

Surfaces, Interfaces and Thin Films

Wednesday, 06.09.2023, Room 114

Time	ID	SURFACES, INTERFACES AND THIN FILMS I: SURFACE SCIENCE Chair: Jiri Pavelec, TU Wien
17:00	201	<p style="text-align: center;">Creation of the elusive carbon allotrope cyclo[18]carbon; a cyclic carbon molecule</p> <p style="text-align: center;"><i>Katharina Kaiser, IBM Research Zurich, Säumerstrasse 4, CH-8803 Rüschlikon</i></p> <p>Cyclo[n]carbons were predicted for decades to exist. Although a synthetic route was elaborated in the 1980's, and glimpses of cyclocarbons were detected in gas phase, they could never be stabilized long enough for characterization. AFM and STM at low temperatures allow triggering certain on-surface chemical reactions by atom manipulation and can facilitate the controlled formation of highly reactive molecules on inert surfaces. Using this approach, we formed cyclo[18]carbon on a thin layer of NaCl. By comparing high-resolution AFM images and AFM simulations of different predicted resonance structures, we identified possible ground state structures of cyclo[18]carbon adsorbed on bilayer NaCl.</p>
17:30	202	<p style="text-align: center;">Intrinsic defects on PtSe₂ vdW single crystals studied with ncAFM</p> <p style="text-align: center;"><i>Igor Sokolovic^{1,4}, Bing Wu², Zdenek Sofer², Aleksandar Matkovic³, Michael Schmid⁴, Ulrike Diebold⁴, Tibor Grasser¹</i></p> <p style="text-align: center;">¹ Institute of Microelectronics, TU Wien ² Dep. of Inorganic Chemistry, University of Chemistry and Technology, Prague, Czech Republic ³ Chair of Physics, Montanuniversität Leoben, Leoben, Austria ⁴ Institute of Applied Physics, TU Wien</p> <p>In this research, surfaces of van-der-Waals-bonded single-crystal PtSe₂ cleaved in ultrahigh vacuum (UHV) were studied with non-contact atomic force microscopy (ncAFM) to simultaneously reveal their atomic and electronic structure. Typical ionic and electronic defects present on the cleaved surfaces were characterized with single-atom precision to reveal the proclivity of the layered Dirac semi-metal PtSe₂ toward different defect types compared to the synthesized single trilayer thin films of semiconducting PtSe₂ and other Pt-based TMDs. Cleaving reveals the intrinsic distribution of defects within the bulk, while such surfaces can also be considered representative of the commonly exfoliated and stacked PtSe₂ thin sheets used in complex heterostructures.</p>
17:45	203	<p style="text-align: center;">Selective adsorption of DHTAP on the nanostructured Cu-CuO stripe phase</p> <p style="text-align: center;"><i>Claudia López-Posadas¹, Antony Thomas², Thomas Leoni², Olivier Siri², Conrad Becker², Peter Zeppenfeld¹</i></p> <p style="text-align: center;">¹ Institute of Experimental Physics, Johannes Kepler University Linz ² Aix-Marseille University, CNRS, CINaM</p> <p>We have studied 5,14-dihydro-5,7,12,14-tetraazapentacene (DHTAP) layers on the regularly patterned Cu(110)-(2x1)O stripe phase. Using Reflectance Difference Spectroscopy (RDS) and Scanning Tunneling Microscopy (STM) we find that the DHTAP molecules preferentially adsorb on the Cu(110) stripes, with their long molecular axis aligned parallel to the [-110]-direction. In contrast, on the subsequently covered Cu(110)-(2x1)O stripes, the DHTAP molecules are aligned parallel to the [001]-direction. The evolution of the RDS signal allows to monitor the sequential adsorption and orientation of DHTAP for different oxygen pre-coverages and, hence, different Cu and CuO stripe widths. Interestingly, beyond the first monolayer, the DHTAP molecules adopt a preferential orientation which critically depends on the initial oxygen coverage.</p>

18:00	204	<p style="text-align: center;">Heterogeneous Photocatalysis: Alcohols on Bare and Metal-decorated Titania(110) and Hematite(012)</p> <p style="text-align: center;"><i>Moritz Eder¹, Ulrike Diebold¹, Ueli Heiz², Gareth Parkinson¹, Jiri Pavelec¹, Philip Petzoldt², Michael Schmid¹, Martin Tschurl²</i> <i>¹ Institute of Applied Physics, TU Wien, ² TU Munich</i></p> <p>We investigated the surface (photo)chemistry of alcohols on TiO₂(110) and recently Fe₂O₃(012) single crystals in ultra-high vacuum. Our studies focused on the role of the metal co-catalyst in the photocatalytic reaction by comparing the reactivity of bare and metal-decorated surfaces. We show that photocatalytic reactions are not merely a couple of redox reactions, but an interplay of thermal and photon-driven steps.</p> <p>On TiO₂(110), the alcohol photoconversion allows for a steady-state production of molecular hydrogen and aldehydes/ketones. We rationalize the findings with a comprehensive mechanism taking into account stoichiometry and charge-carrier dynamics. The identification of surface mechanisms on Fe₂O₃ is less advanced, but there seem to be parallels in the photochemistry.</p>
18:15	205	<p style="text-align: center;">Exploring the surface atomic and electronic structure of the multiferroic Rashba semiconductor Ge_{1-x}Mn_xTe</p> <p style="text-align: center;"><i>Martin Heinrich¹, Juraj Krempasky¹, Matthias Muntwiler¹, Gunther Springholz²</i> <i>¹ Paul Scherrer Institute ² Institut für Halbleiter-und Festkörperphysik, Johannes Kepler Universität, Linz, Austria</i></p> <p>GeTe is a IV-VI semiconductor compound with existing applications in optoelectronics and thermoelectrics. In addition to ferroelectricity and a large Rashba spin splitting in GeTe, doping with Mn atoms introduces ferromagnetism, which makes Ge_{1-x}Mn_xTe a magnetoelectric multiferroic with coupled electric and magnetic polarization and a promising candidate for spintronic applications. In this project, we use synchrotron based photoelectron diffraction (XPD, PhD) and spectroscopy (XPS, ARPES) and scanning tunneling microscopy (STM, STS) to gain a detailed understanding of its surface atomic and electronic structure and the inherent multiferroic couplings.</p>
18:30	206	<p style="text-align: center;">An STM investigation on the CO₂ activation and conversion on Au/MgO(001) ultrathin film</p> <p style="text-align: center;"><i>Francesco Presel¹, Hans-Joachim Freund², Martin Sterrer¹</i> <i>¹ University of Graz, ² Fritz Haber Institut der Max Planck Gesellschaft</i></p> <p>In previous research, we have shown that single-layer Au nanoislands on ultrathin MgO/Ag(001) can catalyze activation of CO₂ to oxalate (CO₂)₂ — a stable intermediate for chemicals and synthetic fuels — even below room temperature.</p> <p>Here we identified with STM the oxalate species present on the surface after reaction, which was only observed in presence of single-layer Au islands after exposure to CO₂ at 200-300 K. Most surprisingly, this species was not located beside the Au islands: being the adsorbate species not mobile on the surface, this suggests that the reaction might involve a complex process, with electrons first tunnelling through the MgO into the gold, then diffusing over MgO.</p>
18:45	207	<p style="text-align: center;">Structure and nanoscale dynamics at carbon materials and interfaces: From organic aromatics to nucleobases</p> <p style="text-align: center;"><i>Philipp Maier¹, Noah J. Hourigan¹, Neubi F. Xavier Jr.², Marco Sacchi², Peter Fouquet³, Anton Tamtögl¹</i> <i>¹ Institute of Experimental Physics, Graz University of Technology ² Department of Chemistry, University of Surrey ³ Institut Laue-Langevin</i></p> <p>The high scattering cross section of neutron and helium beams towards hydrogen provides experimental access to the structure and dynamics of hydrogen containing molecules at carbon materials, including e.g. the molecular motion of water. I will present experimental and theoretical results of hydrogen containing molecules ad-sorbed on carbon surfaces. These include the structure and dynamics of deuterated pyrazine on graphite, providing insight in how the van der Waals interaction between adsorbates and the substrate influences adsorbate structure and stability. Moreover, I will present recent neutron-spin echo measurements of adenine and thymine ad-sorbed on graphite, to better understand hydrogen bond formation in DNA base pairs, tautomerisation rates, and proton tunnelling.</p>

19:00	208	<p align="center">C₂H₄ Adsorption on Clean and Rh-Decorated Fe₃O₄(001) Surface</p> <p align="center"><i>Chunlei Wang¹, Panukorn Sombut¹, Lena Puntischer¹, Manuel Ulreich¹, Jiri Pavelec¹, Matthias Meier^{1,2}, Ulrike Diebold¹, Cesare Franchini^{2,3}, Michael Schmid¹, Gareth Parkinson¹</i></p> <p align="center">¹ Institute of Applied Physics, TU Wien, Austria ² Computational Materials Physics, University of Vienna ³ Alma Mater Studiorum, Università di Bologna, Italy</p> <p>The adsorption of ethylene (C₂H₄) is a crucial step in many important industrial reactions. Recently, novel single-atom Rh₁ heterogeneous catalysts have shown excellent activity and selectivity for hydroformylation reactions (e.g., C₂H₄ + CO + H₂ = CH₃CH₂CHO). However, a fundamental understanding of the catalytic mechanisms remains elusive. As a first step towards this goal, Rh₁ adatoms were deposited on a well-defined single-crystal Fe₃O₄(001) surface, and various surface-sensitive techniques under ultra-high vacuum conditions in combination with density functional calculations were used to investigate the behavior of C₂H₄ adsorption. In addition, the adsorption on clean Fe₃O₄(001) surface is also investigated as control experiments.</p>
19:15	209	<p align="center">Atomic-Level Studies of CO/Rh₁ and (CO)₂/Rh₁ Formation on an Fe₃O₄(001) support</p> <p align="center"><i>Panukorn Sombut¹, Ulrike Diebold¹, Cesare Franchini², Zdenek Jakub¹, Matthias Meier¹, Gareth S. Parkinson¹, Jiri Pavelec¹, Lena Puntischer¹, Michael Schmid¹, Chunlei Wang¹</i></p> <p align="center">¹ TU Wien, ² University of Vienna</p> <p>Understanding the interaction between reactant molecules and “single-atom” active sites is important for comprehending the evolution of single-atom catalysts in reactive atmospheres. Here, we study the interaction between CO and Rh₁ and Rh₂ species supported by Fe₃O₄(001) using DFT and experimental surface science techniques. Stable Rh₁(CO)₁ is formed via CO adsorption at both 2-fold and 5-fold to oxygen-coordinated Rh₁ sites. While DFT suggests Rh₁(CO)₂ to be energetically favorable, only a minority of these are observed experimentally. Instead, the limited Rh₁(CO)₂ is observed experimentally via CO-induced Rh₂ dimer breakup. Experiment and DFT results suggest this process occurs via an unstable Rh₂(CO)₃ intermediate.</p>
19:30		

Thursday, 07.09.2023, Room 114

Time	ID	<p align="center">SURFACES, INTERFACES AND THIN FILMS II: THIN FILMS AND HETEROSTRUCTURES</p> <p align="center"><i>Chair: Chunlei Wang, TU Wien</i></p>
14:00	211	<p align="center">Fabrication of two-dimensional magnets by implanting phyllosilicates with Fe ions</p> <p align="center"><i>Christian Teichert¹, Muhammad Zubair Khan¹, Ulrich Kentsch², Nico Klingner², Gregor Hlawacek², Aleksandar Matkovic¹</i></p> <p align="center">¹ Chair of Physics, Montanuniversität Leoben, ² Helmholtz-Zentrum Dresden-Rossendorf e.V.</p> <p>Recently, we demonstrated weak ferromagnetism in two-dimensional Fe:talc at room temperature and proposed iron-rich phyllosilicates as a promising platform for air-stable magnetic monolayers. Since these minerals are rather rare and hard to synthesize, we suggest ion implantation to tailor the phyllosilicates' magnetic properties. Nonmagnetic, iron-free single-crystalline talc bulk samples were implanted with 50 keV Fe⁺ beams at different substrate temperatures. Ultrathin layers could be exfoliated indicating that the layered crystal structure is maintained after ion irradiation. The Mg-OH Raman peak showed a triplet formation implying a successful substitution of Mg by Fe in the talc layers.</p>

14:30	212	<p style="text-align: center;">Thin Film Structure of the Asymmetric Ph-BTBT-10 Molecule for Application in Organic Thin Film Transistors</p> <p style="text-align: center;"><i>Roland Resel, TU Graz, Yves Geerts, University Libre Brussels</i></p> <p>The class of benzothieno-benzothiophene (BTBT) type molecules are among the best performing organic semiconductors in thin film transistors. The asymmetry of the molecule induces specific thin film forming properties and unique crystallographic features. We see the nucleation of the thermodynamic stable phase at the substrate surface and a transition to a metastable phase at the subsequent film growth. Peak broadening effects could be referred to defects by integration of reversed molecules into the crystal structure. This work reveals that the reversal of the molecular orientation at the substrate surface is the dominant effect in the crystallisation kinetics within thin films.</p>
	210	<i>cancelled</i>
14:45	214	<p style="text-align: center;">Ultrathin $\text{La}_{0.8}\text{Sr}_{0.2}\text{MnO}_3$ films with enhanced magnetic properties</p> <p style="text-align: center;"><i>Gyanendra Panchal, Federico Stramaglia, Frithjof Nolting, Carlos A. F. Vaz, PSI</i></p> <p>We report the effect of inserting LaMnO_3 and $\text{La}_{0.45}\text{Sr}_{0.55}\text{MnO}_3$ buffer layers on the magnetic properties of epitaxial ultrathin $\text{La}_{0.8}\text{Sr}_{0.2}\text{MnO}_3$ films on $\text{SrTiO}_3(001)$ substrate. The LaMnO_3 induces a bulk-like magnetic moments for $\text{La}_{0.8}\text{Sr}_{0.2}\text{MnO}_3$ down to 1 uc thickness, the $\text{La}_{0.45}\text{Sr}_{0.55}\text{MnO}_3$ induces antiferromagnetic order on the first 3 uc $\text{La}_{0.8}\text{Sr}_{0.2}\text{MnO}_3$ and bulk-like moments at larger thicknesses. In both cases, the bulk-like moment is confirmed by a linear increase in the magnetization, with a slope $m = 3.8 \mu\text{B}/\text{Mn}$. XMCD measurements confirm our magnetic results; XLD demonstrate the presence of an orbital reorganization at 3-4 uc. We attribute the full spin polarization of the $\text{La}_{0.8}\text{Sr}_{0.2}\text{MnO}_3$ films to a charge carrier transfer into the adjacent buffer layer.</p>
15:00	215	<p style="text-align: center;">Revealing the electronic structures of SrTiO_3 membranes and related heterostructures</p> <p style="text-align: center;"><i>Hang Li¹, Alla Chikina¹, Nicholas Clark Plumb¹, Nini Pryds², Milan Radovic¹, Ming Shi¹, Shinhee Yun²</i> <i>¹ Paul Scherrer Institute, ² Technical University of Denmark</i></p> <p>Transition metal oxide (TMO) exhibit exotic physical properties, which generally originated from the strong interplay between the charges, spins, orbitals, and lattice degrees of freedom. Therefore, developing methods for manipulating this coupling yields opportunities for realizing many novel quantum phenomena. Recent studies establish routes to exfoliate free-standing TMO membranes, raising a promising method for realizing 2D TMO systems.</p> <p>In this presentation, I'll introduce our new ARPES studies on high-quality SrTiO_3 membranes and SrNbO_3 films grown on as-received STO membranes, showing high spectra quality. Our studies demonstrated that STO membranes are an advantageous platform for 2D electronic systems and can be utilized as a wafer for assembling complex oxide heterostructures.</p>
15:15	216	<p style="text-align: center;">Long Ranged Proximity Induced Interactions in $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}\text{Sr}_2\text{IrO}_4$ Thin Film Multilayers Revealed by X-ray Absorption Spectroscopy</p> <p style="text-align: center;"><i>Jonas Knobel¹, Subhrangsu Sarkar¹, Mathias Soulier¹, Roxana Gaina Capu^{2,1}, Christian Bernhard¹, Fabrice Wilhelm³, Andrei Rogalev³, Peter Nagel⁴, Stefan Schuppler⁴</i> <i>¹ University of Fribourg, ² West University of Timisoara, RO, ³ ESRF, ⁴ KIT</i></p> <p>Heterostructures consisting of the high-T_c superconductor $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ (YBCO) and the iridate Sr_2IrO_4 (SIO) have been predicted to host induced superconducting spin-triplet or Majorana bound states and to find applications in devices such as superconducting diodes.</p> <p>Using X-ray Absorption Spectroscopy, we observe a large charge transfer in multilayers of these materials with holes being transferred from YBCO to SIO, leading to insulating behavior for thin YBCO layers. We also study the influence of the interface on the magnetism of both materials with X-ray circular dichroism.</p> <p>This work provides important insights on the interaction at the interface which is a crucial step towards real life applications and devices made from these heterostructures.</p>

15:30	217	<p style="text-align: center;">Characterization of Atomically Precise Graphene Nanoribbons by Raman Spectroscopy</p> <p style="text-align: center;"><i>Jeong Ha Hwang, Amogh Kinikar, Mickael Lucien Perrin, Roman Fasel, Gabriela Borin Barin, Empa</i></p> <p>Raman spectroscopy has been widely used to characterize graphene nanoribbons (GNRs) as it is possible to probe GNR quality from growth in ultra-high vacuum (UHV) until device integration. However, implementing this technique to study GNRs intrinsic spectroscopic properties remains challenging, as their synthesis requires UHV environment and many of these GNRs are reactive and air-sensitive. Here, we propose a UHV chamber where in-situ growth and Raman characterization are possible. We studied short 7-AGNRs with unique zigzag/armchair aspect ratio that allowed us to investigate the zigzag edge reactivity upon their exposure to air. Further, we will also discuss the effect of controlled oxygen exposure on characteristic Raman transitions of the GNRs.</p>
15:45	218	<p style="text-align: center;">Intercalation of graphene nanoribbons with carbenes in ultra-high vacuum</p> <p style="text-align: center;"><i>Dominik Lüthi ¹, Lin Yang ², Ji Ma ², Akimitsu Narita ^{3,4}, Xinliang Feng ², Pascal Ruffieux ¹, Roman Fasel ¹, Gabriela Borin Barin ¹</i> ¹ Empa, ² TU Dresden, ³ Max Plank Institute for Polymer Research, ⁴ Okinawa Institute of Science and Technology</p> <p>Atomically precise graphene nanoribbons (GNRs) have been synthesized by on surface-synthesis of specific precursors on metallic substrates in ultra-high vacuum (UHV). The enhanced chemical reactivity of zigzag edge states of reactive GNRs has hindered their transfer and device integration. Here, we studied the intercalation of various GNRs with carbenes (BIM) as a promising route towards dry-transfer of GNRs in UHV. The intercalation occurs due to the formation of a dense self-assembled monolayer (SAM) on the surface, causing stochastic intercalation of GNRs. Intercalation also decreases the interaction with the underneath metal, allowing better access to GNRs electronic characterization and open a pathway to study the interaction of nanographenes with other surfaces.</p>
16:00	219	<p style="text-align: center;">Measuring Surface Parameters of Intercalated Graphene and their Correlation with the Substrate Coupling Strength</p> <p style="text-align: center;"><i>Noah J. Hourigan ¹, Giorgio Benedek ², Philipp Maier ¹, Joshua A. Robinson ³, Anton Tamtögl ¹, Maxwell Wetherington ³</i> ¹ Institute of Experimental Physics, Graz University of Technology ² Università di Milano-Bicocca, ³ The Pennsylvania State University</p> <p>Graphene can be grown via chemical vapour deposition on a silicon carbide substrate; thereafter, various elements can be intercalated between the graphene and the substrate. Here, we investigate bilayer graphene atop either intercalated 2D polar gallium, an intercalated hydrogen layer, or a simple carbon buffer layer. Using helium atom scattering (HAS) we probe surface characteristics such as the in-plane thermal expansion relationship, the electronic corrugation, and the electron-phonon coupling strength. We compare how these properties are affected by the intercalated material beneath. Despite HAS exclusively probing the graphene overlayer, we are able to detect subtle differences likely to be related to the substrate coupling strength.</p>
16:15		
16:30		Coffee Break

Time	ID	<p style="text-align: center;">SURFACES, INTERFACES AND THIN FILMS III: METHOD DEVELOPMENT <i>Chair: Moritz Eder, TU Wien</i></p>
17:00	221	<p style="text-align: center;">Distance-Dependence of Orbital Density Mapping Using a CO-Functionalized STM Tip</p> <p style="text-align: center;"><i>Fabian Paschke, Florian Albrecht, Leo Gross, Leonard-Alexander Lieske IBM Research Europe - Zurich</i></p> <p>In this work we use a CO tip to study the appearance of frontier molecular orbitals of pentacene as a function of the tip-sample distance. STM constant-height imaging reveals a transition from p- to s-wave dominated tunneling. We present a simple model that reproduces the distance-dependency due to the symmetry-dependent decay lengths of the CO tip states. The findings provide an additional control knob to identify molecular electronic and spin states, which often requires STM imaging of orbital densities and careful assignment to calculated molecular orbitals.</p>
17:15	222	<p style="text-align: center;">Microwave reflectance calibration in a scanning tunnelling microscope</p> <p style="text-align: center;"><i>Bareld Wit¹, Georg Gramse², Stefan Müllegger¹</i> ¹ <i>Institute of Semiconductor and Solid State Physics, Johannes Kepler University Linz, Austria</i> ² <i>Biophysics Institute, Johannes Kepler University Linz, Austria</i></p> <p>Recent advances in near-field scanning microwave microscopy enable characterisation of nano-scale functional materials, surfaces, and nanoelectronic devices up to GHz frequencies and with sub-micron resolution. Material properties, including dielectric permittivity and dopant concentration have been detected in a microwave-adapted atomic force microscope at ambient conditions. We show our STM-based microwave reflectance set-up and report a quantitative in-situ procedure for impedance calibration in ultra-high vacuum at 8 K. These results open the door to microwave impedance spectroscopic fingerprinting down to the scale of single molecules.</p>
17:30	223	<p style="text-align: center;">Correlation between 2- and 3-dimensional crystallographic lattices for epitaxial analysis</p> <p style="text-align: center;"><i>Josef Simbrunner¹, Jari Domke², Oliver T. Hofmann³, Roland Resel³, Roman Forker², Torsten Fritz²</i> ¹ <i>Medical University Graz</i>, ² <i>Institute of Solid State Physics, Friedrich Schiller University Jena</i> ³ <i>Institute of Solid State Physics, Graz University of Technology</i></p> <p>While the crystalline properties of an epitaxially grown thin film can be studied in three dimensions by X-ray methods like grazing incidence X-ray diffraction (GIXD), the first monolayer is only accessible by surface sensitive methods that allow the determination of a two-dimensional lattice like low-energy electron diffraction (LEED). GIXD measurements with sample rotation on epitaxially grown films are compared with distortion-corrected LEED experiments of molecular monolayers. In this work, a combined experimental approach of GIXD and LEED is introduced which can be used to investigate the effect of the epitaxial monolayer on the evolution of molecular crystals with epitaxial order grown on top.</p>
17:45	224	<p style="text-align: center;">Optimized Infrared Reflection Absorption Spectroscopy for Metal Oxides: Overcoming Challenges of Low Reflectivity and Sub-Monolayer Coverage</p> <p style="text-align: center;"><i>Jiri Pavelec, David Rath, Michael Schmid, Ulrike Diebold, Gareth Parkinson Vienna University of Technology</i></p> <p>This study presents a new Infrared Reflection Absorption Spectroscopy (IRAS) setup for investigating adsorption on "single-atom" catalysts, addressing the challenges of low reflectivity from oxide supports and sub-monolayer coverage of adsorbates. The setup features improvements such as a high numerical aperture, optimized optical path, controlled incidence angle range, and high mechanical stability. Utilizing adjustable aperture plates, the minimum and maximum incidence angles can be varied to optimize the signal for each sample. This new setup successfully demonstrated enhanced signal-to-noise ratio in D₂O and CO absorbance measurements on a rutile TiO₂(110) surface, agreeing with established literature, with significantly reduced measurement time.</p>

18:00	225	<p style="text-align: center;">The Surface Tension of Water in its Pure Vapor</p> <p style="text-align: center;"><i>Alexander Syböck, Jan Balajka, Ulrike Diebold, Jiri Pavelec, Paul Ryan, Michael Schmid</i> Institute for Applied Physics, TU Wien</p> <p>Contaminants and other gases are known to greatly affect surface tension values. We have developed a way to measure the surface tension of ultra-clean liquids in contact with their pure gaseous phases. The liquid is condensed onto a small cryostat in a vacuum chamber. A pendant drop is formed and photographed allowing the surface tension of the ultra-pure liquid to be directly determined. Accurate control of the temperature, pressure and optics of the system is of importance. How these parameters are precisely controlled in the instrument design will be discussed along with initial measurements of ultra-pure water.</p>
18:15	226	<p style="text-align: center;">Surface band-bending response to charge redistribution and adsorbates in the ZnO/electrolyte interface probed by in-situ Spectroscopic Ellipsometry</p> <p style="text-align: center;"><i>Luis Rosillo, Christoph Cobet, Kurt Hingerl, Johannes Kepler Universität Linz</i></p> <p>In this work we look at the response of the surface band-bending of the ZnO single crystal polar faces (0001) and (000-1), in contact with an electrolyte, to a variation of charge at the solid-liquid interface by analyzing the effect of the inner electric fields on the excitonic dielectric function using in-situ spectroscopic ellipsometry.</p> <p>Discrete excitons on ZnO have a binding energy of (~ 60 meV) and in space charge region are significantly sensitive to modifications in the surface dipole moment. Hence, making them a suitable platform to study the response of the band-bending.</p>
18:30	227	<p style="text-align: center;">Quantitative Surface Structure of Water on Hematite: Experiment vs Theory</p> <p style="text-align: center;"><i>Paul Ryan, Matthias Meier, Gareth Parkinson, Ali Rafsanjani-Abbasi, Panukorn Sombut, Chunlei Wang, TU Wien</i></p> <p>Normal incidence X-ray standing waves (NIXSW) was used to directly determine the adsorption height of adsorbed H₂O and OH on the α-Fe₂O₃(012)-(1x1) surface. The H₂O and terminal OH both sit at the same adsorption height (1.45 Å and 1.46 Å respectively). The bridging OH is found sitting essentially in plane with a projected bulk surface (0.01 Å) implying little surface relaxation. This data corroborates our previous AFM study [Jakub 2019] and can be used to benchmark DFT calculations. The most appropriate functionals are those that produce little outward or inward surface relaxation and expensive Hybrid functionals are not necessarily suited for such systems. These findings are inline with our prior work [Meier 2018, Ryan 2020].</p>
18:45	228	<p style="text-align: center;">A Novel Four-Terminal Suspended Device for Nanoscale Thermal Characterization</p> <p style="text-align: center;"><i>Giulio de Vito¹, Rahul Swami¹, Dominik Koch¹, Tathagata Paul², Wenhao Huang², Michel Calame², Bernd Gotsmann³, Ilaria Zardo¹</i> ¹ University of Basel, ² EMPA, ³ IBM Zurich</p> <p>2D-flakes exhibit among the highest thermal conductivity in materials, which make them suitable for heat dissipation in microchip processes. However, it is challenging to produce thin homogenous flakes or transferring one flake onto a target because of the risk of damaging or contaminating the material. Thus, it is important to characterize the intrinsic properties of the materials with a consistent and reliable method. A novel four-terminal device is proposed which involves fabricating suspended four transducers, which can act as thermometer as well as heater, combined with the suspension of an h-BN flake. We demonstrate the capabilities of this novel four-terminal devices through electrical measurements and first results on h-BN flakes.</p>
19:00		END; Transfer to Dinner
19:30		Conference Dinner

ID

SURFACES, INTERFACES AND THIN FILMS POSTER

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Towards dielectric relaxation at a single molecule scale

Stefan Müllegger¹, Simon Feigl¹, Jindrich Nejedly², Eva Rauls³, Michal Samal², Ivo Stary²,
Vitalii Stetsovych¹, Radovan Vranik¹, Bareld Wit¹

¹ Institute of Semiconductor and Solid State Physics, Johannes Kepler University Linz

² Inst. of Organic Chemistry and Biochemistry of the Czech Academy of Sciences, Prague, Czech Republic

³ Institute for mathematics and physics, University of Stavanger, Norway

Recent advances have turned the scanning tunnelling microscope (STM) into a single molecule identification tool. We apply a radio frequency STM to excite a single molecule junction based on a polar substituted helicene molecule by an electric field oscillating at 2 to 5 GHz. We detect the dielectric relaxation of the single molecule junction indirectly via its effect of power dissipation, which causes lateral displacement. From our data we determine a corresponding relaxation time of about 300 ps – consistent with literature values of similar helicene derivatives obtained by conventional methods of dielectric spectroscopy.

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Controlling skyrmion density and formation mechanism by tuning ferromagnetic layer thicknesses in thin film multilayers

Reshma Peremadathil Pradeep¹, Hans Josef Hug^{1,2}, Andrada-Oana Mandru¹

¹ Empa, Swiss Federal Laboratories for Materials Science and Technology

² Department of Physics, University of Basel

With the goal of controlling the skyrmion density and their formation mechanism, which are highly relevant for spintronic devices using skyrmions, we investigate $[Ir(1\text{ nm})/Co(t)/Pt(1\text{ nm})]_n$ multilayers with varying Co-layer thickness. We observe that by increasing the Co layer thickness, domains (at zero field) become narrower, and skyrmion density (in an applied field) increases. This can be explained using the critical material parameter $\kappa = D/4 \cdot \sqrt{AK_{\text{eff}}}$, with D - interfacial DMI constant, A - exchange stiffness and K_{eff} - effective magnetic anisotropy. Skyrmions are thermodynamically stable for $\kappa > 1$. Here, κ increases as the effective anisotropy approaches zero at a critical Co-thickness. Furthermore, two different skyrmion formation mechanisms (shrinking and fission) are observed.

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Magnetoelectric Coupling in $\text{La}_{0.9}\text{Ba}_{0.1}\text{MnO}_3$ / BaTiO_3 Multiferroic Heterostructures Imaged by X-ray Photoemission Electron Microscopy

Gyanendra Panchal¹, Federico Stramaglia¹, Ludovica Tovaglieri², Celine Lichtensteiger²,
Frithjof Nolting¹, Carlos A. F. Vaz¹

¹ Paul Scherrer Institut, ² University of Geneva

We report the direct XPEEM imaging of the magnetic response of a 4.8 nm $\text{La}_{0.9}\text{Ba}_{0.1}\text{MnO}_3$ film to the voltage applied across a 5 nm BaTiO_3 film. Ferroelectric patterns were written on the BaTiO_3 with an AFM in contact-mode and the change in magnetic contrast measured with XPEEM. We observe an increase in the magnetic contrast when going from negative to positive writing voltages. Temperature dependent measurements show a decrease in the Curie temperature for positive voltage above +6 V applied, corresponding to hole-depletion state. The magnetic contrast of the written areas are compared with SQUID-magnetometry results, confirming the behavior for accumulation/depletion states of the $\text{La}_{0.9}\text{Ba}_{0.1}\text{MnO}_3$ for the two polarizations of BaTiO_3 .