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<td>13:30</td>
<td>201</td>
<td>Isolated Pd Sites on PdGa Model Catalyst Surfaces</td>
<td>Jan Prinz 1, Roland Widmer 1, Carlo A. Pignedoli 1, Daniele Passerone 1, Harald Brune 2, Oliver Gröning 1</td>
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<td>1 nanotech@surfaces, EMPA, Überlandstrasse 129, CH-8600 Dübendorf</td>
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<td>2 Institute of Condensed Matter Physics, EPFL, Station 3, CH-1015 Lausanne</td>
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<td>The site-separation principle or &quot;ensemble effect&quot; is a frequently</td>
<td>Discussed point in heterogeneous catalysis research. As the size of metallic clusters on surfaces is reduced, so are the</td>
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<td>presented model catalyst system. A combined experimental-computational approach is presented, revealing adsorption</td>
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<td>characteristics which can be assigned to the different extends of active-site separation on various single crystal</td>
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<td>various single crystal facets.</td>
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<td>13:45</td>
<td>Metal clusters and simple adsorbates on ultra-thin ZrO$_2$/Pt$_3$Zr</td>
<td>Joong Il J. Choi, Wernfried Mayr-Schmölzer, Florian Mittendorfer, Josef Redinger, Ulrike Diebold, Michael Schmid</td>
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<td>Ultra-thin ZrO$_2$ films were prepared by oxidation of a Pt$_3$Zr(0001) crystalline</td>
<td>Results in molecular water binding to Zr. The experimental desorption energy of water is 1.05 eV, and the adsorption strongly depends on the site w.r.t. the substrate. Atomic H forms hydroxyl groups with the surface oxygen atoms; DFT shows a high adsorption energy (2.6 eV). Silver on ZrO$_2$/Pt$_3$Zr(0001) at RT results in clusters with a huge contact angle and (111) orientation.</td>
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<tr>
<td>14:00</td>
<td>203</td>
<td>Mechanics of single molecules</td>
<td>Ernst Meyer, Department of Physics, University of Basel, Klingelbergstr. 82, CH-4056 Basel</td>
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<td>Single molecules are investigated by high resolution force</td>
<td>Microscopy. Accurate positioning gives the opportunity to rotate porphyrin molecules either clock- or anti-clock wise in a</td>
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<td>porphyrin molecules either clock- or anti-clock wise in a</td>
<td>R. Pawlak, S. Fremy, S. Kawai, T. Glatzel, H. Fang, L.-A. Fendt, F. Diederich, and E. Meyer, Directed rotations of single</td>
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<td>controlled manner. Associated dissipation energies are measured</td>
<td>porphyrin molecules controlled by localized force spectroscopy, ACS Nano, 6, (2012), 6318-6324.</td>
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<tr>
<td>14:30</td>
<td>204</td>
<td>Initial steps of indigo film growth on silicon dioxide</td>
<td>Boris Scherwitzl, Adolf Winkler, Roland Resel</td>
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<td>Institute of Solid State Physics, TU Graz, Petersgasse 16, AT-8010 Graz</td>
<td>Studies of the initial stages of organic film growth are essential for a full understanding and best control of building processes of organic microelectronic devices. This contribution focuses on the initial growth behavior of thin indigo films on a silicon dioxide substrate under UHV conditions with respect to sample treatments. Films from sub-monolayer up to multilayer range were created using physical vapor deposition and subsequently analyzed with Auger Electron Spectroscopy, Thermal Desorption Spectroscopy, Atomic Force Microscopy and X-Ray Diffraction. It could be shown that indigo films tend to dewet already at very low coverages and form bulk-like structures bound by hydrogen bonds.</td>
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Effective control of chirality in supramolecular systems is an important challenge towards the assembly of well-defined nano-architectures from the bottom-up. The chirality transfer from single molecules onto 3D- and 2D-crystals is well known, however chirality in case of the 1D-objects (wires) is largely unexplored. Here we present a study based on Scanning Tunnelling Microscopy (STM) and X-Ray Photoelectron Spectroscopy (XPS) measurements and Density Functional Theory (DFT) calculations to understand the formation of 1D conglomerates from enantiopure dicyano functionalized heptahelicene molecules of both chiralities at different, well defined single-crystal surfaces. We show that the main bonding motif can be switched by temperature, substrate or adatom stimuli. We discuss the key driving forces for the formation of well-ordered long-range arrays and the chirality transfer on the single molecule scale as well as onto the 1D conglomerate as a whole. In comparison of experiment and theory, we deepen the insight into the chirality transfer in competition between molecule-molecule and surface-molecule interactions.

In photoelectron emission microscopy (PEEM), the polarization of the exciting light is usually not taken into account, but may reveal valuable information about the anisotropy of the surface. As an example, we studied the growth of alpha-sexithiophene on silver and nickel oxide surfaces. The light of a Hg lamp can only excite electrons from the metal-organic interface, since the ionization potential of the molecules is higher than the available photon energy. Although the molecules do not emit photoelectrons, they are optically anisotropic and act as dichroic filters for the incident light which results in a net anisotropy of the local electron yield measured accross the organic crystallites.

The tomographic analysis of the ARUPS data cube into band (E vs. k) and momentum (k_x vs. k_y) maps reveal changes in both the substrate and molecule electronic structure upon the formation of the pentacene monolayer. In the region down to 1 eV below the Fermi edge the momentum maps clearly show a 5 Å LUMO intensity distribution with a large dispersion of ~ 0.7 eV in the direction of the long molecular axes. This contrasts to the calculated dispersion of a free standing 5 Å monolayer of only 20 meV and a truly significant enhancement of intermolecular dispersion is claimed. The strong periodic potential of the 5 Å overlayer also leads to a remarkable opening of a band gap in the observable substrate sp bands.

Supported by the Austrian Science Foundation (FWF Projects P21330-N20 and P23190-N16). We also thank the staff of Helmholtz-Zentrum BESSY II.
**Ohmic contacts for resistance measurements of ultra-thin metal-on-silicon layers**

*Bernhard Lutzer, Ole Bethge, Christina Zimmermann, Emmerich Bertagnolli*

_Institut für Festkörperelektronik, Technische Universität Wien, Floragasse 7, AT-1040 Wien_

Substrates with a high charge carrier mobility are a key issue in the progress of semiconductor technology and its further scaling. Possible alternative candidates for high-mobility substrates are ultrathin (< 5 nm) metal layers (e.g. lead, gold or silver) on silicon (111) surfaces. The appearance of nearly massless electrons in such structures can be accounted to an overlapping of surface states at the silicon-metal interface [1]. To characterize these thin metal-on-silicon layers, TLM (Transfer Length Method) measurements are used. This method [2] allows specifying the sheet resistance of a layer and the contact resistance of the structure. In this work, different approaches to establish ohmic contacts to the interface layer without interfering with the sensitive ultra-thin metal layer are discussed. Furthermore, measurements of the contact resistance as well as the sheet resistance of different metal layers are shown.

to calculate anisotropic surface dielectric function and then RAS of Cu(110) surface with the latest studied adsorbed water structures. At the end the effect of different adsorption structures on RAS and surface states is studied.

### 17:00 215

**Organic Semiconductors Interfaces Explored With Ab-initio Electronic Structure Methods**

*Peter Puschnig, Institut für Physik, Karl-Franzens-Universität Graz, AT-8010 Graz*

The performance of organic devices depends strongly on the properties of organic-organic and organic-inorganic interfaces. It is shown how density functional theory (DFT) and many-body perturbation theory methods shed light on the electronic properties of organic molecules and their interfaces. First, a simple but powerful relation between the angle-resolved photoemission intensity and the spatial distribution of molecular orbitals will be established. It allows a detailed comparison between theory and photoemission experiments and a benchmarking of exchange-correlation functionals. Second, the model interface between a conducting polymer and graphene is studied at the G0W0 level revealing a band structure re-normalization arising from polarization effects which are absent in DFT.

### 17:30 216

**Solid-solid interfaces in metal oxide nanoparticle ensembles**

*Oliver Diwald, Department of Materials Science and Physics, University of Salzburg, Hellbrunnerstrasse 34/ III, AT-5020 Salzburg*

The exploration of interfacial phenomena in agglomerated oxide nanoparticles and the identification of related synergistic effects are vital to the development of functional particle systems. Semiconducting metal oxide particles and MgO cubes were used as nanoparticulate model systems [2]. We quantitatively characterized the effect of particle powder consolidation on photoelectronic property changes and discussed them in the light of results from first-principles calculations [3].


### 17:45 217

**Single gold nanoparticles as nanoscopic pH-sensors**

*Cynthia Vidal 1, Martin Djiango 1, Calin Hrelescu 1, Thomas A. Klar 1, Andrei I. Mardare 2, Achim Walter Hassel 2*

1 Institute of Applied Physics, Johannes Kepler University Linz, Altenberger Str. 69, AT-4040 Linz
2 Inst. for Chem. Tech. of Inorganic Materials, Johannes Kepler University Linz, Altenberger Str. 69, AT-4040 Linz

We report on the pH-dependence of the reversible oxidation and reduction of single gold nanoparticles. Electrochemical and optical dark field spectroscopy measurements reveal insights in the oxide formation and removal processes. In combination with cyclic voltammetry results, the spectral shift of the nanoparticle plasmon can be correlated with electrochemical phenomena. Changing from an acidic environment to a more basic one, a shift of the hydroxyl reduction potential to lower values is observed. The spectral blue shift of the nanoparticle plasmon attributed to the oxide reduction exhibit the same pH dependence of the reduction potential as measured with cyclic voltammetry.

### 18:00 218

**Efficient random lasing from star-shaped nanoparticles**

*Johannes Ziegler, Martin Djiango, Cynthia Vidal, Calin Hrelescu, Thomas A. Klar*

Institute of Applied Physics, Johannes Kepler University Linz, Altenberger Straße 69, AT-4040 Linz

Random lasing, i.e the emission of narrow bandwidth light, occurs when scattering nanostructures form random resonator cavities that interact with a surrounding gain medium. We investigate random lasing from dye-doped polymer thin films with embedded gold nanoparticles. When the films are excited with ns-pulses in a variable stripe length geometry, we observe the onset of emission with narrow linewidth as well as superlinear behaviour of the peak intensities with increasing pump fluxes. In particular, we examine the influence of differently shaped gold nanoparticles on the random lasing efficiency by comparing star-shaped nanoparticles to other nanoparticle shapes.
Research on nanostructures such as nanowires is of both fundamental and technological interest. Here, we investigated the self-assembly of in-plane SiGe nanowires under various growth conditions and for different compositions. Initially, Ge is deposited in a Stranski-Krastanow growth mode by molecular beam epitaxy on Si(001) substrates. The wires develop during thermal annealing at relatively low temperatures from the initial hut-clusters. The nanowires are terminated by \{105\} facets and are oriented along the \langle100\rangle directions. Lengths >1 micrometer are achieved. The demonstrated in-plane nanowires are promising candidates for nanoelectronic applications with full compatibility with standard Si technologies.

We are interested in controlling the magnetic properties of paramagnetic molecules adsorbed on ferromagnetic substrates. The transition-metal ions in the surface-adsorbed porphyrins / phthalocyanines have a free top site for an additional ligand to bind and to control the magnetic properties of the on-surface complex. We show switching-off, tuning and switching-on the magnetic moments in the adsorbed complexes. Because of the interaction with the surface, the exact outcome of those reactions can be different. The axial-ligand allows to modify this interaction and can thus be used to control the exchange-interaction with the substrate. We combine element specific x-ray magnetic circular dichroism (XMCD) with STM and DFT+U.

The competition between screening of local spins and magnetic interactions of neighbouring spins determines many of the electronic and magnetic properties of dilute magnetic systems. We report on low-temperature scanning tunneling microscopy (STM) and spectroscopy (STS) experiments performed on linear chains of surface-supported hydrocarbon spin-1/2 radicals. The spin chains are prepared by self-assembly of the stable sp magnetic radicals a,g-bisdiphenylene-b-phenylallyl (BDPA) on a single-crystal metal surface under ultrahigh vacuum conditions [1]. Below about 50 K the chains exhibit many of the characteristic properties of the Kondo effect observed by STM-based electron transport experiments at the atomic scale [2]. We find strong evidence for a parallel alignment of neighbouring spins within the chains mediated by the electron gas of the supporting metal substrate.
Spectroscopic imaging of radical chains reveals extended two-dimensional Kondo patterns. They span several nm$^2$ across the substrate area even into regions of the pristine Au substrate, indicating the involvement of surface-state electrons from the substrate. The single adsorbed radicals exhibit a handedness as revealed by topographic STM imaging at the single-molecule level, which leads to an enantio-selective chain growth and the formation of structurally different domains of neighboring radical chains.


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<td>14:15</td>
<td>223</td>
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| **Using AFM nanoindentation to investigate mechanical properties of cellulose fibers in controlled humidities**

Christian Ganser 1,4, Ulrich Hirn 2,4, Robert Schennach 3,4, Christian Teichert 1,4
1 Institute of Physics, Montanuniversität Leoben, Franz Josef - Str. 18, AT-8700 Leoben
2 Inst. of Paper, Pulp and Fibre Technology, TU Graz, Inffeldgasse 23, AT-8010 Graz
3 Institute of Solid State Physics, TU Graz, Petersgasse 16/2, AT-8010 Graz
4 Christian Doppler Laboratory for Surface Chemical and Physical Fundamentals of Paper Strength, TU Graz, Petersgasse 16/2, AT-8010 Graz

In papermaking, fiber-fiber bonds are formed in the wet state and dried consecutively. Thus, it is of interest to investigate mechanical properties of cellulose fibers used in papermaking as a function of relative humidity and in the fully wet state. For this purpose, we chose atomic force microscopy (AFM) nanoindentation because it combines the possibility to gently image the surface before performing actual nanoindentation. Starting at the fully dried state, surface hardness is around 240 MPa and is reduced moderately to 90 MPa at 80% relative humidity and drops further to 3 MPa at the fully wet state.

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| **Helium Atom Scattering Measurements of the Sb(111) Surface**

Michael Mayrhofer-Reinhartshuber, Markus Polanz, Patrick Kraus, Anton Tamtögl, Wolfgang E. Ernst
Graz University of Technology, Petersgasse 16, AT-8010 Graz

The semimetals antimony (Sb) and bismuth (Bi) can be found in a group of compounds, which are part of the recently discovered class of topological insulators [1]. Therefore, an accurate knowledge of their surface structure and dynamics is a prerequisite for further studies in this field. Intriguing properties, in particular subsurface phonon modes of Bi(111), were revealed by our group in previous works [2,3]. Lately, we performed helium atom scattering measurements of the Sb(111) surface. The angular positions and heights of the diffraction peaks were used to calculate the surface corrugation by using the Eikonal- as well as the GR-method. The surface Debye-temperature was found by analyzing elastic measurements at surface temperatures between 100 K and 450 K.


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| **Formation of HCN⁺ in Heterogeneous Reactions of N²⁺ and N⁺ with Surface Hydrocarbons**

Martina Harnisch 1, Alan Keim 1, Zdenek Herman 2, Paul Scheier 1
1 Inst. for Ion Physics and Applied Physics, University of Innsbruck, Technikerstraße 25, AT-6020 Innsbruck
2 J. Heyrovský Institute of Physical Chemistry, Academy of Sciences of the Czech R, Dolejškova 3, CZ-18223 Prague

Ion-surface collisions of low-energy ions of N²⁺ and N⁺ with hydrocarbon-covered room-temperature or heated surfaces of tungsten, carbon-fiber-composite, and beryllium showed significant increase of the ion yield at m/z = 27, not observed in analogous collisions of Ar⁺. This increase is ascribed to formation of HCN⁺ in heterogeneous reactions between N²⁺ or N⁺ and surface hydrocarbons, arising from cracked pump oil. While the formation of HCN⁺ via the reaction with N⁺ occurs barrier-less via an exoergic reaction, the reaction with N²⁺ could only be observed at incident energies above 50 eV suggesting an activation barrier or reaction endothermicity of about 3 - 3.5 eV.

Supported by the FWF project P23657.
100 nm gold films with -30±6 MPa residual stress were exposed to low temperature hydrogen plasma. After the plasma treatment, the films exhibited buckling zones localized inside circular boundaries. This is attributed to compressive stress exerted by the over-pressurized hydrogen gas at the trap zones in the film and at the coating interface. The sidewalls of the circular buckling zones were oriented with an angle of 7.7±1.0° to the substrate, indicating a critical buckling stress of -410±120 MPa. Several methods were investigated to suppress hydrogen-induced buckling. Among these, reducing the impact energy of the ions appeared to be the only effective method.

IV. Oxides

Chair: Ulrike Diebold, TU Wien

16:00 231 Growth and Morphology of Epitaxial MgO Films on GaAs(001)

Anirban Sarkar, Shibo Wang, Markus Gruber, Reinhold Koch
Institut für Halbleiter- und Festkörperphysik, Johannes-Kepler-Universität Linz, AT-4040 Linz

Intermixing at the interface between high-spin-polarization ferromagnetic layers and semiconductor templates is expected to significantly reduce the spin injection efficiency of spin and magnetoelectronics devices and recommends the use of appropriate diffusion barriers. Here we report on the growth of single-crystal MgO films on GaAs(001), which may be utilized as both, spin-filtering tunnel and diffusion barriers. In addition to structural and morphological results we present in-situ stress results that provide direct information on the strain relaxation of the MgO films, which plays a crucial role in the subsequent growth of Heusler films.

16:15 232 Compositional and structural study of homoepitaxial-STO based oxides heterostructures

Mathilde L. Reinle-Schmitt 1, Claudia Cancellieri 1, Andrea Cavallaro 2, Steven J. Leake 1, Christof W. Schneider 1, John A. Kilner 1, Philip R. Wilmott 1
1 Paul Scherrer Institut, Swiss Light Source, CH-5232 Villigen
2 Dep. of Materials, Imperial College London, South Kensington Campus, SW72AZ London, UK
3 Paul Scherrer Institut, Materials Group, CH-5232 Villigen

Complex oxides interfaces, and in particular the interface between LaAlO₃ (LAO) and SrTiO₃ (STO), have been the subject of intensive research in the last years. The unexpected interfacial conductivity between these band insulators may be particularly interesting for future integrated oxide-based electronic devices. Attempts to grow related structures, such as LAO on homoepitaxial-STO layers, or multilayers have been made. However as far as we know the new devices do not generally exhibit similar interfacial properties as standard LAO grown on STO. In this work we try to explain why LAO grown on top of homoepitaxial-STO behaves differently than expected, using low energy ion scattering and surface x-ray diffraction to study the composition and structure of the homoepitaxial-STO layers.

16:30 233 Single Metal Adatoms on Fe₃O₄(001)-(√2x√2)R45°

Gareth Parkinson, Zbynek Novotny, Roland Bliem, Michael Schmid, Ulrike Diebold
TU Wien, Wiedner Hauptstrasse 8-10/134, AT-1040 Wien

The (001) surface of magnetite (Fe₃O₄) exhibits a reconstruction that consists of undulating rows of surface atoms. When metals (Au, Ag, Pd, Ni, Fe) are vapor-deposited on Fe₃O₄ at 300 K, they adsorb as single atoms at specific sites within this reconstructed surface. This provides a unique opportunity for studying single-atom processes: isolated Au atoms [1] are stable against clustering up to 700 K, and one can follow the CO-induced sintering of Pd atoms [2] in real time with Scanning Tunneling Microscopy (STM).
**17:00 234**

**Water Gas Shift Chemistry at the Fe₃O₄ (001) Surface**

Oscar Gamba ¹, Roland Bliem ¹, Zbyněk Novotny ¹, Niclas Johansson ², Michael Schmid ¹, Joachim Schnadt ², Ulrike Diebold ¹, Gareth Parkinson ¹  

¹ Inst. für Angewandte Physik, TU Wien, Wiedner Hauptstr. 8-10/134, AT-1040 Vienna  
² Division of Synchrotron Radiation Research, Lund University, Box 118, SE-22100 Lund

Magnetite (Fe₃O₄) is an important material in heterogeneous catalysis [1], both as an active surface and as a support for metal nanoparticles. The water gas shift reaction, in which CO is oxidized to CO₂ and H₂O is reduced to H₂, is performed over an iron-oxide catalyst. Fe₃O₄ has been identified as the active phase, but important details such as the active intermediates and the reaction pathway are not clear [2]. Using a combination of high pressure XPS and STM, we study the reaction of H₂O and CO on the Fe₂O₃(001) surface and observe formation of formate and methoxy species.


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**17:15 235**

**STM and photoemission study of vacancies and hydroxyls at the SrTiO₃(110)-(4×1) surface**

Stefan Gerhold, Zhiming Wang, Xianfeng Hao, Michael Schmid, Ulrike Diebold  
Institut für Angewandte Physik, TU Wien, Wiedner Hauptstraße 8-10, AT-1040 Wien

The interaction of water with oxide surfaces is of great interest for both fundamental sciences and applications. We present a combined theoretical (DFT) and experimental (STM, photoemission) study of water interaction with a two-dimensional tetrahedrally coordinated TiO₄ overlayer at the SrTiO₃(110)-(4×1) surface. STM, core-level and valence band photoemission spectroscopy studies show that water dissociates at the oxygen vacancies, while it neither adsorbs nor dissociates at the stoichiometric surface. This is in agreement with DFT calculations. By comparisons with other tetrahedrally coordinated surfaces, our study suggests that two-dimensional tetrahedrally coordinated TiO₄ overlayers provide a hydrophobic surface.

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**17:30 236**

**Interface Fermi states of LaAlO₃/SrTiO₃ and related heterostructures**

Claudia Cancellieri ¹, Mathilde L. Reinle-Schmitt ¹, Masaki Kobayashi ¹, Vladimir N. Strocov ¹, Stefano Gariglio ², Jean-Marc Triscone ², Thorsten Schmitt ¹, Philip R. Willmott ¹  
¹ Paul Scherrer Institut, Swiss Light Source, CH-5232 Villigen PSI  
² University of Geneva, DPMC, 24 Quai Ernest-Ansermet, CH-1211 Geneva 4

At the interface between complex oxides, unexpected electronic properties different from those of the constituent bulk materials can arise. A particularly interesting example is the appearance of 2-dimensional conductivity at the interface of the band insulators LaAlO₃ (LAO) and SrTiO₃ (STO) above a critical LAO thickness of 4 unit cells (u.c.). The interfaces of LaAlO₃/SrTiO₃ and (LaAlO₃)_x(SrTiO₃)_{1-x}/SrTiO₃ (LASTO:x/STO) heterostructures have been investigated by soft x-ray photoelectron spectroscopy for different layer thicknesses across the insulator-to-metal interface transition. The valence band and Fermi edge were probed using resonant photoemission across the Ti L₂,₃ absorption edge. We measured clear spectroscopic signatures of Ti³⁺ signal at the Fermi level. Our results show that Ti³⁺-related charge carriers are present in both systems, but only for conducting samples.

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**18:00 237**

**Combined Spectroscopic Study of the Evolution from the Metallic Surface State on SrTiO₃ to the Interface of LaAlO₃/SrTiO₃**

Nicholas Plumb¹, Marco Salluzzo ², Thorsten Schmitt ¹, Ming Shi ¹, Joël Mesot ³, Luc Patthey ⁴, Milan Radović⁵  
¹ Swiss Light Source, Paul Scherrer Institut, CH-5232 Villigen PSI  
² CNR-SPIN, Complesso Universitario Monte S. Angelo, Via Cinthia, IT-80126 Napoli  
³ Paul Scherrer Institut, CH-5232 Villigen PSI  
⁴ SwissFEL, Paul Scherrer Institut, CH-5232 Villigen PSI

The LaAlO₃/SrTiO₃ (LAO/STO) interface famously hosts a metallic electron gas capable of superconducting and magnetic behavior. Recent experiments found that a universal metallic state can also exist on the bare surface of STO itself. This raises the possibility that the two systems are connected, and each may be able to teach us about the origins of metallicity and other properties in the other.
With this in mind, we have combined in situ high-resolution angle-resolved photoemission spectroscopy (ARPES) and soft x-ray ARPES (SX-ARPES), as well as resonant inelastic x-ray scattering (RIXS) in order to understand the electronic structure of the STO surface state and study its evolution during LAO deposition. The results show important similarities – and at least one key difference – between bare STO and LAO/STO interfaces.

**18:15 238 Field-induced migration of oxygen vacancies towards the surface of TiO$_2$ anatase(101)**

Martin Setvin, Philipp Scheiber, Benjamin Daniel, Michael Schmid, Ulrike Diebold
TU Wien, Wiedner Hauptstrasse 8-10/134, AT-1040 Wien

TiO$_2$ is a material known mainly for its photocatalytical properties but it has applications in many other fields – in photoelectrochemical cells, Li-ion batteries, and, possibly, in memristors for data storing. While the rutile phase of TiO$_2$ is well investigated in surface science, the metastable anatase phase is used in most applications and generally considered the technologically more relevant polymorph. Oxygen vacancies (VO) are more favorable in bulk than at the surface of TiO$_2$ anatase(101). As a consequence, an as-prepared anatase(101) surface does not contain any surface VO’s. These can be created at low temperature either by desorbing surface O atoms by means of electron bombardment, or by pulling subsurface VO’s to the surface by means of electric field of the STM tip. We show that O$_2$ adsorption on the anatase(101) surface also promotes migration of bulk VO’s towards the surface.

**18:30 Postersession and Apéro**

**20:00 Conference Dinner**

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**Friday, 06.09.2013, HS 1**

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<td>13:30</td>
<td>241</td>
<td>Observing Graphene grow: In-situ metrology for controlled growth of graphene and carbon nanotubes</td>
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<td><strong>Bernhard Bayer</strong> ¹, <strong>Robert Weatherup</strong> ¹, <strong>Piran Kidambi</strong> ¹, <strong>Raoul Blume</strong> ², <strong>Axel Knop-Gericke</strong> ², <strong>Carsten Baehz</strong> ³, <strong>Robert Schloegl</strong> ³, <strong>Stephan Hofmann</strong> ³</td>
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<td>¹ Dep. of Engineering, University of Cambridge, 9 JJ Thomson Avenue, CB3 0FA Cambridge, UK ² Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 99 DE-14195 Berlin-Dahlem ³ Helmholtz-Zentrum Dresden-Rossendorf, P.O. Box 510119, 99 DE-01314 Dresden</td>
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<tr>
<td>13:45</td>
<td>242</td>
<td>Electronic Structure of Atomically Precise Graphene Nanoribbons</td>
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<td><strong>Pascal Ruffieux</strong> ¹, <strong>Jinming Cai</strong> ¹, <strong>Hajo Söde</strong> ¹, <strong>Nicholas C. Plumb</strong> ², <strong>Luc Patthey</strong> ², <strong>Xinliang Feng</strong> ³, <strong>Klaus Müllen</strong> ³, <strong>Roman Fasel</strong> ¹</td>
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<td>¹ EMPA, Überlandstr. 129, CH-8600 Dübendorf ² Swiss Light Source, Paul Scherrer Institute, CH-5232 Villigen ³ MPI für Polymerforschung, Ackermannweg 10, DE-55128 Mainz</td>
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Graphene Nanoribbons (GNRs) offer great potential for future electronic and optoelectronic devices due to sizable electronic band gaps that are expected for narrow (<10 nm) GNRs. Recently, we reported a bottom-up fabrication protocol based on on-surface chemical routes to colligate and dehydrogenate specifically designed precursor monomers to form N=7 armchair GNRs (7-AGNRs) with atomic precision, a prerequisite for the control of the band gap magnitude [1]. Here, we report scanning tunneling spectroscopy (STS) and angle-resolved photoelectron spectroscopy (ARPES) results.
allowing for the determination of band gap and exact band dispersion of 7-AGNRs [2]. Furthermore, ARPES results are compared to Fourier-transformed STS (FT-STS) results, which additionally give direct access to the unoccupied band dispersion.


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<tr>
<td>14:00</td>
<td>243</td>
<td><strong>Optical characterization of atomically precise graphene nanoribbons</strong></td>
<td>Richard Denk¹, Michael Hohage¹, Jinming Cai², Pascal Ruffieux², Roman Fasel², Peter Zeppenfeld¹</td>
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¹ Experimental Physics, JKU LINZ, Altenbergerstrasse 69, AT-4040 Linz
² nanotech@surfaces, EMPA, Überlandstrasse 129, CH-8600 Dübendorf

Graphene nanoribbons (GNRs) promise high potential for future nanoscale electronic devices. While 2-dimensional graphene is semimetallic, electron confinement and edge effects in narrow (<10nm) GNRs can result in the opening of a band gap. Only recent advances in the bottom-up fabrication of atomically precise GNRs [1] have enabled reliable experimental investigations of well-defined GNRs. We have studied the optical properties of GNRs grown on Au(788) using reflectance difference spectroscopy (RDS), taking advantage of the optical anisotropy due to uniaxial alignment of the GNRs parallel to the step edges of the vicinal Au(788) surface.


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<tr>
<td>14:15</td>
<td>244</td>
<td><strong>Modification of exfoliated graphene: a case study</strong></td>
<td>Markus Kratzer¹, Stefan Klima¹, Andreas Nevosad¹, Christian Ganser¹, Borislav Vasić², Aleksandar Matković², Uroš Ravelić², Radoš Gajić², Christian Teichert¹</td>
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¹ Institute of Physics, Montanuniversität Leoben, Franz Josef Sraße 18, AT-8700 Leoben
² Institute of Physics, University of Belgrade, Pregrevica 118 P.O.Box 68, RS-11080 Belgrade

We investigated graphene (Gr) modifications via direct nanomechanical patterning by the AFM based dynamic plowing lithography (DPL) and the growth of para-hexaphenyl (6P) thin films on SiO2 supported exfoliated graphene. DPL turned out to be a viable tool for the local straining or even cutting of Gr.

Hot wall epitaxy of 6P resulted in temperature and Gr thickness dependent morphologies. While below 360K islands of upright standing molecules and needles of lying molecules coexist, exclusively needles are found above 360K. The Gr layer dependent growth morphologies are attributed to changes of the Gr surface energy with layer number.

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<tr>
<td>14:45</td>
<td>245</td>
<td><strong>In-situ thin film transistor fabrication: Electrical and surface analytical characterization</strong></td>
<td>Roman Lassnig¹, Bernd Striedinger², Alexander Fian², Barbara Stadlober², Adolf Winkler¹</td>
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¹ Solid State Physics, TU Graz, Petersgasse 16, AT-8010 Graz
² Materials, Joanneum Research Weiz, Franz-Pichler-Straße 30, AT-8160 Weiz

The underlying principles affecting performance and lifetime of organic semiconducting devices are still not fully understood. We present analysis on the formation and stability of Pentacene layers in organic field effect transistors (OFET) through a unique combination of organic layer deposition and in-situ electrical and surface analytical characterization during and subsequent to deposition, all performed under ultra-high vacuum conditions. Layer growth and performance parameters, such as layer thickness and device temperature were modified and evaluated. To reach conclusions about the layer growth mechanism and possible growth affecting contaminations, in-situ AES, TDS and ex-situ AFM were performed throughout the device fabrication.
### 15:00 246  
**Valve metal anodic oxides for flexible electronics**

*Andrei Ionut Mardare 1, Christian Siket 2, Martin Kaltenbrunner 2, Siegfried Bauer 2, Achim Walter Hassel 1*

1 ICTAS, Johannes Kepler University Linz, Altenberger Str. 69, AT-4040 Linz  
2 Soft Matter Physics, Johannes Kepler University Linz, Altenberger Str. 69, AT-4040 Linz

The anodic oxides grown on valve metals have a great potential for being used as dielectrics. The use of flexible plastic substrates for physical vapour deposition of valve metals (e.g. Al) is explored. A scanning droplet cell microscope (SDCM) is used for the electrochemical oxidation on the metal surface in a localized manner using both contact and free droplet modes. Direct writing of oxide lines is investigated and the oxide formation particularities as a function of the writing speed are described. The influence of various polymer substrates on the metallic film adhesion and anodic oxides growth is explored.

### 15:15 247  
**Direct writing of high-k metal oxide dielectrics for flexible large area electronics**

*Christian M. Siket 1, Martin Kaltenbrunner 2, Andrei I. Mardare 3, Tsuyoshi Sekitani 2, Takao Someya 2, Siegfried Bauer 1, Achim Walter Hassel 3*

1 Dep. of Soft Matter Physics, Johannes Kepler University Linz, Altenbergerstr. 69, AT-4040 Linz  
2 Department of Electrical Engineering, School of Engineering, University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, JP-1138656 Tokyo  
3 Inst. for Chem. Tech. of Inorganic Materials, Johannes Kepler University Linz, Altenbergerstr. 69, AT-4040 Linz

High-k dielectrics have potential in organic electronics for capacitors and as gate dielectric in field-effect transistors. By employing a scanning droplet cell microscope (SDCM), the direct electro-chemical writing of nm thick aluminium oxide structures is demonstrated, allowing fabrication and patterning in one single step. Metal-insulator-metal (MIM) capacitors and organic field-effect transistors (OFETs) on flexible polyethylene naphthalate (PEN) substrates are fabricated and show high performance. This proofs the applicability of the SDCM for fabrication of large area flexible electronic devices, widening the applicability for micro-electrochemical anodisation.

### 15:30 END
| 253 | **Molecule-Substrate Hybridization Revealed by Angle-Resolved Photoemission Spectroscopy**  
Dario Knebl, Bernd Kollmann, Daniel Lüftner, Peter Puschnig  
Institut für Physik, Karl-Franzens-Universität Graz, Universitätsplatz 5, AT-8010 Graz  
Within the past few years a close relation between the angle-resolved photoemission (ARPES) intensity of oriented molecular films and the spatial distribution of the respective molecular orbital has been demonstrated. So far, experimental ARPES data has been accounted for by neglecting the interaction of molecule with the underlying metal substrates. The remaining, small differences have been tentatively attributed to modifications of the molecular states due to molecule-substrate hybridization. Here, we calculate ARPES intensity maps of the prototypical monolayers PTCDA/Ag(110) and pentacene/Cu(110) by explicitly taking into account molecule-substrate interactions within ab-inito density functional calculations. By comparing simulated ARPES maps with experiment, we shed light on the possibility to extract information about molecule-metal hybridization from ARPES experiments and reveal limitations of the plane-wave final state approximation for such molecular films. |
| 254 | **Initial growth of quinacridone on Ag(111)**  
Thorsten Wagner, Michael Györök, Daniel Huber, Peter Zeppenfeld  
Experimental Physics, Johannes Kepler University Linz, Altenberger Str. 69, AT-4040 Linz  
The organic dye pigment quinacridone (QAC) may play a role as an outsider in view of record breaking organic semiconductors like pentacene or rubrene, but its dominant H-bonds might be a key to innovative device structures. This work focusses on the initial growth of QAC on Ag(111) surfaces at room temperature which has been studied by means of photoelectron emission microscopy (PEEM), STM and LEED. STM images of the as-deposited layer exhibit a simple, row-like stacking of parallel molecules which can be explained by H-bonds between adjacent, flat-lying molecules. After annealing to a temperature of T=550–570 K the structure changes to a stacking of dimers. |
| 255 | **Adsorption of quinacridone on Cu(110) and Cu(110)-(2x1)O surfaces**  
Harald Zaglmayr, Johannes Gall, Lidong Sun, Peter Zeppenfeld  
Inst. f. Experimentalphysik, JKU Linz, Altenbergerstraße 69, AT-4040 Linz  
In this work we studied the adsorption of the organic pigment, quinacridone (QAC) on the Cu(110) and the Cu(110)-(2x1)O reconstructed surface using in-situ reflectance difference spectroscopy (RDS) and ex-situ atomic force microscopy (AFM). In the case of the adsorption on Cu(110) the surface state is quenched linear during the formation of the first monolayer. For higher coverages an absorption feature with negative sign forms at 2.2eV. For the adsorption on the Cu(110)-(2x1)O surface the RD signal shows a higher optical anisotropy for the same amount of material than on the bare Cu(110) surface suggesting the formation of an highly ordered QAC thin film. |
| 256 | **Attachment-limited nucleation and growth of organic films: Pentacene on sputter modified mica (001)**  
Levent Tümbek 1, Alberto Pimpinelli 2, Adolf Winkler 1  
1 Institute of Solid State Physics, Graz University of Technology, Petersgasse 16/A, AT-8010 Graz  
2 Rice Quantum Institute, Rice University, Brockman Hall 337, Houston 77005, Texas, USA  
The morphology of organic thin films is crucial for the functionality of organic electronic devices. Understanding the initial growth and formation of organic thin films requires a detailed description of island nucleation. The island density as a function of the deposition rate and the distribution of the areas of the capture zones of islands measurements are used for determination of critical island size. Here we consider the aggregation of pentacene islands on sputter amorphized mica as a model system for weakly interacting substrates. We show that nucleation and growth is diffusion limited at low deposition rates, and becomes limited by hindered-attachment at high deposition rates. |
Inorganic electronics the detailed structure of the interface is crucial for device performance. In heterojunction photovoltaic cells thin films of two semiconducting materials are sandwiched between conducting electrodes. For the present study poly(3-hexylthiophen-2,5-diyl) (P3HT) is used as hole conductor and poly(9,9-diocetylfluorene-co-benzothiadiazole)(F8BT) as electron-conductor. P3HT films are prepared on optically transparent conducting indium-tin–oxide substrates. The second polymer layer was deposited on top of the P3HT layer by floating and aluminium was used as top electrode. X-ray reflectivity was used to characterise the thickness of the thin films and the interface roughness of F8BT and P3HT. The development of interface roughness was studied as a function of annealing time at 90°C, 100°C and 110°C and 120°C. The interface roughness increases with annealing time (between 2 min and 250 min) and this increase is weakly observable at 90°C, clearly visible at 100°C and drastically enhanced at higher temperatures. The device performance show a clear increase of the efficiency at small annealing times (2 min.) but after that a continuous decrease with the annealing time. This result suggests that increasing interface roughness has a negative influence to the device performance, which is in contradiction to the current model but in line with another experimental observation.
### Optical properties of metal doped ZnO thin films on glass and polymer substrates

Meirzhan Dosmailov, Josef Patek, Gabriela Sbarcea, Mihaela Girtan, Angela Vlad, Marius A. Bodea, Guru V. Naik, Alessandra E. Boltasseva, Thomas A. Klar, Johannes D. Pedarnig

1 Institute of Applied Physics, Johannes Kepler University, Altenbergerstr. 69, AT-4040 Linz
2 Photonics Laboratory, Angers University, 2, Bd. Lavoisier, FR-49045 Angers
3 School of Electrical and Computer Engineering, Purdue University, West Lafayette, IN, 47907, USA

Metal doped ZnO thin films are deposited on glass and polymer substrates by pulsed-laser deposition technique and the optical properties of films are measured in the UV / VIS / NIR range. Doping of films by aluminium or gallium produces transparent conductive oxide layers with high optical transmission in the visible (T) and low electrical resistivity at room temperature ($\rho$). Al doped ZnO films on polyethylene terephthalate foils show excellent properties ($T > 85\%; \rho = 1.3 \text{ m}\Omega \text{ cm}$) and may be used as electrodes for plastic solar cells. Al or Ga doped ZnO films on glass reveal an onset of metallic reflectivity in the near infrared at 1100 nm and a crossover to a negative real part of the permittivity at approximately 1500 nm. In comparison to noble metals, doped ZnO shows substantially smaller losses in the near infrared.

### Negative muonium as a local probe for the detection of the photo-induced inversion of a Ge surface layer


1 Paul Scherrer Institute, CH-5232 Villigen PSI
2 University of Alberta, Department of Physics, Edmonton T6G 2E1, Canada

The controlled manipulation of the charge carrier concentration in nanometer-thin layers is the basis of current semiconductor technology and of fundamental importance for device applications. Here we demonstrate the persistent inversion from n- to p-type in a 200-nm-thick surface layer of germanium wafers by illumination. The inversion with a half-life $> 12 \text{ h}$ is induced at $T = 220 \text{ K}$, and disappears after warming above 280 K. The increase of the hole carrier concentration in the surface layer is detected by low-energy muon spin rotation. We propose accumulation of photo-generated electrons in empty surface acceptor states as the origin of the inversion, and that thermal activation at $T \sim 280 \text{ K}$ liberates the electrons from the surface states.

### Short-Term Metastable Effects in Amorphous Silicon Solar Modules

Ankit Mittal, Marcus Rennhofer, Ingo Riedel

1 Department of Photovoltaic, Austrian Institute of Technology, Donau City Strasse 1, AT-1220 Vienna
2 Institute of Physics, Universität Oldenburg, Carl-von-Ossietzky-Straße 9-11, DE-26129 Oldenburg

A short term metastable effect of the electric parameters in thin film amorphous silicon photovoltaic modules was observed under low irradiation ($\sim 50 \text{ W/m}^2$). The characteristic voltage, fill factor and power output of an amorphous silicon module increases during illumination and relaxes again when stored in the dark. Further, observable changes in the amplitude of this effect after slow thermal annealing (reversed Staebler Wronski effect) at low temperatures were followed. These experiments confirm that the occurrence of the short term metastable effect in amorphous silicon devices is directly correlated to its defect structure.

### Oxide diffusion barriers on GaAs(001)

Shibo Wang, Anirban Sarkar, Reinhold Koch

Institut für Halbleiter- und Festkörperphysik, Johannes-Kepler-Universität Linz, AT-4040 Linz

Thin oxide layers functioning as tunnel contacts and/or diffusion barriers between a ferromagnetic electrode and a semiconductor template are expected to improve the spin injection efficiency by reducing the loss of the electrons' spin polarization at the interface. We present our recent results on the growth and properties of different oxide layers on GaAs(001) substrates, with emphasis on their structure, morphology, stress, strain relaxation, and electrical properties.

### Formation of Tungsten Oxide Nanolayers by (WO$_3$)$_3$ Cluster Condensation on Ag(100)

Thomas Obermüller, Margareta Wagner, Martin Denk, David Kuhness, Svetlozar Surnev, Falko P. Netzer

Surface and Interface Physics, Institute of Physics, Karl-Franzens University Graz, AT-8010 Graz

Ultra thin films of tungsten oxide have been intensively investigated in recent years due to their outstanding properties, enabling applications in heterogeneous catalysis, photoelectrochemistry and electrochromism. The preparation of ultra thin tungsten oxide nanolayers by traditional physical vapor deposition methods is, however, very difficult because of the extremely high melting point of tungsten. Here we propose a new method to
prepare tungsten oxide nanolayers via condensation of \((WO_3)_3\) cluster on a Ag(100) surface, whereby the Ag substrate plays an active catalytic role.

The formation of tungsten oxide nanolayers on a Ag(100) single crystal surface has been studied using STM, LEED and photo electron spectroscopy (PES) with use of synchrotron radiation. A \((WO_3)_3\) cluster beam has been created by sublimation of tungsten trioxide powder in a thermal evaporator under ultra-high vacuum conditions, and has then been directed onto the Ag(100) substrate. It was found that highly ordered extended tungsten oxide layers form when the substrate is heated to temperatures of 500°C, either during or after the deposition, while the tungsten clusters associate into fractal structures, when the substrate is at room temperature. The ordered tungsten oxide layers exhibit distinct Moiré patterns with different orientation and periodicity, which indicates a weak substrate-overlayer bonding. The PES measurements confirm this weak coupling in that the Ag 3d core level peaks remain unchanged, and reveal that the W-oxide stoichiometry is \(WO_3\).

Work supported by the ERC Advanced Grant SEPON.

### 266 Influence of the Ni content in AlCu alloy using the combinatorial approach.

Martina Hafner, Achim Walter Hassel, Andrei Ionut Mardare  
ICTAS, Johannes Kepler University Linz, Altenberger Straße 69, AT-4040 Linz

Al-Cu and Al-Cu-Ni thin film alloys were deposited by thermal evaporation to generate combinatorial material libraries. Investigations were done to characterize the performance of the films and the influence of the Ni content. The films were deposited on glass substrates and their microstructural properties and composition were investigated by SEM, EDX and XRD. The electrochemical behaviour of the thin films were studied by SKP and scanning droplet cell microscopy (SDCM). Electrochemical dissolution experiments were performed using a flow cell and the elements were detected with an AAS.

### 267 Susceptibility measurements of Ni clusters embedded in organic matrices

Mariella Denk, Robert Mittermair, Daniel Queteschnier, Richard Denk, Michael Hohage, Lidong Sun, Peter Zeppenfeld  
Institut für Experimentalphysik, JKU Linz, Altenbergerstr. 69, AT-4040 Linz

Reflectance Difference-Magneto Optic Kerr spectroscopy (RD-MOKE) and Atomic Force Microscopy (AFM) was used to study the morphologic and magnetic properties of organic magnetic molecules, namely, cobalt tetramethoxyphenylporphyn (CoT TPP) on Cu(110)-(2x1)O. Thick layers (≈ 100 nm) of organic molecules were used as host material for Ni cluster growth. The size, shape and distribution of the Ni particles strongly influences their optical and magnetic properties. By using an embedding organic matrix, we try to tune the inter-particle interactions as well as the coupling between the molecules and the metal clusters, which, for instance, will affect the superparamagnetic limit of the nanoparticles.

### 268 Investigation of Single Ni Adatoms on the Magnetite (001) Surface

Roland Bliem, Lukas Pernecky, Zbynek Novotny, Oscar Gamba, Michael Schmid, Ulrike Diebold, Gareth Parkinson  
Institute of Applied Physics, Vienna University of Technology, Wiedner Hauptstraße 8-10/134, AT-1040 Vienna

The investigation of reaction processes on single atom catalysts is a promising approach to unravel the mechanisms which make materials catalytically active. The Fe\(_3\)O\(_4\) (001) surface provides a model system for stable single metal adatoms at room temperature [1,2]. Here we report an STM and XPS study of the Ni/Fe\(_3\)O\(_4\) (001) system. High densities of single Ni adatoms remain stable up to 225°C, at which point they become incorporated in the Fe\(_3\)O\(_4\) lattice. The reactivity of the single Ni atoms toward CO, H\(_2\)O, O\(_2\), and H\(_2\) will be described and compared to Pd and Au [2].


### 269 Investigation of Exchange Coupled Composites with Scanning Transmission X-ray Microscopy

Phillip Wohlhüter ¹, Stephanie Stevenson ¹, Eugenie Kirk ¹, Carlos Vaz ¹, Christoforos Moutafis ¹, Jörg Raabe ¹, Patrick Matthes ², Christian Schubert ², Karl Güdel ², Harald Özelt ³, Thomas Schrefl ³, Manfred Albrecht ², Laura Heyderman ²  
¹ Paul Scherrer Institut, CH-5232 Villigen PSI  
² Institut für Physik, TU Chemnitz, Reichenhainer Str. 70, DE-09126 Chemnitz  
³ Fachhochschule St. Pölten, Matthias Corvinus-Straße 15, AT-3100 St. Pölten

Novel exchange coupled composites incorporating a hard and a soft magnetic layer have the potential for a number of applications including magnetic recording, sensors, MRAM and oscillators. We investigate the magnetic behaviour of ferromagnetic L10 FePt thin films exchange coupled to soft ferrimagnets, including
FeGd and FeTb, using Scanning Transmission X-ray Microscopy (STXM), which allows us to probe each layer individually, and magnetic force microscopy (MFM). Using a luminescence detection scheme, we are able to determine the magnetic domain configuration using STXM. From MFM measurements we find a compositional dependence of the domain structure in the ferrimagnetic films.

270 Spin resolved photoemission spectroscopy of Fe$_3$O$_4$: The effect of surface structure

Jiří Pavelec, Zbyněk Novotný, Martin Setvín, Michael Schmid, Ulrike Diebold, Gareth Parkinson
Institute of Applied Physics, Vienna University of Technology, Wiedner Hauptstr. 8-10/134, AT-1040 Vienna

Ever since DFT calculations have predicted half metallicity, magnetite (Fe$_3$O$_4$) has been considered an ideal spintronics material. Reported spin polarizations at $E_{\text{Fermi}}$ obtained from spin resolved photoemission spectroscopy (SPES) vary between 20 and 80 %. One potential problem is the surface sensitivity of SPES which probes a mixture of bulk and surface properties. We report SPES measurements for differently terminated Fe$_3$O$_4$ (001) surfaces and show that the surface structure has little impact on the measured spin polarization near $E_{\text{Fermi}}$. With ~25% our value is in line with previous measurements, suggesting magnetite is not a true half-metal.

271 Charge behavior on insulating monocrystallic surfaces by Kelvin probe force microscopy

Monika Mirkowska ¹, Markus Kratzer ², Christian Teichert ², Helmut Flachberger ¹
¹ Chair of Mineral Processing, Montanuniversität Leoben, Franz Josef Straße 18, AT-8700 Leoben
² Institute of Physics, Montanuniversität Leoben, Franz Josef Straße 18, AT-8700 Leoben

Detailed knowledge on the contact charging behavior of dielectric materials is of great interest for technological applications like tribocharging separation. The underlying mechanisms are still not well understood. The charging of quartz and calcite single crystal surfaces upon contact with an Atomic Force Microscope tip has been investigated using Kelvin Probe Force Microscopy. It turned out that the charging is strongly influenced by the sample history. Especially contact with different forms of water (bulk water or humid air) and sample heat treatment change the charging/discharging behavior significantly.

272 Stabilization of explosive compounds on metallic surfaces

Stefan Ralser, Michaela Hager, Thomas Möst, Paul Scheier
Ionenphysik, Universität Innsbruck, Technikerstrasse 25, AT-6020 Innsbruck

Previous experiments on explosives like RDX, TNT or PETN in gas phase have shown that these molecules decay easily into several fragments upon low-energy electron attachment. These unimolecular decompositions are rather time consuming (several µs) and can be quenched when the molecules are embedded in helium nano droplets. With the use of a variable temperature scanning tunneling microscope, electron induced fragmentation of explosives is investigated for molecules adsorbed on single crystal metal surfaces. This work is supported by the FWF project P23657

273 Characterizations of HOPG and Graphene Treated with Low Temperature Hydrogen Plasma

Baran Eren, Marcin Kisiel, Laurent Marot, Rémy Pawlak, Thilo Glatzel, Urs Gysin, Roland Steiner, Ernst Meyer,
Department Physik, Universität Basel, Klingelbergstrasse 82, CH-4056 Basel

Hydrogen LTP exposed HOPG and SLG is characterized with various experimental techniques such as photoelectron spectroscopy, Raman spectroscopy and scanning probe microscopy. Photoemission measurement of HOPG resembles features similar to those of cubic diamond. STM image of HOPG has various atomic scale charge density patterns were observed, which might be associated with different C-H conformers of graphane. Combined AFM-KPFM images of SLG show local work function variations of 60 meV as a result of hydrogenation, without any contribution from topography. Raman maps of SLG reveal a I(D)/I(G) of over 4 at hydrogenated zones, which 0 for the pristine parts.

274 Characterization of thin two-element compound material films by time-of-flight Low Energy Ion Scattering

Dietmar Roth, Dominik Goebel, Peter Bauer
Institut für Experimentalphysik, Johannes Kepler Universität Linz, Altenbergerstraße 69, AT-4020 Linz

Low Energy Ion Scattering (LEIS) is a versatile tool for surface analysis. In LEIS, the target material is bombarded by noble gas ions (primary energy: 500 eV – 10 keV), and the energy spectra of backscattered projectiles are analyzed. In this contribution, we present an analysis of nanometer films of two-element compound materials (e.g. TiN) by time-of-flight Low Energy Ion Scattering (TOF-LEIS). The following questions shall be addressed:
How precisely can the film thickness be determined? Is it possible to obtain information about, e.g., film roughness/thickness variation? To what extent are the results influenced by uncertainties in the stopping power?

275 Indication of phonon-assisted electron-hole relaxations on Sb(111) and Bi(111) in iHAS measurements

Patrick Kraus 1, Michael Mayrhofer-Reinhartshuber 1, Anton Tamtögl 1, Giorgio Benedek 2, Wolfgang E. Ernst 1
1 Institut für Experimentalphysik, Graz University of Technology, Petersgasse 16, AT-8010 Graz
2 Donostia International Physics Centre (DIPC), Paseo Manuel de Lardizabal 4, ES-20018 San Sebastián / Donostia

Approximations are a fundamental part of scientific work. Without them the systems under investigation would be far too complex and complicated to obtain results. The more important it is to know where these approximations begin to fail. Recently, a strong Kohn-like anomaly was found in the phononic dispersion relation of Bi2Se3 [1]. The supposed nesting vectors connect spin-opposing states on both of the sides of the Dirac cone which are non-equivalent. Thus the electron needs to undergo a non-adiabatic transition to make the softening of the phononic mode possible. This is even more problematic, since transitions that break the adiabatic approximation are not accessible by standard DFPT methods. Recent studies on the (111) surfaces of the semimetals antimony and bismuth revealed deep and narrow strongly pronounced features [2]. The positions of those apparent sudden phonon softenings correspond to an electronic relaxation between the opposite sides of the inner Rashba-split cone [3]. The necessary helicity of 1 which the electron needs to complete this transition can be supplied by a phonon. The helicity exchange between a phonon and an electron is only possible in materials with a strong spin-orbit interaction. Complete measurements of the anomalies found in Sb(111) and Bi(111) will be presented and compared with the relevant electronic data.


276 Determination of atmospheric corrosion of coated steel surfaces by in situ infrared reflection absorption spectroscopy (IRRAS)

Maurizio Musso 1, Johannes Steiner 1, Gerald Luckeneder 2, Hubert Duczaczek 2, Heinz Gsaller 3
1 Fachbereich Materialforschung und Physik, Universität Salzburg, Hellbrunnerstrasse 34, AT-5020 Salzburg
2 voestalpine Stahl GmbH, Forschung und Entwicklung, voestalpine-Straße 1, AT-4020 Linz
3 voestalpine Stahl GmbH, Umwelt- und Betriebsanalytik, voestalpine-Straße 1, AT-4020 Linz

Infrared reflection absorption spectroscopy (IRRAS) is a sensitive technique for measuring thin layers on metallic surfaces. The principal goal of this IRRAS study was the development of a reproducible and reliable in situ measurement procedure for the determination of corrosion of coated steel surfaces.

277 Al-Si thin films for hydrogen reference materials

Cezarina Cela Mardare, Andrei Ionut Mardare, Achim Walter Hassel
ICTAS, Johannes Kepler Universität, Altenbergerstraße 69, AT-4040 Linz

Finding reference materials for hydrogen trapped in metals is an ongoing issue. Thin films of silicon were deposited in vacuum by thermal evaporation. Loading of the Si layer with hydrogen was performed by filling the vacuum chamber with formic gas to a pressure close to the atmospheric one. Subsequently, an aluminium layer was deposited for trapping the hydrogen and to hinder its further release by the formation of native Al2O3 when the sample is exposed to air. The blocking properties of Al2O3 were assessed by measuring the hydrogen release during hot extraction with or without the aluminium coating.

278 Reactive co-sputtered Cu based thin film oxide libraries

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The development of new materials is of great interest for finding new property combinations. Thin films offer a wide range of applications benefiting from the special properties due to the preparation method. In this work Copper based laterally graded thin film material libraries were prepared on glass substrates. The films were produced by reactive co-sputter deposition using two component sectioned targets consisting of Copper and a second metal. Surface analyses determining the composition gradient as well as the microstructure were done by SEM and EDX. Furthermore measurements to determine the contact potential of the sample were performed using a scanning Kelvin Probe.