Tuesday, 01.09.2015, Room EI 10

Time	ID	Surfaces, Interfaces and Thin Films I *Chair: Martin Setvin, TU Wien*
16:00	201	**Differential Optical Spectroscopy for Surface Science** *Peter Zeppenfeld, Institute of Experimental Physics, Johannes Kepler University Linz* Conceptually very simple optical methods, namely Reflectance Difference Spectroscopy (RDS/RAS) and Differential Reflectance Spectroscopy (DRS), can provide valuable insight into the structure and growth of ultrathin films in straight correlation with their electronic, optical and other physical or chemical properties. Notably, differential optical spectroscopies can achieve sub-monolayer sensitivity and are capable of monitoring kinetic processes on surfaces in real time. This will be illustrated in selected examples dealing with the fabrication and optical characterization of functional layers, such as reconstructed surfaces [1,2], graphene nanoribbons [3], and ultrathin molecular films [4,5]. While the spatial resolution in the UV-VIS range is naturally limited, microscopic information on the structure and electronic properties can be obtained from complementary surface science techniques such as STM and Photoemission Electron Microscopy (PEEM). As an outlook, I will describe how optical spectroscopy and PEEM can be combined into a single experiment, thus enabling truly parallel optical and photoelectron spectroscopy at a local scale. [1] L.D. Sun et al., Phys. Rev. B 69, 045407 (2004) [2] M. Bachmann et al., Appl. Surf. Sci. 258, 10123 (2012) [3] R. Denk et al., Nat. Commun. 5:4253 (2014) [4] L.D. Sun et al., Phys. Chem. Chem. Phys. 14, 13651 (2012) [5] L.D. Sun et al., Phys. Rev. Lett. 110, 106101 (2013)
16:30	202	**Spin spectroscopy of molecular quantum dots with a radio frequency scanning tunneling microscope** *Stefan Wiespointner-Baumgarthuber, Stefan Müllegger, Stefano Tebi, Giulia Serrano, Reinhold Koch* *Institut für Halbleiter und Festkörperphysik, JKU Linz, Altenbergerstr. 69, AT-4040 Linz* In the second half of the 20th century two investigation techniques emerged that both revolutionized science and technology in their fields: electron/nuclear magnetic resonance (MR) exhibiting a superior energy resolution and scanning tunneling microscopy (STM) providing spatial resolution at the atomic length scale. In order to benefit from both, the superior spatial resolution of the STM and the exceptional energy resolution of resonance techniques, we developed a radio frequency (rf) STM based on a commercial low-temperature STM upgraded by a home-built rf spectroscopic system. Here, we report the excitation of electron, nuclear and combined electron/nuclear spin transitions by resonant rf tunneling in single molecular quantum dots.
16:45	203	**Charge exchange of He backscattered from metals and metal oxides in Low Energy Ion Scattering** *Barbara Bruckner, Dominik Göbl, Carlos Celedon, Dietmar Roth, Peter Bauer* *Institut für Experimentalphysik, Johannes Kepler Universität, Altenbergerstraße 69, AT-4040 Linz* Low energy ion scattering (LEIS) analyzes the composition and structure of outermost atomic layers when the sample of interest is bombarded with noble gas ions at energies between 0.5 and 10 keV. In this contribution, the influence of oxygen on charge exchange is investigated: a metal sample (Al, Fe, Ta) was exposed to oxygen until further exposure did not lead to changes in the measured backscattering ion yield, which corresponds to a surface oxide. From this, one can obtain information about surface composition and charge exchange between He and O in different oxides.

17:00	**204**	**In-situ atomic-scale control of the pulsed-laser growth of a polar perovskite oxide** *Stefan Gerhold, Michele Riva, Michael Schmid, Ulrike Diebold* *Institute of Applied Physics,TU-Wien, Wiedner Hauptstrasse 8-10, AT-1040 Wien* By combining PLD, high-pressure RHEED, in-situ STM, XPS,and LEIS, we investigate the growth of perovskite oxides on the polar $SrTiO_3$(110) surface, whose structure can be tuned by control of the Sr/Ti stoichiometry [1]. We follow the homoepitaxial growth on the $SrTiO_3$(110)-(4×1) [2] surface, consisting of ordered rings of TiO_4 tetrahedra, and on octahedrally-terminated (2x4)/(2x5)-$SrTiO_3$(110) [3]. Anisotropic diffusion is observed for the adspecies, whose preferential direction is determined by the surface structure. Moreover, kinetic barriers limit mobility across boundaries separating different surface structures. By tuning growth parameters, such as laser intensity, fluency and frequency, background oxygen pressure, and substrate temperature we can achieve either layer-by-layer or step-flow growth, with the TiO_x structures of the topmost layer continuously floating to the surface of the film. [1] Wang, et al, PRB83, 155453(2011); [2] Wang, et al, PRL111, 056101(2013); [3] Wang, et al, submitted
17:15	**205**	**ALD grown bilayer gate stacks for Schottky-barrier Si and Ge MOSFETs** *Bernhard Lutzer, Christina Zimmermann, Ole Bethge, Emmerich Bertagnolli* *Institute for Solid State Electronics, Floragasse 7/1, AT-1040 Wien* In recent years ALD (Atomic Layer Deposition) has been successfully established as a thin layer deposition technique in semiconductor technology. This contribution is about using ALD-grown oxide stacks (Al_2O_3, HfO_2, Y_2O_3) utilized as gate insulator material for Schottky-barrier MOSFETs with thickness control in the nanoscale [1]. The advantage of using ALD is the high quality interface in between the high permittivity oxide and the semiconductor surface which is crucial for a high carrier mobility in the inversion channel. Electrical measurements of MOSFETs and -CAPs are discussed showing very promising results by using a bilayer gate stack design. [1] Suntola, T., Thin Solid Films, 1992. 216(1): p. 84-89.
17:30	**206**	**Electrical Characterization of Yttrium Oxide grown by Atomic Layer Deposition for Germanium based MOS Devices** *Christina Zimmermann, Ole Bethge, Bernhard Lutzer, Emmerich Bertagnolli* *Institute for Solid State Electronics, TU Wien, Floragasse 7, AT-1040 Vienna* Due to the shrinking of device dimensions according to Moore's law the introduction of high-k oxides was necessary in order to reduce high leakage currents. Atomic Layer Deposition (ALD) is the preferred technique for the growth of high-k oxides due to the outstanding step coverage, homogeneity, and oxide quality. In this contribution the ALD-grown high-k oxide Y_2O_3 is applied on next generation Ge based Metal-Oxide-Semiconductor devices for lowering the interface trap density (Dit) and leakage current. Insitu X-Ray Photoelectron Spectroscopy is provided for revealing interfacial mechanisms responsible for low Dit in the range of 10^{10} to 10^{11} $eV^{-1}cm^{-2}$.
17:45	**207**	**Functional modulated structures based on transition metal doped nitrides** *Giulia Capuzzo [1], Thibaut Devillers [1], Andreas Grois [1], Andrea Navarro-Quezada [1], Mauro Rovezzi [2], Tomasz Dietl [3], Maciej Sawicki [3], Alberta Bonanni [1]* *[1] Institut für Halbleiter-und-Festkörperphysik, JKU Linz, Altenbergerstr. 69, AT-4040 Linz* *[2] European Synchrotron Radiation Facility, 6 rue Jules Horowitz, FR-38043 Grenoble* *[3] Institute of Physics, Polish Academy of Sciences, al. Lotników 32/46, PL-02668 Warszawa* Group-III nitrides have already raised to the position of strategic semiconductors for opto- and high-power electronics. The addition of magnetic functionalities is expected to open striking views for both fundamental and application-oriented research [1]. We discuss here the interplay between the distribution of magnetic ions and shallow impurities in III-nitrides, that allows controlling their magnetic [2] and optical [3] properties. [1] A. Bonanni and T. Dietl, Chem. Soc. Rev. 39, 528 (2010); [2] W. Stefanowicz et al, Phys. Rev. B 89, 205201 (2014); [3] T. Devillers et al., Scientific Reports 2, 722 (2012).
18:00		***Postersession and Aperitif***
19:45		***Public Lecture***

Time	ID	Surfaces, Interfaces and Thin Films II *Chair: Christian Teichert, Uni Leoben*
13:30	**211**	**Subsurface Cation Vacancy Stabilization of the Magnetite (001) Surface** *Peter Blaha, Institute of Materials Chemistry, Technische Universitat Wien* Iron oxides play an increasingly prominent role in heterogeneous catalysis, hydrogen production or spintronics. The material interface can be performance-limiting in these applications, so it is vital to understand the atomic-scale structures for iron oxide surfaces. The Fe_3O_4(001) surface undergoes a well-known $\sqrt{2}$ x $\sqrt{2}$ R45 reconstruction, which was explained previously due to orbital ordering of the sub-surface Fe-oct atoms. However, such a model cannot explain the site-selective adsorption of various metal atoms on this surface. Inspired by the common occurrence of non-stoichiometry in iron oxides, we developed a subsurface cation vacancy structure model, which arises from replacing two Fe-oct from the third layer by an interstitial Fe-int with tetrahedral coordination in the second layer. This model is thermodynamically more stable than previous models, explains the site-selective metal adsorption and was verified by quantitative LEED and STM measurements. This hitherto unobserved stabilization mechanism occurs because the iron oxides prefer to redistribute cations in the lattice in response to oxidizing or reducing environments.
14:00	**212**	**An Atomic Scale View of Metal-Assisted Redox Reactions on Fe_3O_4-Supported Au and Pt Catalysts** *Gareth Parkinson, Roland Bliem, Jessica van der Hoeven, Oscar Gamba, Jiri Pavelec, Michael Schmid, Ulrike Diebold* *Institute of Applied Physics, TU Wien, Wiedner Hauptstrasse 8-10, AT-1040 Wien* Scanning tunneling microscopy is used to study the morphology of Pt/Fe_3O_4 and Au/Fe_3O_4 model catalysts exposed to CO, H_2, O_2 at 550 K. In the case of Pt, CO reacts with the support at the cluster perimeter creating holes in the Fe_3O_4 terrace. O_2 dissociates on the metal and spills over onto the support, where it reacts with Fe from the bulk forming islands of Fe_3O_4(001). A similar dissociation and spillover effect in H_2 leads to hydroxylation of the surface. For Au, no holes are observed with CO, but O_2 leads to island growth, indicating O_2 dissociation occurs.
14:15	**213**	*cancelled*
14:30	**214**	**SMSI in inverse model catalysts: ZrO_2 on Pt and Rh** *Joong Il Jake Choi, Ulrike Diebold, Michael Schmid* *Institute of Applied Physics, TU Wien, Wiedner Hauptstr. 8-10/E134, AT-1040 Wien* ZrO_2 is a catalyst support and a catalyst itself. In studying oxide-supported metal catalysts understanding the metal-oxide interaction is essential. Following model system studies on single trilayer zirconia films and the growth of metal clusters, here we present STM and LEED studies on multi-layer zirconia films on Pt(111) and Rh(111). Zirconia dewets the substrate upon annealing. In between the zirconia islands, we find trilayer oxide films when annealed in UHV but these films disappear when annealed in oxygen. This counter-intuitive phenomenon is known as the strong metal-substrate interaction (SMSI) effect and can can be explained by an under-stoichiometric ZrO_{2-x} ultra-thin film forming in UHV.

14:45	**215**	**Manipulation of diffusion paths of Pd atoms through silica thin films on Ru(0001) by hydroxylation** *Sascha Pomp [1], William Kaden [2], Martin Sterrer [1], Hans-Joachim Freund [2]* *[1] Institute of Physics, University of Graz, Universitätsplatz 5, AT-8010 Graz* *[2] Fritz-Haber-Institut, MPG, Faradayweg 4-6, DE-14195 Berlin* In the present study a SiO_2 bilayer film was grown on a Ru(0001) single crystal substrate and applied to investigate possibilities of manipulation of diffusion paths for Pd atoms through the film. A fraction of Pd atoms deposited by vapor deposition penetrates through the clean SiO_2 film and remains trapped at the SiO_2/Ru(0001) interface. Controlled hydroxylation of the SiO_2 surface, which was achieved by electron bombardment of adsorbed ice layers, allows to suppress Pd diffusion through the film. Relevant parameters for this process as well as the fate of hydrogen, which is formed in the ice layers during electron bombardment, will be discussed.
15.00	**216**	**A Surface Science Approach to Catalyst Preparation** *Martin Sterrer, Institute of Physics, University of Graz, Universitätsplatz 5, AT-8010 Graz* Oxide-supported metal nanoparticles represent an important class of heterogeneous catalysts. Their catalytic activity depends on various parameters such as nanoparticle size, morphology, or nature of the support. Maximizing the abundance of active sites is the primary goal for catalysis and is achieved by choosing appropriate catalyst preparation conditions. Surface science models of heterogeneous catalysts have greatly contributed to a deeper understanding of catalytic reactions on surfaces. However, while these models are typically prepared under ultrahigh vacuum conditions, the preparation of technical catalysts is based on wet-chemical procedures. In this talk, I will address the issue of catalyst preparation and present results of our surface science approach to supported metal catalyst preparation utilizing thin, single-crystalline oxide films as substrates. Results will be presented for Au and Pd nanoparticles on MgO(100) and Fe_3O_4(111) supports.
15:30	**217**	**Vortex Assisted Growth of Metallic Nanowires in Superfluid Helium Droplets** *Alexander Volk [1], Philipp Thaler [1], Andreas W. Hauser [1], Daniel Knez [2], Werner Grogger [2], Ferdinand Hofer [2], Wolfgang E. Ernst [1]* *[1] Institute of Experimental Physics, TU Graz, Petersgasse 16, AT-8010 Graz* *[2] Institute f. Electron Microscopy and Nanoanalysis, TU Graz, Steyrergasse 17, AT-8010 Graz,* Helium droplets provide an ideal matrix for the aggregation of tailored metallic nanoclusters and nanowires. The vortex guided growth process of the wires in the superfluid helium environment is not fully understood yet. Silver represents a special case among the metals studied so far since no continuous wires were detected after surface deposition, which was attributed to some unexplained barrier formation by the helium. We have explored the growth process of silver nanowires in detail and show by high resolution transmission electron microscopy in combination with computer simulations under which conditions continuous nanowires are obtained.
15:45	**218**	**Formation of Ag-Au core-shell clusters in superfluid helium nanodroplets studied by atomic resolution electron tomography** *Philipp Thaler [1], Georg Haberfehlner [2], Alexander Volk [1], Gerald Kothleitner [2], Wolfgang E. Ernst [1]* *[1] Institute of Experimental Physics, TU Graz, Petersgasse 16, AT-8010 Graz* *[2] Institiute f. Electron Microscopy and Nanoanalysis, TU Graz, Steyrergasse 17, AT-8010 Graz* The past decades have seen an increasing interest in metal nanoparticles, and especially in core-shell systems which offer great prospects in many fields of nanophysics, ranging from nanoelectronics to catalysis. We utilize superfluid helium droplets to grow Ag-Au core-shell nanoparticles and to deposit the resulting structures under soft-landing conditions. Using atomic resolution electron tomography, we can clarify the structure and composition of our particles on an atomic level. This detailed analysis shines light on the growth process of the nanoparticles and will allow deliberate tuning between single core and multi-core structures in future experiments.
16:00		***Vollversammlung Fachausschuß OGD***
16:05		***Coffee Break***

Time	ID	Surfaces, Interfaces and Thin Films III *Chair: Ulrike Diebold, TU Wien*
16:30	221	**Optimizing pentacene thin-film transistor performance: Temperature and surface configuration induced growth modifications** *Roman Lassnig [1], Michael Hollerer [1], Bernd Striedinger [2], Alexander Fian [2], Barbara Stadlober [2], Adolf Winkler [1]* *[1] Institute of Solid State Physics, TU Graz, Petersgasse 16, AT-8010 Graz* *[2] MATERIALS-Institute, Joanneum Research Weiz, Franz-Pichler-Straße 30, AT-8160 Weiz* Many underlying principles affecting critical organic thin-film transistor parameters are not understood in satisfactory detail. We present in situ electrical and surface analytical, as well as ex situ atomic force microscopy studies on temperature and surface condition induced pentacene layer growth modifications, leading to the selection of optimized deposition conditions and entailing performance improvements. Based on these results the desired organic layer thickness was determined as the deciding factor for optimal deposition parameter selection. A mixed 350 K and 200K, 8 monolayer pentacene device increased the attainable mobility by a factor of 4 compared to single temperature processes.
16:45	222	**1,4-Phenylene Diisocyanide (PDI) Adsorption on Metals Investigated by SFG and STM: From Single Crystals to Supported Nanoparticles** *Ahmed Ghalgaoui, Martin Sterrer* *Institute of Physics, University of Graz, Universitätsplatz 5, AT-8010 Graz* We have investigated the adsorption of 1,4-Phenylene Diisocyanide ((PDI), NC-C_6H_4-NC) on single crystal metal surfaces (Au(111) and Pt(111)) and metal nanoparticles supported by an insulting layer (Au\FeO\Pt(111)). Both, gas-phase and liquid-phase deposition methods were applied. The role of PDI concentration and Au nanoparticle size on the surface structure/adsorption mode of PDI has been investigated by Scanning Tunneling Microscopy (STM) and Broad Band Sum Frequency Generation (BBSFG) Spectroscopy. The influence of the metallic substrate and nanoparticle size on the adsorption geometry will be discussed. In particular, we will show that PDI adsorption changes the morphology of the Au(111) surface.
17:00	223	**Island shape anisotropy of organic thin films on ion-beam irradiated rippled substrates** *Markus Kratzer [1], Dominik Wrana [2], Konrad Szajna [2], Franciszek Krok [2], Christian Teichert [1]* *[1] Institute of Physics, Montanuniversitaet Leoben, Franz Josef Straße 18, AT-8700 Leoben* *[2] Institute of Physics, Jagiellonian University, Lojasiewicza 11, PL-30348 Krakow* We investigated the growth of the organic semiconductor para-hexaphenyl (6P) on highly anisotropic, rippled TiO_2 templates prepared by ion bombardment. 6P islands have been observed featuring clear shape anisotropy and discrete island widths according to the ripple wavelength. These observations are addressed to anisotropic detachment of molecules differently bound to the island rim at ascending and descending substrate steps. The average island length-to-width ratio could be tuned by adjusting the ripple length. Further, a strong diffusion anisotropy along and perpendicular to the ripples was found to be responsible for an increasing island density with decreasing ripple length.
17:15	224	**Single molecules of Sexiphenyl on In_2O_3(111)** *Margareta Wagner [1], Michael Ramsey [2], Martin Sterrer [2], Lynn A. Boatner [3], Ulrike Diebold [1]* *[1] Technische Universität Wien, Wiedner Hauptstr. 8-10/134, AT-1040 Wien* *[2] Karl-Franzens-Universität Graz, Universitätsplatz 5, AT-8010 Graz* *[3] Oak Ridge National Laboratory, USA-Oak Ridge, 37831* Indium oxide is one of the most important TCOs and commonly used as a contact material. Sexiphenyl (6P) is a rod-like molecule and twice as long as the substrate surface lattice parameter. Here, the adsorption of 6P is investigated with STM. We show that 6P has a specific adsorption site, but no well-ordered monolayer is formed. In empty states STM, the single 6P appears as a zig-zag line at bias voltages below +2 V. At +2 V the appearance becomes straight which is associated with the LUMO. At +2.7 V the shape changes again into two blobbs, corresponding to the LUMO+1.

17:45	**225**	**Interplay of weak interactions in the condensation of xenon: Atom by atom investigations in quantum boxes** *Seyedeh Fatemeh Mousavi [1], Sylwia Nowakowska [1], Aneliia Wäckerlin [1], Shigeki Kawai [1], Toni Ivas [2], Jan Nowakowski [3], Shadi Fatayer [4], Christian Wäckerlin [5], Thomas Nijs [1], Ernst Meyer [1], Jonas Björk [6], Meike Stöhr [7], Lutz Gade [8], Thomas Jung [3]* *[1] Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel* *[2] EMPA, Überlandstrasse 129, CH-8600 Dübendorf* *[3] Laboratory for Micro and Nanotechnology, Paul Scherrer Institute, CH-5232 Villigen* *[4] IBM Research Zürich, CH-8803 Rüschlikon* *[5] ICMP, EPFL, Station 3, CH-1015 Lausanne* *[6] Department of Physics, Chemistry and Biology, IFM, Linköping University, SE-58183 Linköping* *[7] Zernike Inst. for Advanced Materials, University of Groningen, Nijenborgh 4, NL-9747 Groningen* *[8] Anorganisch-Chemisches Institut, Uni Heidelberg, Im Neuenheimer Feld 270, DE-69120 Heidelberg* Due to the fundamental importance of condensation processes it is essential to investigate their evolution in an atom by atom manner as it is well established 'in-silico' and experimentally by mass spectrometry in cluster physics. Uniquely, structural information is available by studying condensation atom by atom in so called "quantum boxes" and by analyzing the structure of condensates by Scanning Tunneling Microscopy. Our investigations provide unprecedented insight into Xe condensation and reveal delicate interplay of competing directional and non-directional interactions in emergence of condensate structure. Also unique data for comparison with and analysis of quantum mechanical models is obtained.
18:00	**226**	**Polarization dependent photoelectron emission and optical reflectance of organic thin films on metallic surfaces** *Andrea Navarro Quezada, Markus Aiglinger, Ebrahim Ghanbari, Thorsten Wagner, Peter Zeppenfeld, Inst. for Experimental Physics, Johannes Kepler Universität Linz, Altenberger Str. 69, AT-4040 Linz* The optical and electronic properties of π-conjugated organic materials are important due to their fundamental and technological significance. Despite the improvement in performance of prototype devices, precise understanding and control of thin film growth on metallic surfaces is still a matter of debate. In this work, we use photoelectron emission microscopy (PEEM) and differential reflectance spectroscopy (DRS) simultaneously during the growth of perflouro-pentacene molecules on a Ag(110) surface. While PEEM studies the film morphology on the μm scale, DRS monitors the temporal evolution of the optical properties during deposition. By employing the polarization dependence of both techniques, information on the molecular orientation is obtained.
18:15	**227**	**Switching individual azobenzene-based molecules on metallic and insulating surfaces** *Simon Jaekel [1], Christophe Nacci [1], Knud Seufert [1], Robert Lindner [2], Angelika Kühnle [2], Stefan Hecht [3], Leonhard Grill [1]* *[1] Department of Physical Chemistry, University of Graz, Heinrichstraße 28/5, AT-8010 Graz* *[2] Institute for Physical Chemistry, Johannes-Gutenberg University Mainz, Düsbergweg 10 - 14, DE-55099 Mainz* *[3] Department of Chemistry, Humboldt-University Berlin, Brook-Taylor-Str. 2, DE-12489 Berlin* Studying single molecular switches is of interest for a better understanding of fundamental physical and chemical processes, but also in regards of their possible use in molecular nanotechnology [1]. A prototype conformational switch is azobenzene, which switches between trans and cis isomers at the central N=N bond. In the past years various studies have shown that the switching process can be induced either by light, by the tunneling electrons or the electric field in the junction [2,3]. We present results on azobenzene-based switches that were decoupled from the substrate by bulky side groups and measurements on insulators. [1] C. Joachim et al., Nature 408, 541 (2000); [2] Choi et al., Phys. Rev.

18:30	**228**	**Helium atom scattering measurements revealing the full phononic dispersion of Sb(111)** *Patrick Kraus, Florian Apolloner, Christian Gösweiner, Wolfgang E. Ernst* *Institut für Experimentalphysik, TU Graz, Petersgasse 16, AT-8010 Graz* We have measured the phonon dispersion relation for antimony at 160 K and 300 K in two high symmetry directions using inelastic HAS. The resulting phonon dispersion shows acoustic modes up to 10meV and optical modes between 15 and 20 meV. Additional modes in the acoustic region are visible due to a strong electron-phonon coupling, which allows for charge density oscillations of the surface electron cloud induced by the movement of atoms in the bulk. The dispersion relation also reveals a new mode below the Rayleigh mode, resulting in an upshift of the latter by roughly 0.5 meV compared to the simulations.
18:45	**229**	**Surface Chemistry of Oxygen and Water on Anatase TiO_2 (101)** *Martin Setvin [1], Benjamin Daniel [1], Michael Schmid [1], Ulrich Aschauer [2], Annabella Selloni [3], Ulrike Diebold [1]* *[1] TU Wien, Wiedner Hauptstrasse 8-10/134, AT-1040 Wien* *[2] ETH Zürich, Wolfgang-Pauli-Strasse 27, CH-8093 Zürich* *[3] Princeton University, 08544 Princeton NJ, USA* Reaction between O_2 and H_2O molecules adsorbed on anatase TiO_2 (101) surface was studied by a combination Scanning Tunneling Microscopy (STM) and Density Functional Theory (DFT). We identify terminal OH groups as the final and stable product of the reaction. DFT indicates that the reaction runs as long as the surface provides enough excess electrons. The number of electrons necessary for single reaction steps is discussed. We further characterize OOH groups as important metastable reaction intermediates. The work was supported by the Advanced ERC grant “OxideSurfaces”.
19:00		
19:15		***Transfer to Dinner***
20:00		***Conference Dinner***

Thursday, 03.09.2015, Room EI 9

Time	ID	Surfaces, Interfaces and Thin Films IV *Chair: Peter Zeppenfeld, JKU Linz*
14:00	**231**	**Tailoring the nature and strength of electron-phonon interactions in the $SrTiO_3$(001) two-dimensional electron liquid** *Zhiming Wang, Swiss Light Source, Paul Scherrer Institute, CH-5232 Villigen PSI* *& Department of Quantum Matter Physics, University of Geneva* Surfaces and interfaces offer new possibilities for tailoring the many-body interactions that dominate the electrical and thermal properties of transition metal oxides. Here, we use the prototypical two-dimensional electron liquid (2DEL) at the $SrTiO_3$(001) surface to reveal a remarkably complex evolution of electron-phonon coupling with the tunable carrier density of this system. At low density, where superconductivity is found in the analogous 2DEL at the $LaAlO_3/SrTiO_3$ interface, our angle-resolved photoemission data show replica bands separated by 100 meV from the main bands. This is a hallmark of a coherent polaronic liquid and implies strong long-range coupling to a single longitudinal optical phonon mode. In the overdoped regime the preferential coupling to this mode decreases and the 2DEL undergoes a crossover to a more conventional metallic state with weaker short-range electron-phonon interaction. These results place constraints on the theoretical description of superconductivity and allow for a unified understanding of the transport properties in $SrTiO_3$-based 2DELs

14:30	**232**	**Electronic characteristics of adsorbate-adsorbent hybrid states in one-dimensional molecular structures on Cu(111)** *Jun Zhang [1], Matthias Muntwiler [1], Thomas Jung [1], Abdelkader Kara [2]* *[1] Paul Scherrer Institute, CH-5232 Villigen PSI* *[2] University of Central Florida, 32816 Orlando, USA* The organic/metal interface, important to organic-based electronic and optoelectronic devices, represents a unique system in that more localized molecular orbitals of molecular structures closely interact with the extended states in the metallic substrate. Remarkably, this can give rise to new electronic states which are partially localized to the footprint of the molecules. Here, we investigate the interaction between a molecular state of dicyanoanthracene and the Shockley surface state of the Cu(111) surface by scanning tunneling microscopy and spectroscopy. Comparing differently sized and differently interacting aggregates, we discuss the emergence of a hybrid state between the shifted surface state and the LUMO of the molecule.
14:45	**233**	**Size quantization signatures in graphene quantum point contacts** *Florian Libisch [1], Bernat Terres [2], Larisa Chizhova [1], Dennis Jörger [2], Stefan Engels [2], Joachim Burgdörfer [1], Christoph Stampfer [2]* *[1] Institute for Theoretical Physics, TU Wien, Wiedner Hauptstraße 8-10/136, AT-1040 Wien* *[2] JARA-FIT and 2nd Inst. of Physics, RWTH Aachen, Otto-Blumenthal Str. 2, DE-52056 Aachen* Graphene shows a number of exceptional properties, but the demonstration of graphene quantum point contacts has proven very challenging. Recent developments in fabricating high-mobility graphene-hexagonal boron nitride sandwich structures should allow the study of quantum confinement of Dirac electrons in quasi-one dimensional (1D) graphene systems. Here we show joint experimental and theoretical work on ballistic transport of confined Dirac fermions in graphene quantum point contacts. Reproducible kinks in the conductance are associated with size quantization at the quantum point contact. Comparing the evolution of the observed kinks with magnetic field to theoretical predictions confirms size quantization as their origin.
15;00	**234**	**Intercalation-based decoupling and characterization of bottom-up fabricated graphene nanoribbons** *Okan Deniz, Carlos Sanchez Sanchez, Roman Fasel, Pascal Ruffieux* *nanotech@surfaces, EMPA, Überlandstrasse 129, 8600 Dübendorf* The missing band gap of graphene is major obstacle for electronic applications. Graphene nanoribbons (GNRs) establish such a band gap by quantum confinement. The needed atomic precision is achieved by on-surface bottom-up synthesis [1] which allows GNRs with width-controlled band gaps and various edge topologies. However the process requires a metallic substrate, which inhibits to directly access the GNRs' intrinsic electronic properties due to screening effects and the predominance of the substrate contributions in scanning tunneling spectroscopy (STS) [2]. Intercalation of a decoupling layer (i.e. silicon) allows for direct access to unperturbed electronic structure of GNR structures with different width and edge topologies. [1] Nat. Lett. 466,470-473 (2010); [2] PRB,91,045429 (2015)
15:15	**235**	**Controlling ligation and dimensionality in on-surface coordination polymers by ad-atom specific reactions** *Aisha Ahsan [1], Aneliia Wäckerlin [1], Christian Wäckerlin [2], Jan Nowakowski [2], Sylwia Nowakowska [1], Jonas Björk [3], Shadi Fatayer [1], Jan Girovsky [2], Thomas Nijs [1], Susanne Martens [4], Armin Kleibert [5], Meike Stöhr [6], Nirmalya Ballav [7], Thomas Jung [2], Lutz Gade [4]* *[1] Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel* *[2] Laboratory for Micro- and Nanotechnology, Paul Scherrer Institute, CH-5232 Villigen PSI* *[3] Department of Physics, Chemistry and Biology, IFM, Linköping University, 83, SE-58183 Linköping* *[4] Anorganisch-Chemisches Inst., Univ. Heidelberg, Im Neuenheimer Feld 270, DE-69120 Heidelberg* *[5] Swiss Light Source, Paul Scherrer Institute, CH-5232 Villigen PSI* *[6] Zernike Inst. for Advanced Materials, University of Groningen, Nijenborgh 4, NL-9747 Groningen* *[7] Department of Chemistry, Indian Institute of Science Education and Research, IN-411008 Pune* The formation of on-surface coordination polymers is typically determined by a) type and geometry of molecular building blocks, b) involved functional groups, and c) substrate. Depending on ad-atom choice, a complex pattern of coordination structures of DPDI molecules forms. The coordination

		reaction can be controlled in stages of temperature activated on-surface dehydrogenation (-H, -3H) subsequently forming endo- or exo-ligands (concave or convex arrangement of ligating atoms) from DPDI. The ligand type determines the dimensionality of formed assemblies, as revealed in detail by STM, XPS, NEXAFS and DFT studies and allow us to draw conclusions on the formation mechanisms.
15:30	**236**	**Adsorption of fullerenes on metal surfaces: Vacancy patterning and patterning vacancies** *Alexander Kaiser [1], Francesc Vines [2], Francesc Illas [2], Marcel Ritter [3], Frank Hagelberg [4], Michael Probst [1]* *[1] Inst. für Ionenphysik & Angewandte Physik, Univ. Innsbruck, Technikerstr. 25/3, AT-6020 Innsbruck* *[2] Dep. de Química Física, Universitat de Barcelona, c/Matri i Franques 1, ES-08028 Barcelona* *[3] Institute for Basic Sciences in Engineering Science, University of Innsbruck, Technikerstraße 13, AT-6020 Innsbruck* *[4] Dep. of Physics and Astronomy, East Tennessee State University, 37614 Johnson City TN, USA* A DFT study including van der Waals dispersion reveals the potential of vacancies in metal surfaces to be anchor points for controlled self-assembly of adsorbate molecules in a user-defined pattern. However, energetic criteria also indicate the formation of regular adsorbate-induced vacancies after self-assembly on clean surfaces. Both mechanisms are investigated on the example of fullerene adsorption on Al(111), Au(111), and Be(0001) surfaces with and without vacancies of various sizes. Calculated vacancy-adatom formation energies are given as well. [Nanoscale 6 (2014) 10850]
15:45	**237**	**Assembly of functional molecules - or how to overcome the repulsion between porphins on noble metal surfaces** *Knud Seufert [1], Felix Bischoff [2], Yuanqin He [2], Willi Auwärter [2], Johannes V. Barth [2], Leonhard Grill [1]* *[1] Institut für Chemie, Karl-Franzens-Universität Graz, Heinrichstrasse 28, AT-8010 Graz* *[2] Physik Department E20, TU München, James-Franck-Str.1, DE-85748 Garching* The self-assembly of molecules is essential en route to ordered and utile organic structures - a groundwork of molecular electronics. An archetype of such a functional building block is the porphyrin as it plays a key role in fundamental processes in nature. Here we present a study on porphins, the parent compound of all porphyrins, adsorbed on coinage metal single crystals. While a dominating repulsive intermolecular interaction is present on Au(111), Ag(111) and Cu(111), the herringbone reconstruction on gold has an influence on the assembly. The repulsion can be overcome by coadsorption or a modification of the substrate.
16:00	**238**	**Atomistic Interface Modeling in III-V Semiconductor Superlattices** *Jürgen Maier [1], Hermann Detz [2], Gottfried Strasser [1]* *[1] Center for Micro- and Nanostructures, TU Wien, Floragasse 7, AT-1040 Vienna* *[2] Austrian Academy of Sciences, Dr. Ignaz Seipel-Platz 2, AT-1010 Vienna* The interface quality between layers of a III-V semiconductor superlattice structure is known to influence electronic transport or optical transitions and therefore the device performance. Optimization of epitaxial growth processes also requires detailed insight into interface formation. We use atomistic simulations to find the energetically best interface configuration, analyze structural features as well as strain across the heterojunction. In this model, atoms are placed within an ideal zincblende lattice and then allowed to relax using a Metropolis Monte Carlo simulation with empirical interaction potentials. Preliminary results show good agreement with experimental data on local strain on InAs/GaSb and InAs/AlSb superlattices.
16:15	**239**	**On the mechanism of photoconductivity in atomically thin MoS_2** *Dmitry Polyushkin, Marco Furchi, Andreas Pospischil, Thomas Müller* *Institute of Photonics, Vienna University of Technology, Gusshausstr. 27-29/E387, AT-1040 Vienna* We report a photoconductivity study of biased mono- and bilayer molybdenum disulfide field-effect transistors. We identify photovoltaic and photoconductive effects. The photovoltaic effect is described as a shift in transistor threshold voltage due to charge transfer from the channel to nearby molecules. The photoconductive effect is attributed to the trapping of carriers in band tail states in the molybdenum disulfide itself. A simple model is presented that reproduces our experimental observations. Our findings offer design and engineering strategies for atomically thin molybdenum disulfide photodetectors, and we anticipate that the results are generalizable to other transition metal dichalcogenides as well.

16:30		***Coffee Break, END***
19:45		***Public Lecture***

ID	Surfaces, Interfaces and Thin Films Poster
251	**Vector piezoresponse force microscopy for analysing the orientation distribution function of ferroelectric domains** *Michael Lasnik [1], Sören Röhrig [2], Markus Kratzer [1], Marco Deluca [2], Christian Teichert [1]* *[1] Institut für Physik, Montanuniversität Leoben, Franz-Josef-Strasse 18, AT-8700 Leoben* *[2] Materials Center Leoben Forschung GmbH, Roseggerstraße 12, AT-8700 Leoben* The orientation distribution function (ODF) of the domains in ferroelectric ceramics is an important figure of merit for analysing and improving the behaviour of commercial piezoelectric actuators. Piezoresponse Force Microscopy (PFM) is a common tool for investigating piezoelectric domain patterns. By measuring the out-of-plane and in-plane components of the domains a three-dimensional reconstruction of the domain polarization can be obtained (Vector-PFM). Here, differently polarized lead zirconate titanate ceramics were investigated by Vector-PFM. Based on the material's piezoelectric tensor, the orientations of the domains are obtained and from multiple measurements on a certain sample, the ODF can be determined.
252	**Growth morphologies of small polar molecules on silicon dioxide and graphene** *Benjamin Kaufmann [1], Markus Kratzer [1], Tony Lelaidier [2], Olivier Siri [2], Aleksandar Matković [3], Radoš Gajić [3], Conrad Becker [2], Christian Teichert [1]* *[1] Institute of Physics, Montanuniversitaet Leoben, Franz Josef Straße 18, AT-8700 Leoben* *[2] CINaM, Aix Marseille Université, Campus de Luminy Case 913, FR-13288 Marseille* *[3] Inst. of Physics, Dep. for Solid State Physics, University of Belgrade, Pregrevica 118, RS-11080 Belgrade* We investigated the growth morphologies of the polar organic molecule dihydrotetraazapentacene (DHTAP) on SiO_2 and exfoliated graphene. The morphology of ultra-thin films grown by hot wall epitaxy was analyzed using atomic force microscopy. The morphologies arising between 290 K – 390 K exhibit a strong temperature dependence. Above substrate temperatures of 330 K, the molecules tend to build either curved needle-like structures or terraced islands. At lower growth temperatures, the islands are smaller having no organized structure and no needles are found. On graphene, the islands are reduced in height compared to those grown on SiO_2.
253	**Angle-resolved photoemission spectroscopy (ARPES) simulations of benzene on Pd(110)** *Bernd Kollmann, Peter Puschnig, University of Graz, Universitätsplatz 5, AT-8010 Graz* Angle-resolved photoemission spectroscopy (ARPES) is a powerful technique to investigate the electronic structure of organic films at the interface to metallic surfaces. However, the experimental data is sometimes difficult to interpret. Here, we investigate the electronic structure of a benzene ring adsorbed on a Pd(110) surface. After exploring the energetically most favorable adsorption sites by making use of state-of-the-art van-der-Waals corrected DFT calculations, we perform ARPES simulations for several substrate-adsorbate-geometries which are compared to experiment. We further discuss the applicability of the plane wave approximation for the final state for such rather small molecules and present an approach which allows us to go beyond the plane wave approximation.
254	**TiO_2 nanotube arrays for photovoltaic application** *Krunoslav Juraić [1], Milivoj Plodinec [2], Davor Gracin [2], Sigrid Bernstorff [3]* *[1] Institute of Inorganic Chemistry, Graz University of Technology, Stremayrgasse 9/IV, AT-8010 Graz* *[2] Ruđer Bošković Institute, Bijenička c. 54, HR-10000 Zagreb* *[3] Elettra-Sincrotrone Trieste, SS 14, km 163.5, IT-34149 Trieste* Conversion efficiency of solar cells can be significantly improved by using oriented nanorod-like materials on top of transparent conductive oxide. For this purpose we prepared TiO_2 nanotube arrays by anodizing titanium thin film deposited on ZnO covered glass substrate. In this work we will present results of structural analysis of TiO_2 nanotube arrays obtained by Raman spectroscopy, Scanning electron microscopy and Grazing Incidence Small Angle X-ray Scattering and Wide Angle Scattering. It will be also discussed possible application in dye sensitized and perovskite solar cells.

255 AFM and KPFM investigation of high strength aluminum brazing sheets

Michael Huszar [1], Thomas Kremmer [1], Markus Kratzer [2], Paul Oberhauser [3], Helmut Antrekowitsch [1], Christian Teichert [2]
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High strength aluminum brazing compounds used in car-cooler systems become susceptible to corrosion after brazing. An intermediate layer has to be inserted to separate the 4xxx filler-material from the 7xxx base-material. The effectivity of this layer in preventing corrosion was investigated using atomic force microscopy (AFM) and Kelvin probe force microscopy (KPFM). Samples were subjected to a simulated brazing cycle and exposed to a corrosive medium. The investigations revealed the presence of cathodic inclusions in the Al-matrix. Further, a line of up to 3 μm wide holes is formed at the transition between intermediate layer and base material.

256 Graphene-based integrated photonics

Simone Schuler [1], Andreas Pospischil [1], Marco Mercurio Furchi [1], Markus Humer [2], Romain Guider [2], Thomas Fromherz [2], Thomas Müller [1]
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[2] Institut für Halbleiter und Festkörperphysik, JKU Linz, Altenbergerstr. 69, AT-4040 Linz

Graphene, a two dimensional material made out of carbon atoms, provides unique physical properties and is a promising candidate for integrated optoelectronics. We demonstrate a waveguide integrated graphene photodetector on a standard SOI waveguide [1]. Operation over a wide wavelength range is achieved with a responsivity of 0.03 A/W for a 25×25 µm² bilayer graphene. The absorption efficiency can be further improved taking advantage of the local field enhancement of a slot waveguide. At the same time, the waveguide can be used to locally inject carriers in the graphene where the photocurrent is generated within a pn-junction.

[1] A. Pospischil et al., Nat. Phot. 7, 892 (2013)

257 Electrochemistry of Iron Oxide Model Surfaces

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Single-crystalline oxide thin films supported by metals are a well-accepted class of model system for studying fundamental aspects of oxide surface and thin oxide layer chemistry and physics. In the present contribution, we report on our efforts to expand this model approach to electrochemical studies on well-ordered oxide surfaces. Single-crystalline FeO(111) and Fe_3O_4(111) films were grown under ultrahigh vacuum conditions on a Pt(111) substrate and subsequently transferred into air or brought into contact with aqueous solutions. We have tested the stability of the oxide layers in these environments and characterized their electrochemical properties by cyclic voltammetry. Finally, the surface morphology and potential-dependent surface structure changes were investigated in-situ by electrochemical scanning tunneling microscopy.

258 Charge dependent adsorption of carbon dioxide on fullerenes

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In the following work the charge-dependent adsorption of CO_2 on cold (0.37 K), charged buckminsterfullerens (C_{60}) was investigated. It has been shown that the packing density in the first solvation shell around the fullerene is increased by a factor of ≈ 25% for positively charged C_{60} in comparison to negatively charged species. This was confirmed in both, mass spectrometric experiments, as well as theoretical investigations.

259

Creating Ordered Indium Adatoms on the In_2O_3(111) surface

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Indium oxide is one of the most important TCOs but little is known about the fundamental surface properties. Here the In_2O_3(111) surface of single crystals is investigated with STM. The In_2O_3(111) surface can be transformed from a oxidized surface to one that is covered by single indium adatoms forming a (1 × 1) superstructure. Also the room temperature deposition of iron onto the oxidized surface results in adatoms forming a (1 × 1) superstructure. These iron-induced adatoms are not discernible from In adatoms in STM. It is hypothesized that In is pushed to the surface by strongly interacting Fe atoms.

260

Ion-beam-induced magnetic and structural phase transformation of fcc Fe thin films

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Ultrathin fcc Fe films on Cu(100) have been studied for their unique capability of magnetic (non- magnetic to ferromagnetic) and structural (fcc to bcc) transformation upon ion beam irradiation. This opens the possibility of direct writing of magnetic patterns by focused ion-beams. The simplicity of direct focused ion beam writing of ferromagnetic elements embedded in a nonmagnetic thin film makes these films an ideal candidate for the fabrication of magnetic nanostructures. However, pure fcc Fe films undergo a spontaneous transformation when their thickness exceeds ~2 nm (10 ML) [1]. We showed it is possible to grow transformable $Fe_{78}Ni_{22}$ films on Cu(100) without a limit in its thickness [2]. The next step was to grow transformable films on a variety of substrates while using Cu(100) buffer layer. We present the experimental results of $Fe_{78}Ni_{22}$/Cu(100) on Si(100) [3] and $SrTiO_3$(100) [4].

[1] J. Thomassen, et al., Phys. Rev. Lett. 69, 3831 (1992). [2] J. Gloss, et al., Appl. Phys. Lett. 103, 262405 (2013). [3] I. Hashim, et al., Appl. Phys. Lett. 63, 2833-2835 (1993). [4] A. J. Francis, et al., Thin Solid Films 496, 317-325 (2006).