Sb atoms for the even number of KBr layers. Thus the ultrathin KBr film acts as an atomic scale "sieve" facilitating, depending on the film thickness, tunneling to the one or the other sublattice at the interface. The "sieve" effect may be introduced as a correction to the "dielectric model" explained above because the atomically resolved modulation observed in the STM constant height mode is less than 10% as compared to the apparent step height.

🔹 🌒 🔰 Oral Presentation

THERMALLY INDUCED REACTIONS BETWEEN A GaN(0001) SUBSTRATE AND HAFNIUM LAYER

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The growth of hafnium films on n-GaN(0001) surface with native oxide was investigated using surface-sensitive techniques. The electron affinity of the cleaned n-GaN(0001) surface amounts to 3.4 eV. It is shown that hafnium creates a continuous and stable layer on GaN substrate. Thermal treatment of Hf/GaN system causes decomposition of GaN and reaction of hafnium with atomic nitrogen from the substrate. XPS spectra demonstrate the reaction by a strong shift of the N 1s and Hf 4f lines. An attempt for bringing on the same reaction with molecular nitrogen under pressure of 1.2×10^{-6} mbar was not successful. UPS spectra show a metallic character of the hafnium adlayer in such instances. The experiment confirms that the N₂ atmosphere does not react efficiently with hafnium despite a relatively high partial pressure. Formation of hafnium and nitrogen compounds at hafnium film during annealing follows the reaction with atomic nitrogen derived from decomposition of the GaN substrate.
Oral Presentation

TUNING THE STRUCTURE OF ULTRATHIN FeO ISLANDS ON Ru(0001) BY OXIDATION/REDUCTION

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Ultrathin iron oxide (FeO) films epitaxially grown on Pt(111) exhibit unique electronic [1], magnetic [1,2] and catalytic [3] properties not observed for bulk iron oxides. The catalytic activity is mainly related to the presence of undercoordinated iron atoms at the edge and defect sites within FeO and, therefore, is particularly high for well-dispersed FeO islands [4].

We studied ultrathin FeO islands grown on another close-packed metal substrate – Ru(0001) – by room temperature iron deposition and postoxidation in molecular oxygen. Such preparation procedure was shown to lead to the formation of well-dispersed and well-ordered FeO islands [5]. The performed scanning tunneling microscopy (STM), low energy electron microscopy (LEEM), local low energy electron diffraction (micro-LEED) and X-ray photoelectron spectroscopy (XPS) experiments reveal that the structure of the islands can be additionally tuned by oxidative and reducing treatments. Regarding potential catalytic activity, UHV annealing was found to increase the number of undercoordinated iron sites (CUFs) [4] at the perimeter of FeO islands and within the islands, which makes FeO/Ru(0001) an interesting model system for further catalytic studies.

[1] L. Giordano et al., Phys. Rev. B 76 (2007) 075416.

[2] N. Spiridis et al., Phys. Rev. B 85 (2012) 075436.

[3] Y.-N. Sun et al., Angew. Chem. Int. Ed. 49 (2010) 4418.

[4] Q. Fu et al., Science **328** (2010) 1141.

[5] G. Ketteler et al., J. Phys. Chem. B 107 (2003) 4320.

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Program Overview

Oral Presentation

STRUCTURAL AND MAGNETIC PROPERTIES OF TRANSITION METAL OXIDE THIN FILMS GROWN ON Ru(0001)

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Transition metal oxides (TMO) are promising candidate materials for future spintronic devices. Their properties arise from the interaction between transition metal and oxygen ions in a given structure which are very sensitive to different bond length and angles, as well as to their particular cationic distribution. However, their properties in thin film form, as required for the use in microelectronic devices, are often disappointing, since interface and surface effects, as well as defects can play strong roles. Thus, a detailed understanding of magnetic and transport properties of ultrathin films at such scale are needed, which enables us to optimize the fabrication methods.

Here we demonstrate a route for preparing high quality ultrathin ternary transition metal oxide films on a metallic substrate. Mixed nickel, iron and cobalt oxides have been grown on Ru(0001) by high temperature oxygenassisted molecular beam epitaxy. The nucleation and growth process are observed in real time by means of Low Energy Electron Microscopy (LEEM), which enables to optimize of the growth parameters. A comprehensive characterization is performed combining LEEM and LEED for structural characterization and PEEM (PhotoEmission Electron Microscopy) with synchrotron radiation for chemical and magnetic analysis via X-ray Absorption Spectroscopy, X-ray Magnetic Circular Dichroism and X-ray Magnetic Linear Dichroism (XAS-PEEM, XMCD-PEEM and XMLD-PEEM, respectively).

Depending on the chosen stoichiometry and conditions, either spinel ferrites or monoxides of rocksalt structure can be prepared. The spinel ferrites show ferromagnetic contrast. While the monoxide one present long range antiferromagnetic ordering with the Néel temperature above the room temperature. The high crystalline and morphological quality of prepared films result in optimized properties with respect to films grown by other methods, such as magnetic domains which are larger by several orders of magnitude.



Oral Presentation

MOLECULAR SELF-ASSEMBLY OF PORPHYRINS ON Au(111) PRECOVERED BY COPPER AND SULPHATE

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The selforganization of porphyrin molecules TMPyP and sulphate on the copper precovered Au(111) surface was investigated in solution with the use of electrochemical scanning tunneling microscopy and cyclic voltammetry. The experiments were carried out at different copper coverages [1-4]. The first stages of the underpotential deposition lead to the formation of a $(\sqrt{3}\times\sqrt{3})R30^{\circ}$ sulphate structure on 2/3 ML and 5/3 ML of Cu and a $(\sqrt{3}\times\sqrt{7})$ R19° sulphate structure on pseudomorphic 1 ML of Cu. In the overpotential deposition region the formation of copper multilayers with characteristic sulphate induced Moiré structure was observed. A "charge inversion" effect within the interface layers serves as a template for adsorption of organic TMPyP cations. An ordered molecular layer exhibiting domain structure was imaged by STM after the formation of the complete pseudomorphic Cu monolayer. At multilayer Cu coverages the growing order of porphyrin molecules with hexagonal (hex) and square (sqr) local arrangement was observed (Fig. 1). An imbalance between the copper deposition and desorption current suggests the formation of CuTMPyPmetalloporphyrins. The comparison of EC-STM and CV results obtained for porphyrins deposited on Cu/Au(111) and Cu(111) is presented [5].

- [1] B. Madry, K. Wandelt, M. Nowicki, Surface Science 637-638 (2015) 77.
- [2] B. Madry, K. Wandelt, M. Nowicki, Electrochimica Acta 217 (2016) 249.
- [3] B. Madry, K. Wandelt, M. Nowicki, Applied Surface Science 388 (2016) 678.
- [4] B. Madry et al., Encycl. Inter. Chem., Surf. Sci. Electrochem. 5 (2018) 281.
- [5] B. Madry et al., Topics in Catalysis 61 (2018) 1335.



Fig.1. Porphyrin molecules on multilayer Cu deposit on Au(111).

Invited Lectures

Oral Presentation

PROPERTIES OF ULTRATHIN Pt LAYERS ON Cu(111) REVEALED BY AES, LEED AND DEPES

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The investigations of Pt on Cu(111) [1] were carried out to reveal the growth mode and crystalline structure of the adsorbate with the use of Auger electron spectroscopy (AES), low energy electron diffraction (LEED), and directional elastic peak electron spectroscopy (DEPES) [2-4]. 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 1 ML of Pt show the formation of the compressed adlayer. 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 islands. Experimental DEPES data were compared to theoretical results obtained with the use of the multiple scattering (MS) calculations [4,5] for different adsorption geometries including the Pt and Cu intermixing at the interface in a form of the Cu₃Pt alloy [6,7]. The quantitative analysis of the data made by R-factor calculations enabled the determination of Pt domain populations already at 1 ML and 6 ML.

- [1] A. Miszczuk et al., J. Elect. Spec. Rel. Phen. 223 (2018) 29.
- [2] S. Mróz, M. Nowicki, Surface Science 297 (1993) 66.
- [3] M. Nowicki, Vacuum 54 (1999) 73.
- [4] I. Morawski et al., Surf. Sci. Rep. (2019), doi.org/10/1016/j.surfrep.2019.05.002
- [5] I. Morawski, M. Nowicki, Physical Review B 75 (2007) 155412.
- [6] P.C. Dastoor et al., Surface Science 588 (2005) 101.
- [7] R. Belkhou et al., Surface Science 297 (1993) 40.



Nanostructured Surfaces

Oral Presentation

Pb INTERCALATION OF GRAPHENE ON Ru(0001) – AES, LEED AND DEPES STUDY

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Auger electron spectroscopy (AES), low energy electron diffraction (LEED) and directional elastic peak electron spectroscopy (DEPES) [1,2] were used to investigate graphene (Gr) on Ru(0001) before and after the intercalation by Pb. AES recorded during the continuous Pb adsorption on clean and Gr precovered Ru(0001) shows early stages of the Pb monolayer nucleation, as well as the decrease of the sticking coefficient of Pb after the graphene layer formation. The intercalation is proved by the recording of the Auger signal from Pb at such high temperature as 1100°C, far above melting point of Pb. The LEED pattern recorded for Gr/Ru(0001) shows the large (12×12) unit cell of graphene overlayer, which corresponds to the (11×11) substrate unit cell [3]. The intercalation of the graphene layer by Pb significantly weakens the intensity of the superstructure reflexes. However, some low intensity satellite spots suggest the presence of a quasi-free standing graphene layer. The DEPES anisotropies for Gr/Ru(0001) reflect the six-fold symmetry pattern without any distinct maxima, which confirms the formation of a large adsorbate unit cell. After the intercalation the DEPES anisotropies reveal the six-fold rotational and reflection symmetry pattern, which is very similar to the $(\sqrt{7}\times\sqrt{7})$ of the Pb-Ru(0001) structure [4].

[1] S. Mróz, M. Nowicki, Surface Science 297 (1993) 66.

[2] I. Morawski et al., Surf. Sci. Rep. 74 (2019) 178.

[3] S. Marchini, S. Gunther, J. Wintterlin, Physical Review B 76 (2007) 075429.

[4] M. Jurczyszyn et al., Encycl. Inter. Chem., Surf. Sci. Electrochem. 1 (2018) 496.

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Oral Presentation

2D SELF-ASSEMBLED NANOMATERIALS – COMPUTER SIMULATIONS AND EXPERIMENT

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The fabrication of 2D nanomaterials with a precisely defined structure and interesting physicochemical properties is currently one of the most important challenges for modern materials chemistry. The use of bottom-up techniques, which are based on the spontaneous self-assembly of simple organic molecules on flat surfaces, seems to be particularly promising for this purpose. This is related to the large variety of molecules that can be used as elementary building blocks of advanced supramolecular structures. Nowadays, however, the construction of new 2D nanomaterials is based mainly on the trial and error methods, which are time-consuming and requires numerous test experiments. This is especially true for conformationally flexible molecules with several functional groups, which on flat surfaces can exist as racemates or mixtures of different conformers. In order to better understand the main factors that have a decisive influence on the morphology of above-mentioned supramolecular structures, it seems rational to use computer simulations. Particularly suitable for this purpose are coarsegrained Monte Carlo simulations, in which molecules are modelled in a simplified way but their most important parameters like shape, size and distribution of functional groups are preserved. Herein we present our recent theoretical investigations in the field of on-surface supramolecular chemistry and compare them with corresponding experimental data obtained with the use of Scanning Tunneling Microscopy.

[1] D. Nieckarz, P. Szabelski, Chem. Commun. 54 (2018) 8749.

Nanostructured Surfaces

Oral Presentation

DFT STUDY ON THE STRUCTURE OF ULTRATHIN FeO FILMS ON Ru(0001)

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Ultrathin iron oxide (FeO) films on Pt(111) exhibit unique electronic and catalytic properties originating from a strong film-substrate interaction [1,2]. Similar films can be also grown on Ru(0001) [3], however, those are way less studied. Here, we present the results of DFT calculations on the structure of FeO/Ru(0001). The experimentally observed films exhibit long-range Moiré superstructure with characteristic high-symmetry regions. Therefore, the calculations were performed not only for different oxide stackings (arrangement of Fe and O layers), but also for different oxide registries with respect to the substrate. It was found, that the systems with Fe atoms at the FeO-Ru interface and antiferromagnetic arrangement of Fe layers are the energetically most favorable ones – independently on the film thickness and Moiré high-symmetry region. These findings are in agreement with experimental STM and XPS results.

[1] E. D. L. Rienks et al., Physical Review B **71** (2005) 241404(R).

[2] L. Giordano et al., The Journal of Physical Chemistry C 114 (2010) 21504.

[3] G. Ketteler and W. Ranke, The Journal of Physical Chemistry B 107 (2003) 4320.

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Invited Lectures

Oral Presentation

HEXAGONAL BORON NITRIDE NANOMESH STRUCTURE TUNED BY GOLD-RHODIUM SURFACE ALLOY

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Hexagonal boron nitride (h-BN) monolayer on the Rh(111) substrate has a periodically corrugated "nanomesh" structure. On the other hand, h-BN layer on a clean Au(111) substrate is atomically flat. By forming surface alloys of Au-Rh in different compositions on a Rh(111) substrate, we report on the gradual tunability of the nanomesh morphology of h-BN [1], which can be useful for various nanopatterning applications. Increasing the Au amount in the surface alloy results in reduced pore diameter and corrugation of the h-BN layer [1]. The experimental findings are confirmed by density functional theory calculations: The energetically preferred ordered (2×1) Au-Rh surface alloy [2,3] is reconstructed, and Rh is accummulated below the pore of h-BN.

[1] R. Gubó et al., Phys. Chem. Chem. Phys. 20 (2018) 15473.

[2] L. Óvári et al., Phys. Chem. Chem. Phys. 18 (2016) 25230.

[3] K. Palotás et al., J. Phys. Chem. C 122 (2018) 22435.

Oral Presentation

APPLICATION OF *IN-SITU* XPS SPECTROSCOPY FOR ANALYSIS THE CHEMISTRY OF PLASMA NITRIDED TiO₂ NANOTUBES

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Highly ordered nitrogen-doped titanium dioxide nanotubes (N-TiO₂ NTs) were fabricated by anodic oxidation of Ti foil at constant voltage (25 V) in glycerol based electrolyte containing ammonium fluoride [1]. The following step-wise procedure consisting of 4 steps was applied: (1) plasma nitriding of $TiO_2 NT$ (in as-received sate), (2) heat treatment at 450°C / 2h in vacuum, (3) plasma nitriding of annealed TiO₂ NT at 450°C, (4) heat treatment at 450°C / 2 h in vacuum. All steps of this procedure were monitored by XPS method in situ. As a result chemical shifts of the N 1s XPS peak were observed after each step. Usually, after plasma treatment the BE-peak position of nitrogen was close to 400.0 eV (NH_x species), but after heat treatment the negative BE shifts were recorded. The negative shift in the nitride direction (397.0 eV) is crucial as an effective way of incorporating nitrogen into the TiO₂ lattice [2,3]. This phenomenon also influenced on the change of the modified Auger parameter (α ') to a lower value in comparison to undoped TiO₂ NTs, which suggests the formation of certain chemical bonds between titanium, nitrogen and oxygen atoms. Present experimental procedure leads to substitutional N doping. The XPS results provide an unambiguous characterization of the electronic states associated with N-impurities in TiO₂ NTs and a realistic picture of the processes occurring in the solid under plasma nitriding treatment.

[1] P. Roy et al., Angew. Chem. Int. Ed. **50** (2011) 2904. [2] C. Di Valentin et al., Chem. Phys. **339** (2007) 44.

[3] R. Asahi et al., Chem. Review 114 (2014) 9824.



Oral Presentation

FORMATION AND OPTICAL PROPERTIES OF THIN TIN AND GOLD FILMS PRODUCED BY PVD METHOD

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The aim of the research was to study the kinetics of growth of gold and tin thin layers. For this purpose, the Au and Sn layers with thicknesses of 2.5 nm, 5 nm and 10 nm were deposited on the silicon substrates, at a pressure below $2 \cdot 10^{-5}$ mbar, using the thermal vapor deposition method.

It was noticed that the microstructure and growth mechanism of thin films strongly depend on the deposition conditions (e.g. deposition rate, temperature) [1]. Therefore, the studied layers were prepared at two different deposition rates (0.05 Å/s and 2.50 Å/s).

It was found that the change of the microstructure of layer has a significant impact on the change of its optical properties [1,2]. Therefore, the produced layers have been tested in terms of microstructure and optical properties using Atomic Force Microscopy (AFM) and Spectroscopic Ellipsometry (SE), respectively.

Research of growth mechanism and morphology of layers are necessary for the production of nanostructured materials under controlled conditions to obtain systems with specific optical, mechanical and chemical properties [3].

[1] T. Rerek, et al., Thin Solid Films 670 (2019) 86.

[2] T. Rerek, et al., Appl. Surf. Sci. 451 (2018) 32.

[3] F. Ruffinio et al., J. Appl. Phys. **107** (2010) 104321.

Program Overview



Oral Presentation

REDUCTION OF Fe₃O₄ FILMS ON Pt(111) - SURFACE STRUCTURE VS. COMPOSITION

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The (111) surfaces of magnetite become very heterogeneous when the condition of their formation are far from the equilibrium [1,2]. The inhomogeneities, termed as "biphase", have a strong tendency to order in a quasi-hexagonal structure with a periodicity 3-6 nm. To better recognize the atomic structure and depth composition associated with the observed biphase superstructures we have systematically studied the effect of surface reduction of magnetite Fe₃O₄(111) films [3]. The stoichiometry of the magnetite films was modified by deposition of metallic Fe, followed by UHV annealing.

The films were grown on a Pt(111) single crystal. The film surface structure was analyzed using LEED and STM, whereas the composition was determined by *in situ* conversion electron Mössbauer spectroscopy (CEMS). The stoichiometric Fe₃O₄(111)/Pt(111) 5-nm films displayed electronic and magnetic properties characteristic for bulk magnetite.

The addition of iron resulted in a modification of the surface structure from the regular $Fe_3O_4(111)$ termination to the bi-phase reconstruction. Whereas the LEED pattern weakly depended on the amount of iron added, STM showed successive biphase structures, identified with atomic resolution and explained within a coherent model. CEMS revealed that the composition of a 5 nm film, initially only weakly dependent on the amount of Fe, abruptly changed above 2 ML of ad-Fe.

[1] M. Paul et al., Phys. Rev. B 76 (2007) 075412.

[2] N. Condon et al., Phys. Rev. B 55 (1997) 15885.

[3] N. Spiridis et al., J. Phys. Chem. C 123 (2019) 4204.

The work supported by the National Science Centre, Poland, Grant 2016/21/B/ST3/00861



Oral Presentation

IMPACT OF SUBSTRATE TEMPERATURE ON OPTICAL CONSTANS OF CHROMIUM NANO-FILMS

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The present investigation focuses on the process of preparation of chromium nanofilms by resistive heating method in vacuum. Chromium nano-films were prepared, onto ultrasonically cleaned glass substrates, by thermal evaporation in vacuum, under a pressure of 1×10^{-6} Torr at substrate temperatures $T_s=22^{\circ}C$ and $180^{\circ}C$. The chromium nanofilms were characterized by Ratio Recording Spectrophotometer, the films, at lower thicknesses, were transparent compared to those at higher thicknesses, in the range (5 - 30) nm, for the visible wave-length region of incident radiation, (300-700) nm. The optical measurement that was made on the films included transmittance for different film thicknesses at different wavelength of incident radiation, in the range for the films deposited at both T_s. With this data, we have estimated the optical constants like reflectance (R%), transmittance (T%), refractive index (n), extinction coefficient (k), absorption coefficient (α), real part of permittivity (\in ') and imaginary part of permittivity $(\in")$ for chromium nano-films. The optical constants were found to be very sensitive to the film thickness as well as wave-length of incident photon. It is found that the reflectivity of chromium films deposited at $T_s=180$ °C is found to be about 10% more than that deposited at $T_s=22$ °C. A comparison and conclusion will be drawn between the optical parameters films deposited at both the substrate temperatures.

[1] A. H. A. Mohamed, Int. J. Phys. Sci. **7** (2012) 2102.

[2] A. J. M. Siqueiros et al., Revista Mexicana De Fisica **45** (1999) 593 PACS: 78.66.w; 78.66.Bz; 81.15.Ef

Oral Presentation

HYDROGEN INFLUENCE ON SURFACE MORPHOLOGY OF 4H-SiC{0001} SURFACES

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The wide band-gap semiconductor silicon carbide has attracted a great interest during the past decades because of number of properties which make it very attractive for many applications in electronic devices. For electronic applications purposes hexagonal 4H-SiC is the preferred polytype. The (0001) surfaces of the hexagonal polytype 4H-SiC are structurally equivalent to the Si(111) surface for which hydrogenation has proved to be the method to produce unreconstructed, extremely flat, H-terminated surfaces. The hydrogen atoms attach to semiconductor dangling bonds thus providing the surface chemically and electronically passivated. Moreover, as the SiC crystal is grown in hydrogen atmosphere its presence influences the reaction of Si and C atoms with surfaces influencing the quality of grown crystal. In previous density functional theory (DFT) studies of the changes in the surface atomic and electronic structure resulting from hydrogen coverage ranging from a submonolayer to one monolayer [1] it was shown that an adsorbed monolayer of H almost completely suppresses relaxation of the SiC surface atomic layers.

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-unitcell or single-unit-cell height. DFT studies of the atomic structure and morphology of the atomic steps formed in the [10-10] and [11-20] directions on the Si- and the C-terminated surfaces [2] identified atomic structure of the most favourable energetically steps. In presented research the adsorption of hydrogen on those steps was studied. Various adsorption sites on the lower and upper terrace as well as at the step edge were considered. The most favourable energetically sites were found depending on the terrace width. Then, the influence of adsorbate on the atomic and electronic structure of both the step edges and the terraces was examined.

E. Wachowicz, A Kiejna, J. Phys.: Condens. Matter **24** (2012) 385801.
 E. Wachowicz, T. Ossowski, and A. Kiejna, Appl. Surf. Sci. **420** (2017) 129.



^orogram Overview

Oral Presentation

ON THE STRUCTURE OF ULTRATHIN FeO FILMS ON Ag(111)

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Ultrathin transition metal oxide films grown on single crystal supports exhibit unique properties not observed for the corresponding bulk oxides [1]. These properties, originating mainly from the low-dimensionality and the interaction with the substrate, make those films similar to other supported 2D materials with bulk counterparts. Ultrathin iron oxide (FeO) films, for example, were shown to exhibit unique electronic, catalytic and magnetic properties that depend on the metal single crystal support used. Ag(111) has always been considered a promising candidate for FeO growth, as it has the same surface symmetry as FeO(111), only ~5% lattice mismatch, is considered a weakly-interacting and is relatively resistant to oxidation. However, the reports on the growth and structure of FeO on Ag(111) are scarce and often contradictory to each other.

We used scanning tunneling microscopy (STM), low energy electron diffraction (LEED) and X-ray photoelectron spectroscopy (XPS) to study ultrathin FeO films grown on Ag(111) using different preparation procedures. We observed the formation of a previously unreported Moiré superstructure with a 45 Å periodicity, as well as other reconstructed and reconstruction-free surface species. The experimental results obtained by us and other authors indicate that the structure of FeO/Ag(111) may depend on the preparation conditions. We also performed density functional theory (DFT) calculations on the structure and properties of a conceptual reconstruction-free FeO film on Ag(111). The results indicate that such a film, if successfully grown, should exhibit tunable thickness-dependent properties, being substrate-influenced in the monolayer regime and free-standing-FeO-like when in the bilayer form.

[1] G. Pacchioni, Chem. Eur. J. 18 (2012) 10144.

This work was financially supported by the Foundation for Polish Science (First TEAM/2016-2/14 (POIR.04.04.00-00-28CE/16-00) project co-financed by the European Union under the European Regional Development Fund). T.P. and A.K. acknowledge computer time granted by the ICM of the Warsaw University (Project G44-23).

Oral Presentation

Pb NANOCHAINS ON THE Si(113) SURFACE

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Surface morphology plays an important role in predicting and controlling growth of low-dimensional systems. Arrays of structures that are uniform and oriented in only one direction throughout a large area focus particular interest. They are used to search and study new phenomena such as the Fermi liquid theory or the Peierls distortion.

Vicinal substrates are promising templates for the growth of low-dimensional nanostructures since they are able to form long-range anisotropic onedimensional order [1]. Among many, the Si(113) surface reveals pronounced structural anisotropy and reconstructs to form stable superstructures.

In this contribution we investigate crystallographic and electronic structure of the Si(113) surface covered with Pb. Reflection high energy electron diffraction (RHEED) and scanning tunneling microscopy (STM) are used for a study of morphology and crystallographic structure of the surface. Its electronic properties are investigated with angle resolved photoelectron spectroscopy (ARPES). Deposition of 1.5 ML Pb with subsequent annealing at 300°C leads to distinct well-ordered areas and formation of one-dimensional atomic Pb chains. The Pb nanostructures show anisotropic metallic bands with parabolic dispersion along direction parallel to the step edges. The observed close proximity between electronic bands makes this ensemble a good candidate for the investigation of the Rashba effect. The experimental results are supported by density functional theory (DFT) calculations.

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







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• • • Poster Presentation • • •

FORMATION OF SODIUM BROMIDE LAYERS ON Ag(111) TO CHARACTERIZE CARBENE MOLECULES

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During the last few decades notable efforts have been made in exploring the self-assembly of organic molecules on metal surfaces, in which the adsorbed molecules can significantly influence the electronic properties of the metals underneath by forming chemical bonds. On non-metal layers such as alumina or NaBr films, the molecules exhibit quite different self-assembly manner and electronic properties from those adsorbed directly on metal surfaces. The insulating layers screen the conduction electrons of the supporting metals and thereby modify their surface potential. In contrast, besides of organic molecules, imaging and understanding of active radicals is important as they are short-lived intermediates in almost all chemical reactions, but because of their limited life time, there is very little fundamental knowledge about it. However, radicals on metal surface tend to lose their character due to the strong interaction with metal atoms. To avoid this problem salt surface might help to keep their property constant.

We have grown sodium bromide (NaBr) layers on Ag(111) at room temperature. By variable temperature (100-350 K) fast scanning-STM, we are investigating layer formation, atomic resolution, defects and a moiré pattern. The NaBr layers grow on the surface directly as a bilayer and then consequently third and fourth single layers depending on different deposition rates. The atomic resolution of NaBr bilayer has a surface orientation along the (100) plane with a lattice constant of 0.41 nm. The Na atom are shown as depression and Br atom as protrusion when imaging with the metal tip. But, the metal tip can easily capture a Br atom and create a single vacancy on the surface. In comparison with bare metal tips, the chemically modified Br tips yield drastically enhanced spatial resolution as well as contrast reversal in STM topographies, implying that Na atom imaged as protrusions rather than Br atoms. Due to the lattice mismatch with the metal surface, the layer creates a properly visible moiré pattern with Ag(111). These layers serve as support for the organic and inorganic molecules we are investigating. We want to look at radicals, which cannot be produced and then deposited on surface. Therefore, we have chosen a diazo (C=N=N) protected precursor (organic molecule) to produce the radicals by activating light. We have deposited these diazo protected organic molecules on metal and also NaBr surface at 100-110 K and imaged at 120-140 K. Recent progress will be present in the contribution.

Poster Presentations



Nanostructured Surfaces

Poster Presentation

MICROSCOPIC VIEW OF TIN PHTHALOCYANINE ADSORPTION ON THE RUTILE TiO₂(011) SURFACE

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The adsorption and assembling process of organic molecules on semiconductor surface often determine final properties of a device where the organic-inorganic interface plays a crucial role (for example in DSSC – dye sensitized solar cells). Among the molecules considered as appropriate dyes, functionalized porphyrin-like molecules as well as phthalocyanine species are often studied. Particularly interesting is their adsorption behaviour at room temperature for coverage greater than monolayer. The adsorption behavior of tin phthalocyanine (SnPc) on the (011) face of rutile TiO_2 was studied via scanning probe microscopy at room temperature. Deposited molecules form a commensurate structure (A-type phase), which evolves into another incommensurate structure (B-type phase) as a result of sample annealing. Both structures exhibit two mirror domains with respect to the [01-1] direction. Kelvin probe force microscopy indicates that SnPcs aligned in Atype phase adsorb in tilted geometry with the tin atom directed towards the surface. The molecules in B-type phase hold their molecular board upright mimicking the structure of corresponding molecular crystal. Comparison with other metalized phthalocyanines could shed a light on role of central atom in adsorption process.

Oral Presentations

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OXYGEN ADSORPTION, SUBSURFACE OXYGEN LAYER FORMATION AND REACTION WITH HYDROGEN AND CARBON OXIDE ON SURFACES OF A Pt-Rh ALLOY NANOSIZED CRYSTAL

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The adsorption of oxygen and its catalytic reactions with hydrogen and carbon oxide on Pt-17.4 at.% Rh nanosized crystal were studied by Field Emission Microscopy (FEM) and Field Ion Microscopy (FIM) techniques in the 600-700 K temperature range. Both techniques use samples prepared as sharp tips, apexes of which mimick a single nanoparticle of catalyst in size and morphology.

Our observations suggest that oxygen adsorption on Pt-Rh samples leads to the formation of subsurface oxygen layer. Initially, the subsurface oxygen layer is formed beneath the {113} planes for O₂ exposure of about 3 L (Langmuirs). For large oxygen doses around 100 L, the change of the tip morphology was observed and subsurface oxygen layer was believed to accumulate also beneath the surface of high Miller index areas between the {012} and {011} poles of the hemispherical tip.

The subsurface oxygen could have been effectively removed from the subsurface layers by subsequent exposure of the sample to H_2 . This phenomenon was observed as sudden, eruptive change of the FEM pattern brightness. The reaction resulted in the recovery of the initial field emission pattern, observed before any exposure of the sample to O_2 . This result clearly indicates that the oxygen accumulation-reduction process is completely reversible in the case of reaction with hydrogen.

Contrarily, exposure of the sample with subsurface oxygen layer to CO resulted in the recovery of the FEM pattern of the clean tip only for small amounts of adsorbed oxygen, while for large O_2 doses the initial field emission pattern did not recover.



Poster Presentations

Nanostructured Surfaces

Oster Presentation

INVESTIGATION OF INTERFACE FORMATION OF INDIUM ON AN ORGANIC THIN FILMS DEPOSITED ON DIFFERENT SUBSTRATES USING PHOTOELECTRON SPECTROSCOPY COMBINED WITH CHEMOMETRIC METHODOLOGY

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The application of multivariate chemometric analysis to enhance information available from photoelectron spectra of the indium metal on organic semiconductor layers: phthalocyanine (CuPc) and tris (8-hydroxyquinoline) aluminum (Alg₃) interface formation is demonstrated. Indium was evaporated gradually on thin organic films by increasing the thickness of the contact interface. In previous studies [1] of the In/CuPc formation, we presented evidence of the coexistence of two types of indium phases, "reactive" and "unreactive", whose behavior is of particular importance when used in organometal-based devices. The key information about chemically meaningful compounds has been gained in graphical form by a PCA biplot, which allows for a visual determination of the characteristic peak positions. Moreover, the effect of the substrate onto the In/CuPc interface formation was studied by looking at InSb and graphite (HOPG) as substrates for CuPc deposition. In this communication we present an observation of In/Alq₃ interface formation on metal single crystal (Mo(100)). The proposed chemometric approach allows us to compare our current results with the results for In/CuPc and in this way the degree of interaction between thin CuPc and Alq₃ layers and embedded indium on this organic medium is evaluated.

[1] G. Balcerowska-Czerniak et al., J. App. Phys. 124 (2018) 075302.

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STRUCTURAL AND ELECTRONIC PROPERTIES OF Sb ATOMIC CHAINS ON Si(553) WITH Pb NANORIBBONS

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Topological insulators and their symmetry protected boundary states could be crucial for future nanoelectronics due to possibility of achieving nondissipative transport. In this context low-dimensional Sb nanostructures (i.e. atomic chains or nanoribbons) need a thorough study. However, fabrication of quasi-1D Sb structures is challenging due to preferred sublimation of Sb from source in a form of clusters. In order to overcome this problem one can use Pb as surfactant which enhances surface diffusion length and changes surface energy necessary to dissociate Sb clusters. Therefore as a template for Sb atomic chains we used very well ordered anisotropic Si(553) surface with Pb nanoribbons [1].

Atomic structure of the Si(553)-Pb surface was studied with RHEED and STM methods, whereas ARPES and STS methods were applied to characterize electronic structure. We observed that after deposition of 0.23 ML of Sb at room temperature the atomic chains of Sb were grown. The chains were aligned parallel to the Si(553) step edges and parallel to the Pb chains. Their lattice constant was the same as Si interatomic distance in [110] direction of the substrate. The presence of Sb atomic chains caused replacement of a set of one-dimensional parabolic bands of the Si(553)-Pb substrate into a single 1D-band. Results of tunneling spectroscopy measurements showed that the Sb atomic chains exhibit metallic character.

[1] M. Kopciuszyński, et al., Phys. Rev. B 88 (2013) 55431.

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Poster Presentations

Oster Presentation

In/Alq₃/HOPG STUDIED BY UPS AND XPS

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The results of investigations of thin layers of indium on tris(8hydroxyquinolato)aluminum (Alq₃) are presented in this report. The studies were carried out *in situ* in ultrahigh vacuum. Alq₃ layers were formed by vacuum evaporation on the surface of highly oriented pyrolytic graphite (HOPG). The HOPG substrate was chosen as an unreactive and conductive one to force the amorphous Alq₃ growth. The formation of multilayers was monitored using a quartz microbalance. The measured (mass) deposition rate was 0.075-1.0 nm/min. The growth of indium film on Alq₃ was examined by X-ray photoelectron spectroscopy (XPS) (C 1s, N 1s, O 1s and In 3d core levels) and ultraviolet photoelectron spectroscopy (UPS) in HeII regime. Measurements were taken using Scienta R3000 analyzer and intensities for XPS and UPS peaks were calculated using CasaXPS software.

The presence of a thin indium layer on the Alq₃ surface does not substantially modify the valence band structure of Alq₃ although it does peaks broadening in both, XPS and UPS spectra and the formation of the gap states is also observed. During the deposition of indium, energy position differences as well as the shape changes of the characteristic In 4d peaks (and other valence levels) as a function of the indium layer thickness are observed which suggest different metallic phases. The results were compared to previous ones obtained on other substrates.

G. Balcerowska-Czerniak et al., J. Appl. Phys. **124** (2018) 075302.
 Y. Park, J. Lee, S.K. Lee, D.Y. Kim, Appl. Phys. Lett. **79** (2001) 105.



🕐 🌒 🕘 Poster Presentation 🖉 🌒 🔍

USE OF NANOSTRUCTURED In₄Se₃ CRYSTAL (100) SURFACE AS A TEMPLATE FOR OBTAINING AN ARRAY OF NANOWIRES

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There are a lot of methods for obtaining nanowires (NWs) and other nanosized structures on flat or textured substrate surfaces, which use the phenomenon of self-assembling. Among them is a class of methods for the formation of nanostructures referring to the technology of the vapor - liquid - solid phase or vapor - solid - solid phase. They are based on the properties of the rearrangement of thin metal films deposited on the substrate surface, under the action of elevated temperatures, in nanosized droplets, through a dewetting process. The disadvantage of most of them is the need to pre-create a topographic pattern on the substrate surface by mechanical influence, such as indentation, scribing or by lithographic methods, as well as restrictions on the minimum size of nanostructures, which are, in particular, due to the resolution of the methods of a topographic pattern obtaining.

Our work aims at the creation of NWs with predicted parameters such as diameter, length and period in the array (i.e., matrix of NWs) on (100) surface of In₄Se₃ layered semiconductor single crystal using its furrowed structure, which acts as a high resolution template for the formation of NWs. The NWs were investigated using data obtained at room temperature with an Omicron NanoTechnology STM/STS System in UHV better than 10^{-10} Torr. Indium deposition was conducted with application of EFM-3 thermal evaporator. We observed self-assembling in the deposited coverage towards array of NWs directed along *c* axis of the surface lattice due to the subsequent thermal activation. Besides, the factor affecting the formation of NWs is the presence of In⁺ atoms in the structure of In₄Se₃ crystal.

Poster Presentations

Poster Presentation

ONE-DIMENSIONAL MOLECULAR CHAINS OF QUINACRIDONE ON Ag(100): STM AND SPA-LEED INVESTIGATIONS

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One-dimensional molecular aggregates are of high interest because they often show specific and pronounced coupling effects for electronic excitations, e.g. in optical spectra. One molecule that is already known to form such structures on the Ag(111) surface is the prochiral quinacridone (QA) [1]. Here, we report on the temperature dependent growth of QA chains and the structure of the condensed monolayer of QA on the Ag(100) surface by spot profile analysis low energy electron diffraction (SPA-LEED) and scanning tunnelling microscopy (STM).

QA grows on Ag(100) at low temperatures in short, curvy, heterochiral chains containing many defects. The bonding motif are intermolecular hydrogen bonds. Upon warming, the chains transform into long, straight, homochiral chains showing interesting interactions between the two enantiomers. The condensed monolayer of QA on Ag(100) is very similar to the one on Ag(111) investigated by Wagner et al. [1]. It consists of domains of parallel homochiral chains with the distance between the chains depending on the coverage. This structure is metastable. Upon annealing at 500 K it transforms into a two-dimensional, heterochiral, commensurate structure. It consists of homochiral dimers forming periodically indented, heterochiral and closely packed chains.

[1] Th. Wagner et al., The Journal of Physical Chemistry C 188 (2014) 10911-10920.

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MOLECULAR SWITCHES ON METALLIC SURFACES

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The project relies on the implementation of a molecular switch [1-3] in the form of a phthalocyanine (H₂Pc) molecule adsorbed on the Ag(100) surface. This molecule changes its conductive state in the process of hydrogen tautomerization as recorded with the aid of an STM tip. The process of switching of a molecule is reversible, and the reaction position is well determined. A similar phenomenon of molecular switching, also using an STM tip, has already been demonstrated [4] for a similar molecule (naphthalocyanine), but on a different substrate, i.e. an ultrathin insulating layer (NaCl bilayer) on a Cu(111) surface. However, so far the process of molecular switching has never been explored for a H₂Pc molecule adsorbed on the Ag(100) surface.

First-principle calculations are performed based on density functional theory (DFT) using the FIREBALL code [5], whereas calculations of the transport properties employ the nonequilibrium Green function (NEGF) technique [6]. Performed calculations consist in modelling of the process of hydrogen tautomerization of a H₂Pc molecule on the Ag(100) surface and analyzing the changes in the spatial distribution of molecular orbitals that are responsible for the difference in the recorded tunneling current.

[1] W. Auwärter et al., Nat. Nanotechnol. 7 (2011) 41.

[2] K.P. Dou et al., Front. Phys. 12 (2017) 127303.

[3] P. Liljeroth et al., Nat. Nanotechnol. 7 (2012) 5.

[4] P. Liljeroth et al., Science **317** (2007) 1203.

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

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

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SILICENE ON ULTRATHIN GOLD LAYERS

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Silicene is a new, two-dimensional material with a honeycomb lattice that may host Dirac fermions [1]. This silicon analogue of graphene has a big advantage that is the possibility of band gap opening by applying the external electric field. Unfortunately, silicene is a metastable material and its synthesis has to be done on a supporting material. In many cases the interaction with the substrate suppresses the existence of Dirac cones [2].

To overcome this limitation several different substrates for silicene growth were proposed. For example: Ag(111), Au(111) and Si(111) with $\sqrt{3}\times\sqrt{3}$ reconstructions induced by Ag or Bi atoms. However, the experimental realization of silicene on those substrates is disputable and only in the case of silicene/Au(111) bands with linear dispersion were observed in the electronic structure [3].

In this contribution we report a new approach for the formation of silicene. Contrary to traditional methods, where silicon is deposited from a Si source onto a monocrystalline substrate we were able to form Si honeycomb structure on the top of several monolayer thick gold film utilizing the surface segregation process of silicon atoms in Au/Si system. In this method we only apply a mild annealing of Au/Si(111) substrate and silicene forms on the top of gold layer. This is accompanied with the appearance of new bands in the electronic structure that reveal linear dispersion.

[1] S. Cahangirov et al., Phys. Rev. Lett. 102 (2009) 1.

[2] R. Quhe et al., Sci. Rep. 4 (2014) 5476.

[3] S. Sadeddine et al., Sci. Rep. 7 (2017) 1.

This work was supported by the National Science Centre under Grant No.2018/29/B/ST5/01572.

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INVESTIGATION OF Pt AND Mn THIN FILMS ON Si(111) SURFACE

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Thin layers of platinum and manganese on semiconductors have a wide application in microelectronics. Platinum is known for its chemical stability, and is commonly used as catalyst and, moreover, its silicon compounds are successfully applied in devices based on Schottky barrier [1]. Thin films of manganese and manganese oxides on semiconductors have been proved to have ferromagnetic properties, which is crucial for spintronic applications [2]. However, incorporating these metal/semiconductor systems into microelectronic devices requires in particular knowledge about their growth mechanism and surface morphology of the manufactured systems.

In this study changes of structural, morphological and chemical properties of Pt and Mn thin films (formed *in situ* by deposition from handmade effusion cells heated indirectly by electron bombardment) on Si(111) surface were investigated in wide range of temperatures (from room temperatures up to 1200 K) under UHV conditions (with base pressure lower than 1×10^{-9} mbar) using X-Ray Photoelectron Spectroscopy (XPS) and Low Energy Electron Diffraction (LEED).

M. C. Li et al., Materials Chemistry and Physics 80(3) (2003) 620 – 624.
 M. Aouassa et al., Applied Surface Science 428 (2018) 1056 – 1060.

Poster Presentations

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SURFACE TERMINATION REVEALED BY DIRECTIONAL ELASTIC PEAK ELECTRON SPECTROSCOPY

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In this work the results of investigations concerning the termination of the Ru(0001) surface are presented [1]. All experiments were carried out with the use of a retarding field analyser. The cleanness of the sample was monitored by Auger electron spectroscopy. After the cleaning procedure the long-range order of surface atoms was proved by the observation of sharp diffraction spots with the use of low energy electron diffraction. The short-range order of atoms within the surface-near region was investigated with the use of directional elastic peak electron spectroscopy [2-5]. The experimental intensity distributions presented as stereographic projections were recorded for different energies of the primary electron beam E_p . The six-fold symmetry intensity pattern observed in all intensity plots reflected the contribution of A and B terminated terraces of the Ru(0001) surface. The quantitative analysis of the experimental data, presented in the form of stereographic distributions and azimuthal profiles, performed by means of contrast values of intensity maxima, showed the equal population of A and B terminated terraces. The data are discussed in the context of single and double steps on Ru(0001) and face centered cubic (111) samples, and the theoretical distribution for the A terminated Ru(0001) surface obtained with the use of the multiple scattering theory [6] is presented.

[1] S. Kovalchuk et al., J. Elec. Spec. Rel. Phen. 233 (2019) 77-82.

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

[3] M. Nowicki, Phys. Rev. B 69 (2004) 245421.

[4] M. Jurczyszyn et al., Encycl. Inter. Chem., Surf. Sci. Electrochem. 1 (2018) 496.

- [5] I. Morawski et al., Surf. Sci. Rep. 74 (2019) 178.
- [6] I. Morawski, M. Nowicki, Phys. Rev. B 75 (2007) 155412.



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UNUSUAL STRUCTURAL PHASE TRANSITIONS IN THE CRYSTAL OF {[N₂H₅]₃CdCl₅}_n

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Our last studies revealed that the reaction of $CdCl_2 \cdot 2.5H_2O$ with an excess of hydrazine hydrate and hydrochloric acid leads to the formation of a crystal $\{[N_2H_5]_3CdCl_5\}_n$ of the polymeric structure. Preliminary studies on the crystal structure at room temperature were undertaken by Braibanti and Tiripicchio [1]. On the basis of DSC, single crystal X-ray diffraction experiments and optical observation, we found that the crystal exhibits several structural phase transitions. On heating run at 328 K the crystal undergoes a phase transition of the ferroelastic type from the monoclinic to the orthorhombic phase. Afterwards, upon cooling the two structural phase transitions at about 322 K and 319 K are observed, where crystal adopts orthorhombic symmetry. The presented phase transitions are unique due to the fact the first heating run results in different structural changes compared to those observed during subsequent heating.

In the studied crystal $[N_2H_5]^+$ ions and 1D chains built up from dimeric $\{Cd_2Cl_{10}\}_n^{6-}$ units occur. As a result of phase transitions the change of positions of cations and partial disorder of cations as well as Cl ions is observed.



Figure. The crystal structure of {[N₂H₅]₃CdCl₅]_n at 340 K. Hydrogen atoms have been omitted for clarity due to the disorder of hydrazine ions.
Symmetry codes: (i) 0.5+x, 1.5-y, 0.5-z; (ii) x, 1.5-y, z; (iii) -0.5+x, 1.5-y, 0.5-z.

[1] A. Braibanti, A. Tiripicchio, Gazz. Chim. Ital. **96** (1966) 1580.

Poster Presentation

APPLICATION OF THE MULTIPLE SCATTERING FORMALISM TO THE QUANTITATIVE ANALYSIS OF DEPES RESULTS FOR Ru(0001) AND Pt(111)

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Directional elastic peak electron spectroscopy (DEPES) [1-4] was used to reveal the short range order within the surface-near region of Ru(0001) and Pt(111). Experiments were performed at primary electron beam energies from 0.7 keV till 1.8 keV. DEPES signal was recorded for the wide range of polar θ (from -80° till 80°) and azimuthal φ (from 0° till 180°) angles and then transformed to two-dimensional DEPES maps using stereographic projection. The three-fold and six-fold symmetry intensity pattern observed in DEPES distributions for Pt(111) and Ru(0001), respectively, reflects the crystallinity of samples. Theoretical DEPES distributions were obtained by the application of the multiple scattering (MS) theory [5]. In calculations three parameters were varied, namely: the inelastic mean free path of electrons [6], the radius around the emitter and the radius of smoothing [4,7]. The comparison of the experimental and theoretical DEPES results was performed by an R-factor analysis. The contribution of subsequent layers to the DEPES signal and the role of the surface termination in the calculated distributions for both samples is discussed.

- [1] S. Mróz, M. Nowicki, Surface Science **297** (1993) 66.
- [2] M. Nowicki, Physical Review B 69 (2004) 245421.
- [3] M. Jurczyszyn et al., Encycl. Inter. Chem., Surf. Sci. Electrochem. 1 (2018) 496.
- [4] I. Morawski et al., Surf. Sci. Rep. 74 (2019) 178.
- [5] I. Morawski, M. Nowicki, Physical Review B 75 (2007) 155412.
- [6] S. Tanuma et al., Surface and Interface Analysis 17 (1991) 927.
- [7] M. Jurczyszyn et al., Materials Characterization **93** (2014) 94.



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DYNAMIC PROPERTIES OF TOPOLOGICAL ATOMIC CHAINS

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Atomic wires and low-dimensional systems are of great interest nowadays and there are many different methods of fabricating atomic chains like for example MCBJ (Mechanically Controlled Break Junction) and vicinal surfaces [1]. As the thinnest electric conductors they can found many possible applications in nanoelectronics and quantum computing. There is also a big interest of topological insulators that reveal new interesting phases of matter different with ones that we are familiar with [2]. Unlike 2D and bulk materials, one-dimensional topological insulators reveal protected states that can be found only on the edges of system and band gap inside [3,4].

Here we discuss dynamic electrical properties of topological chains in Su-Schrieffer-Heeger model with tight binding Hamiltonian and evolution operator formalism. We show transitions between trivial and non-trivial topological phases. We analyse the formation process of topological edge states and study the influence of external impurities (like adatoms or coupled chains) on the system conductance. We also study transient effects in normal and topological chains and show that they reveal the memory effect after e.g. breaking the chain or due to different initial occupations.

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

[2] S. Sachdev, Quantum Phase Transitions, Cambridge University Press, Cambridge (2000).

[3] J. K. Asboth et al., A Short Course on Topological Insulators Springer, Switzerland, (2016).

[4] M. Kurzyna et al., Journal of Applied Physics, doi: 10.1063/1.5080651 (2019).

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Poster Presentations

Poster Presentation

EC-STM AND CV INVESTIGATIONS OF Au(110) IN ACID SOLUTIONS

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Surface structures formed on the Au(110) electrode in the base 0.1 M H₂SO₄ solution were studied by electrochemical scanning tunneling microscopy (EC-STM) and cyclic voltammetry (CV). At negative sample potentials current peaks observed in cyclic voltammograms reflect the formation and lifting of the well known 2×1 and 3×1 surface reconstructions as reported in [1]. These surface row structures were monitored *in situ* by STM. With increasing the sample potential the surface reconstruction is lifted. At even higher sample potentials the oxidation process of the Au(110) surface occurs, which is reflected by a characteristic anisotropic surface observed in STM images.

Knowing that the formation of the surface structures depends on both the sample potential and the composition of the solution, which leads to the adsorption of different ions, the EC-STM and CV measurements were also conducted in different acid solutions. Cyclic voltammograms and STM images, the latter recorded at selected sample potentials are presented and discussed.

[1] K. Yoshida, et al., Electrochim. Act. 139 (2014) 281-288.

This work was supported by National Science Centre, Poland, under Grant No.2018/02/X/ST3/00666.

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A NEW CUSTOM-MADE SAMPLE HOLDER FOR HIGH-TEMPERATURE AND *IN SITU* APPLICATION OF MAGNETIC FIELDS IN A PHOTOEMISSION ELECTRON MICROSCOPE

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We present a new custom-made sample holder system for its use in Elmitec Low Energy and PhotoEmission Electron Microscopes. It comprises two different sample holder bodies: one with a filament for electron bombardment heating up to more than 1500 K and another one with integrated electromagnets for the *in situ* application of small magnetic fields either inplane or out-of-plane. The sample itself is placed on a platelet with a central top hat shape which is transferred between both holder types. Thus it is possible to prepare or grow samples at elevated temperatures and then investigate their behavior under magnetic fields without ever leaving the ultra-high vacuum system.

This design opens up new possibilities for the study of magnetic properties of surfaces, thin films and nanostructures which cannot be exposed to air. As an example of the performance of the setup we present the growth of magnetite on Ru(0001) by high temperature oxygen-assisted molecular beam epitaxy. The nucleation and growth process are observed in real time by means of Low Energy Electron Microscopy (LEEM), which enables to optimize the growth parameters. Imaging of the magnetic domain distribution of the resulting magnetite microstructures is done via XMCD-PEEM (X-ray Magnetic Circular Dichroism Photoemission Electron Microscopy). Finally, the switching characteristics of individual magnetite microstructures under applied field was investigated. Our results illustrate the feasibility to change the magnetic state of the *in-situ* grown materials at tens of nm scale resolution.



Figure 1. 3D model of the design of hightemperature part of exchangeable sample holder.

Invited Lectures

Poster Presentations

Oster Presentation

TITANIUM AND ITS OXIDES ON SELECTED SURFACES: SILICON(100), GRAPHITE(0001) AND GRAPHENE/4H-SiC(0001) FOR APPLICATIONS IN OLED TECHNOLOGY

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In the first step of the experiment Ti was deposited by means of ion sputtering technique in high vacuum coating system on given surfaces: Si(100), HOPG(0001) and graphene/4H-SiC(0001). We were focused on studying the interactions of titanium and its oxides with the used substrates. Then the interfaces were studied through atomic force microscopy (AFM), X-ray photoelectron spectroscopy (XPS), ultraviolet photoelectron spectroscopy (UPS), scanning tunneling microscope (STM) and Raman spectroscopy. The research was aimed at modification of electron properties of graphene, which we plan to use as transparent cathode in OLED technology. We proved that deposition by means of ion sputtering technique is not suitable way of deposition for graphene substrate – introduction of defects in graphene was observed by Raman spectroscopy. Interesting compounds were also detected (e.g. TiSi₂, TiSiO_x).

Aforementioned results were the reason for the change in the deposition method of titanium – in the second step Ti was thermally deposited in UHV system (without contact with air atmosphere) on graphene/4H-SiC(0001). However, the research on this interface should be continued, because the most important in the context of OLED applications is the manipulation the work function (WF) on interface. The obtained WF values for Ti-modified graphene/4H-SiC(0001) were lower than 3 eV which is very promising for OLED cathode but the origin for so low WF must be clarified.

The work was co-financed by the Polish National Science Centre under the grant No. UMO- 2016/21/B/ST5/00 984.

Invited Lectures

Oster Presentation

SURFACE CHARACTERIZATION OF THIN M₀S₂ FLAKES ON Si SUBSTRATES

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Thin MoS₂ crystals with several atomic layers deposited on Si substrates were synthesized through mechanical exfoliation [1]. The resulting Mo sulfide flakes were then analyzed ex situ using combination of Auger electron spectroscopy (AES), elastic-peak electron spectroscopy (EPES) and scanning electron microscopy (SEM) in order to characterize their surface chemical composition, electron transport phenomena and surface morphology. Prior to EPES measurements, the Mo sulfide surface was sputter-cleaned and amorphized by 3 kV argon ions, and the resulting S/Mo atomic ratio varied in the range 1.80-1.88, as derived from AES. The SEM images revealed single crystalline small-area (up to 15 µm in lateral size) Mo sulfide flakes having polygonal or near-triangular shapes. Such irregular-edged flakes exhibited high crystal quality and thickness uniformity. The inelastic mean free path (IMFP), characterizing electron transport, was evaluated from the relative EPES using Au reference material for electron energies E = 0.5-2keV. Experimental IMFPs, λ , determined for the AES-measured sulfide surface compositions were approximated by the simple function $\lambda = kE^p$, where k and p were fitted parameters. Additionally, these values were compared with IMFPs resulting from the TPP-2M predictive equation for all the measured surface compositions, and also for stoichiometric MoS₂ composition. Excellent agreement was found between the experimental and predicted IMFPs.

[1] W. L. Spychalski et al., J. Phys. Chem. C 121 (2017) 26027.
Poster Presentation

ELECTRONICS OF Ba ADSORBED ON Ge(001)

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An ordered alkaline earth sub-monolayer on a clean Si(001) surface provides a template for growth of the atomically sharp, crystalline Si-oxide interface that is ubiquitous in the semiconductor device industry. It has been suggested that submonolayers of Sr or Ba on Ge(001) could play a similar role as on structurally identical Si(001), overcoming known limitations of the Ge(001) substrate such as amorphization of its oxidation layers.

We have performed *ab-initio* density functional theory (DFT), plane-waves, pseudopotential computational studies on the electronic properties of the Ba/Ge(001) adsorption system [1]. Previously we have examined the adsorption and organization of Ba atoms on the Ge(001) surface as a function of temperature and coverage using ultrahigh vacuum (UHV) scanning tunneling microscopy (STM) measurements and total energy DFT calculations [2,3]. In this work we supplement these studies by analyzing the corresponding electronic structures. We demonstrate in particular that the key role in the formation of the extended on-top and incorporated phases is played by predominantly ionic Ba-Ge interaction and not by the direct Ba-Ba interaction. This, along with the calculated electronic structures, explains the ordered aggregation of the Ba adatoms in the form of the zig-zag chain-like structures observed in STM measurements.

[1] A. Puchalska et al., Appl. Surf. Sci. 481 (2019) 1474.

[2] W. Koczorowski et al., Phys. Rev. B 91 (2015) 235319.

[3] W. Koczorowski et al., Phys. Rev. B 93 (2016) 195304.

Invited Lectures



• • • Poster Presentation • • •

THE Au(100) SURFACE AS A TEMPLATE FOR PENTACENE ADSORPTION

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The unreconstructed Au(100)–(1×1) surface has squared lattice with lattice constant 2.88 Å. However the topmost layer of the surface usually reconstructs into quazi-hexagonal (hex) structure. The unit cell is huge, complicated and close to $c(28\times48)$. The distance of gold atom in topmost layer to its nearest neighbors vary with the position of the atom in the atomic row. Recently it was shown that the coexistence of (1×1) and hex phases in the same first layer is possible [1].

Pentacene (PEN) belongs to polycyclic aromatic hydrocarbons and consists of five benzene rings. The adsorption of PEN on noble metal surfaces attracts a lot of attention due to, on the one hand, the capacities of such systems into organic electronic devices. On the other hand metal-organic interfaces are model systems in fundamental investigations [2].

By utilizing scanning tunneling microscope (STM) we study the selforganization of PEN on Au(100). Our results reveal the ordered domains creation of PEN molecules onto two coexisted phases. Regardless the surface phase, the molecular axis is aligned along [011] surface crystallographic directions. The molecules vertical arrangement depends on surface phase. On the reconstructed surface area PENs appear with various apparent heights. On the unreconstructed surface the apparent height of the molecules is homogenous. The presence of domains on both gold phases reveal that the adsorption of PEN might not lift the surface reconstruction.

[1] A. Trembulowicz et al., Nanotechnology **30** (2019) 045704.
[2] L. Bartels, Nat. Chem. **2** (2010) 87-95.

62

Poster Presentation

EC-STM AND CV INVESTIGATIONS OF Au(111) IN SULPHURIC ACID SOLUTION

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Electrochemical scanning tunneling microscopy (EC-STM) and cyclic voltammetry (CV) were applied to investigate an Au(111) electrode immersed in 0.1 M H₂SO₄ in a wide potential window from the hydrogen evolution reaction (HER) till the surface oxidation (dissolution). Different preparation protocols of the solution including degassing with Ar and applying different potentials to the sample were used. STM images recorded in-situ at negative sample potentials with respect to the Pt/PtO reference electrode reveal the well-known sulphate free reconstructed Au(111)- $(23\times\sqrt{3})$ surface with the characteristic herringbone pattern. At increased potentials sulphate adsorption leads to the lifting of the surface reconstruction and first the formation of a disordered sulphate layer. At sample potentials above E=200 mV the well resolved long range ordered ($\sqrt{3}\times\sqrt{7}$) sulphate structure is observed [1,2], until at even more positive potential values the surface oxidation leads to the formation of empty islands and two dimensional Au islands, the later originating from the redeposition of previously dissolved Au. The investigations were performed with and without Ar pressure in the STM chamber. The decrease of an ion current at negative sample potentials was observed with each potential cycle under small Ar pressure, while the lack of Ar resulted in the gradual current increase with the number of potential scans. The influence of the solution preparation procedure on the various current maxima and the overall shape of the cyclic voltammograms, as well as the associated electrochemical reactions are discussed.

B. Madry, K. Wandelt, M. Nowicki, Applied Surface Science **388** (2016) 678.
B. Madry, K. Wandelt, M. Nowicki, Electrochimica Acta **217** (2016) 249.



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MICROSTRUCTURE AND OPTICAL PROPERTIES OF THIN COPPER FILMS PRODUCED BY THE PVD METHOD

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The Cu thin films (12 nm, 25 nm and 35 nm) were deposited on Si(100) crystals by a thermal evaporation at a pressure of 10^{-5} mbar. The metal films were grown with a rate of 0.05, 0.50 and 5.00 Å/s. The effective complex dielectric function of the produced layers, $\langle \tilde{\epsilon} \rangle = \langle \epsilon_1 \rangle + i \langle \epsilon_2 \rangle$, was determined using the spectroscopic ellipsometry (SE) technique. These measurements were carried out in a photon energy range from 0.6 eV to 6.5 eV for three angles of incidence (65°, 70°, 75°) using the V-VASE (J. A. Woollam Co., Inc.) device. The surface topography of copper films was investigated using the atomic force microscope Innova from Bruker. The X-Ray Diffraction (XRD) measurements were performed using the Phillips X'Pert system with Cu K α radiation (λ =1.5418 Å) and the X'Celerator Scientific detector. The chemical composition of the deposited layers was estimated using the X-ray photoelectron spectroscopy (XPS) technique. The photoelectrons were detected by a VG Scienta R3000 spectrometer.

The optical and microstructural properties of the produced Cu films strongly depend on the conditions of growth. The higher values of plasma energy and the mean time between collisions of electrons as well as lower values of optical resistivity were obtained for the thickest metallic films deposited at the highest deposition rate. All the synthesized films exhibit nanogranular structure. The XPS measurements revealed no presence of contaminations in the copper layer.

Nanostructured Surfaces

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SURFACE CHARACTERISATION BY THE X-RAY PHOTOELECTRON SPECTROSCOPY COMBINED WITH THE DIELECTRIC AND SPECIFIC HEAT STUDY IN DMAGaS CRYSTAL

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Dimethylammoniumgalium sulfate hexahydrate $(CH_3)_2NH_2Ga(SO_4)_2 \cdot 6H_2O$ – DMAGaS is an organic-inorganic compound from a big family of crystals which are extensively studied because of their interesting structural phase transitions, at $T_{c1} = 136$ K and at $T_{c2} = 118$ K.

The phase transition at T_{c1} is of the first-order type, close to tricritical one. The crystal belongs to monoclinic system with point group symmetry 2/m above T_{c1} and m below T_{c1} . The phase transition at T_{c2} is the first-order type. At T_{c1} para-ferroelectric phase transition of the order-disorder type is connected to an ordering of the dimethylammonium cations. At T_{c2} , due to rearrangement of dimethylammonium cations, ferroelectric properties disappear.

In this work the results of a dielectric and calorimetric study of DMAGaS crystal combined with the surface characterisation by the X-ray Photoelectron Spectroscopy (XPS) are presented. The chemical composition of the surface region and the ferroelectric properties as well as specific heat characterisation are described.

65

• • • • Poster Presentation • • •

MOLECULAR INSTABILITY OF CoPc IN ORDERED LAYER ON Ag(100) DURING STM MEASUREMENTS

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Cobalt-phthalocyanines (CoPcs) are macrocyclic coordinative compounds which exhibit, as another transition metal phthalocyanines (MPcs), remarkable thermal and chemical stability [1]. Nowadays contacts of MPcs with metal substrates are widely studied. On the one hand such metal-organic interfaces are model systems for experimental and theoretical investigations, on the other hand, they are prototypes of organic electronic devices. Scanning tunneling microscope (STM) is useful tool for structural and electronic property investigations of MPc-metal interfaces, however the STM tip can modify the molecules. In STM images the CoPc molecule in direct contact with metal substrate usually appears as a four-leaf feature. The cobalt atom is visible as a bright center during filled state imaging [2].

We show the results of study on stability of CoPc molecules caused by the STM tip. Only molecules in the ordered domains and in direct contact with the Ag(100) substrate have been investigated. During measurements (STM scanning) some molecular instability has been observed, which concerns mainly CoPc metallic core i.e. cobalt atom. It manifests in a few ways. In the slightest ones, planar and/or vertical shifts from its appropriate position occur. The most destructive effect is extraction of Co and dragging it away from not only the molecule cavity but from the molecule itself. This, actually, changes the molecule identity. The molecular cavity is then very quickly filled by cobalt atom. The fourth type of observed instability is the shift of Co atom within particular molecule. In this case, the Co atom is moved from the CoPc center to the ligand.

G. de la Torre et al., Chem. Commun. **2000** (2007) 2000-2015.
J. M. Gottfried, Surf. Sci. Rep. **70** (2015) 259–379.

Nanostructured Surfaces

Oster Presentation

STRUCTURE SENSITIVITY OF THE INITIAL OXIDATION OF RHODIUM: XPS AND PEEM STUDIES

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New instability phenomena in H_2 oxidation on Rh [1] have refocused the attention to rhodium surface oxides. However, in the most studies efforts are traditionally concentrated on low-Miller-index Rh surfaces, whereas the highly stepped surfaces are much less studied. Particularly, the anisotropy of the initial oxidation of such surfaces is not adequately explored, despite the evident importance of the issue: differently oriented facets of a catalytic particle may exhibit different chemical states during the reaction.

A new *surface structure library* approach, based on local analysis of individual µm-sized domains of a polycrystalline foil, where each domain is crystallographically characterized by EBSD [2], allows such access, e.g. by spatially resolved XPS. Since all the domains belong to the same sample, such an approach provides identical conditions for each of the differently oriented surface regions.

In the present contribution, anisotropy of the surface oxidation of Rh is studied in the 10⁻⁵ mbar pressure range and in the temperature range of 573 to 773 K by spatially resolved XPS and by PEEM, using the *kinetics by imaging* approach [3] and a polycrystalline Rh foil as a *surface structure library*.

- [1] Y. Suchorski et al., Nature Comm. 9 (2018) 600.
- [2] Y. Suchorski, G. Rupprechter, Cat. Lett. 148 (2018) 2947.

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



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DETERMINING THE WORK FUNCTION OF ULTRATHIN FeO(111) FILMS ON Ag(111)

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Noble metals and bulk iron oxides are well-known catalysts of many industrially-relevant chemical reactions. Recently, much attention has been paid to the studies of ultrathin iron oxide films grown on noble metal single-crystalline supports. It is well-established that such systems exhibit properties that differ from those of the corresponding bulk materials. Experimental and theoretical studies revealed that ultrathin FeO(111) films grown on Pt(111) exhibit superior catalytic activity in the CO oxidation reaction compared to clean Pt(111) [1,2]. This activity is related, among other factors, to the decrease of the work function of Pt(111) induced by the presence of FeO(111) film.

We used scanning tunnelling microscopy (STM) operating in the dI/dz spectroscopy mode to determine the work function of ultrathin FeO(111) films grown on Ag(111) [3]. The results indicate that FeO layer increases the work function of Ag(111), which may have strong implications on the catalytic activity of this system.

Y. Sun et al., J. Catal **266** (2009) 359.
Y. Sun et al., Angew. Chem. Int. Ed. **49** (2010) 4418.
M. Lewandowski et al., Nanomaterials **8** (2018) 828.

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THE GROWTH OF MANGANESE SULFIDE THIN FILM ON Ru(0001)

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The investigations of growth of manganese sulphide thin film on the Ru(0001) surface in ultra-high vacuum are reported. The low energy electron diffraction (LEED), Auger electron and X-ray photoelectron spectroscopies (AES and XPS) were used to characterise the atomic and electronic structure of the sulphide films. A few nanometer-thick films were prepared by the multiple cycles of deposition of several Mn layers and sequential exposition to S vapour. This procedure was based on the literature data for the formation of 3d transition metal oxides films in similar adsorption systems. The influence of the different exposition time of the Mn films to S flux, substrate temperature during preparation and post annealing on thin film structure are discussed. Furthermore, the problem of co-adsorption of oxygen on the structure of sulphide thin films is also addressed.

Dral Presentations

Poster Presentations

69



